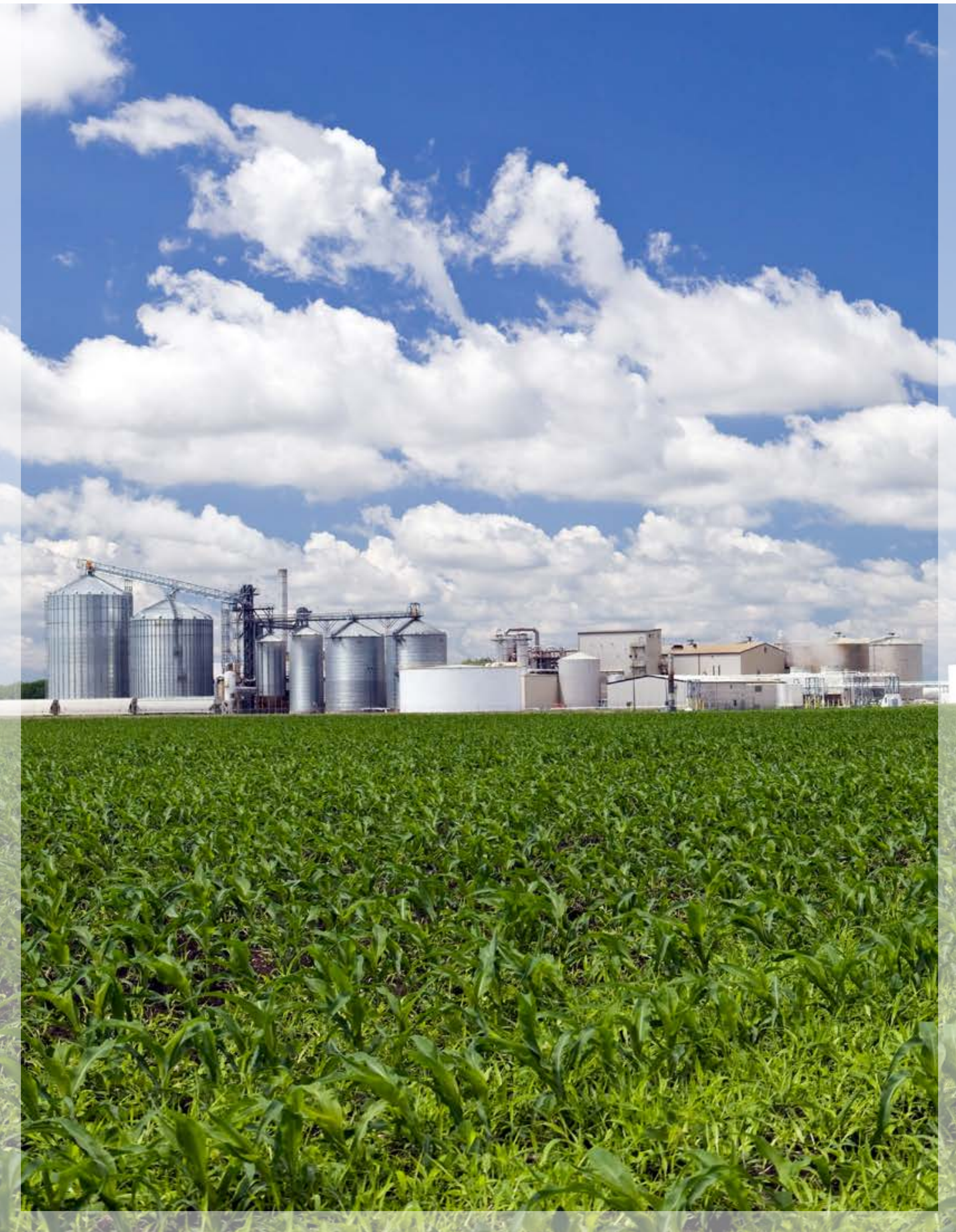
U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

2023 PROJECT PEER REVIEW

U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE



INTRODUCTORY LETTER

Dear colleagues,

In the spring of 2023, the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) Bioenergy Technologies Office (BETO) continued its long-standing commitment to transparency by executing the 11th biennial external review since 2005 of its research, development, and demonstration (RD&D) portfolio. Conducted in accordance with EERE Peer Review guidelines, the review provides an external assessment of the projects in BETO's portfolio and recommendations on BETO's overall technology focus and strategic direction. Results of the Project Peer Review will be considered in programmatic and funding opportunity decision-making.

This review is critical to the success of BETO's mission to develop and demonstrate technologies to accelerate reduction of greenhouse gas (GHG) emissions through the cost-effective, sustainable use of renewable carbon resources across the U.S. economy. At BETO, we are committed to accountability in project management and our role as stewards of taxpayer dollars aimed at achieving high-impact results. The Peer Review is an invaluable opportunity for independent reviewers to rigorously evaluate the approach, impact, and progress and/or outcomes of projects in the BETO portfolio, as well as the program strategies that guide technology area development. Further, it is a unique opportunity for external stakeholders to hear, in a compact and consistent format, about achievements from every corner of the portfolio.

The 2023 Peer Review comprised two levels of review: (1) individual projects were scored based on approach, impact, and progress and outcomes; and (2) each technology area portfolio was evaluated for overall strategy and progress. This report contains the results of both levels of review and the inputs of approximately 400 participants in the Peer Review process, including principal investigators, reviewers, and BETO's staff and contractors.

BETO thanks all the reviewers who participated in this review, as well as the 586 attendees of the Project Peer Review event. Our reviewers include some of the most experienced and knowledgeable experts in the bioenergy community, and we appreciate their insights and recommendations. Achieving the objectives of BETO depends on the effective management of all projects in BETO's existing portfolio and on the appropriate focus and structure of future initiatives. BETO values the input of all stakeholders in the bioenergy sector and looks forward to working with them in the years ahead to continue progress on the path toward building a successful bioenergy industry.

Sincerely,

Valerie Reed

Valerie Reed
Director, Bioenergy Technologies Office
Office of Energy Efficiency and Renewable Energy
U.S. Department of Energy

EXECUTIVE SUMMARY

The Bioenergy Technologies Office (BETO) within the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy supports the research, development, and demonstration (RD&D) of technologies aimed at mobilizing domestic renewable carbon resources for the reduction of greenhouse gas emissions across the U.S. economy. BETO systematically prioritizes RD&D into technology opportunities across a range of emerging scientific breakthroughs and technology readiness levels in the subprogram areas illustrated in Figure 1. This approach supports a diverse portfolio while developing the most promising and widely applicable technologies, testing technologies as integrated processes, and demonstrating integrated processes to support scale-up. These technologies will use a broad variety of renewable carbon resources to produce increasing volumes of biofuels and bioproducts. More information on BETO's mission, goals, and strategic approaches can be found in the Bioenergy Technologies Office Multi-Year Program Plan.[1]

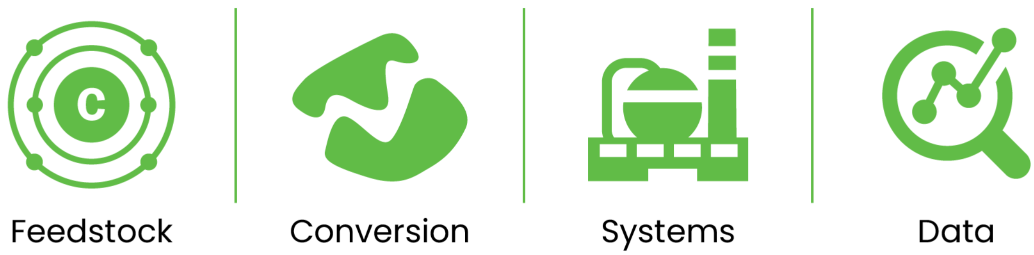


Figure 1. Bioenergy RD&D technologies

The biennial Peer Review process enables external stakeholders to provide feedback on the responsible use of taxpayer funding and develop recommendations for the most efficient and effective ways to accelerate the development of a bioenergy industry. This report includes the results of the Project Peer Review meeting held on April 3–7, 2023, in Denver, Colorado.

[1] BETO. 2023. *Bioenergy Technologies Office Multi-Year Program Plan*. Washington, D.C.: BETO. DOE/EE-2698. https://www.energy.gov/eere/bioenergy/articles/2023-multi-year-program-plan.

ACRONYMS AND ABBREVIATIONS

2,3-BDO	2,3-butanediol
3HB	3-hydroxybutyrate
3-HP	3-hydroxypropionic acid
6HDI	hexamethylene diisocyanate
7HDI	heptamethylene diisocyanate
AAD	arrested anaerobic digestion
AAS	Advanced Algal Systems
ABF	Agile BioFoundry
ABPDU	Advanced Biofuels and Bioproducts Process Development Unit
ABS	acrylonitrile butadiene styrene
ACSC	Advanced Catalyst Synthesis and Characterization
AD	anaerobic digestion
ADM	Archer Daniels Midland
AFT	American Farmland Trust
AI	artificial intelligence
AMMTO	Advanced Materials and Manufacturing Technologies Office
AMP	antimicrobial peptide
ANL	Argonne National Laboratory
AnMBR	anaerobic membrane bioreactor
ANOVA	analysis of variance
AOP	annual operating plan
APAD	advanced pretreatment and anaerobic digestion
ARC	Alder Renewable Crude
ARPA-E	Advanced Research Projects Agency – Energy
ARS	Agricultural Research Service
ASEC	Affordable and Sustainable Energy Crops
aTc	anhydrous tetracycline
ATD	alcohol to diesel
ATEC	Algae Technology Educational Consortium
ATJ	alcohol to jet
ATP	adenosine triphosphate
AUDACity	Arizona State University's direct air capture polymer-enhanced cyanobacterial bioproductivity
AVAP	American Value-Added Pulping
AWOEx	Advanced Wet Oxidation and Steam Explosion
AzCATI	Arizona Center for Algae Technology and Innovation
BAT	Biomass Assessment Tool
BDO	butanediol
BDT	bone dry ton
BEA	beta zeolite
BEEPS	BioEnergy Engineering for Products Synthesis
BEIOM	Bio-based circular carbon economy Environmentally-extended Input-Output Model
beta-KA	beta-ketoadipic acid

BETO	Bioenergy Technologies Office
BFL	Bioenergy Feedstock Library
BFNUF	Biomass Feedstock National User Facility
BHET	bis(2-hydroxyethyl terephthalate
BIC	Biofuels Information Center
BiCRS	biomass with carbon removal and storage
BILT	Biofuel Infrastructure, Logistics, and Transportation
BioC2G	Bio-Cradle-to-Grave
BIP	Biofuels Infrastructure Partnership
BKDL	ß-keto-d-lactone
BMP	best management practice
BNL	Brookhaven National Laboratory
BNSBA	Biofuels National Strategic Benefits Analysis
BOTTLE	Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment
BP	budget period
BPA	bisphenol A
BPM	bipolar membrane
BSM	Biomass Scenario Model
BTG	Biomass Technology Group
BTX	benzene, toluene, xylene
BUoB	best use of biomass
C1	one-carbon
C2+	two-carbon-plus
C4PE	Catalytic Carbon Conversion Center of Piloting and Excellence
CA	carbonic anhydrase
CapEx	capital expenditures
CAPSLOC	Combined Algal Processing for the Synthesis of Liquid Oleofuels and Products
CAS	conventional activated sludge
CBP	consolidated bioprocessing
CCC	countercurrent chromatography
CCE	carbon conversion efficiency
CCPC	Consortium for Computational Physics and Chemistry
CCS	carbon capture and storage
CCUS	carbon capture, utilization, and storage
CDM	Catalyst Deactivation Mitigation for Biomass Conversion
CEH	continuous enzymatic hydrolysis
CEJST	Climate and Economic Justice Screening Tool
CELF	co-solvent enhanced lignin fractionation
CF	carbon fiber
CFAnMBR	cloth filter anaerobic membrane bioreactor
CFB	circulating fluidized bed
CFC	carbon fiber composite
CFD	computational fluid dynamics
CFEP	carbon-fiber-reinforced epoxy composite

CFP	catalytic fast pyrolysis
CFRP	carbon-fiber-reinforced polymer
ChemCatBio	Chemical Catalysis for Bioenergy Consortium
CHJ	catalytic hydrothermolysis jet
CMA	critical material attribute
CNG	compressed natural gas
CO_2e	carbon dioxide equivalent
CO_2ER	CO_2 electrochemical reduction
CO_2RUe	CO_2 Reduction and Upgrading for e-Fuels Consortium
CoA	coenzyme A
COD	chemical oxygen demand
COF	covalent organic framework
Co-Optima	Co-Optimization of Fuels & Engines
CoPc	cobalt phthalocyanine
CORSIA	Carbon Offsetting and Reduction Scheme for International Aviation
CPD	Catalyst Property Database
CPP	critical process parameter
CQA	critical quality attribute
CRADA	cooperative research and development agreement
CRF	chemical-recovery-free
CRISPRa	CRISPR activation
CRISPRi	CRISPR interference
CSTR	continuous stirred-tank reactor
CSU	Colorado State University
CTT	cubical triaxial tester
CUBI	Catalytic Upgrading of Biochemical Intermediates
CUWP	Chemical Upcycling of Waste Plastics
CVWRF	Central Valley Water Reclamation Facility
DAC	direct air capture
DARPA	Defense Advanced Research Projects Agency
DBTL	design-build-test-learn
DEI	diversity, equity, and inclusion
DEIA	diversity, equity, inclusion, and accessibility
DEIP	diversity, equity, and inclusion plan
DEM	discrete element modeling
DFA	directed funding award
DFO	directed funding opportunity
DFT	density functional theory
DIC	dissolved inorganic carbon
DISCOVR	Development of Integrated Screening, Cultivar Optimization, and Verification Research
D-LEWT	distributed low-energy wastewater treatment
DMA	data, modeling, and analysis
DMCO	dimethyl cyclooctanes
DMR	deacetylation and mechanical refining
DOE	U.S. Department of Energy

DRIFTS	diffuse reflectance infrared Fourier transform spectroscopy
EAST	Emerging and Supporting Technologies
ECS	Empire Comfort System
ECO_2R	electrochemical reduction of CO_2
EEDIP	Energy and Environment Diversity Internship Program
EEEJ	energy equity and environmental justice
EERE	Office of Energy Efficiency and Renewable Energy
EJ	environmental justice
EJScreen	Environmental Justice Screening and Mapping Tool
EMPLOY	Environmentally extended Multi-regional Projection of Lifecycle and Occupational energY futures
EOL	end of life
EPA	U.S. Environmental Protection Agency
EPSCoR	Established Program to Stimulate Competitive Research
EROI	energy return on investment
ETAP	Escaped Trash Assessment Protocol
EtOH	ethanol
EXAFS	extended X-ray absorption fine structure
FAIR	findable, accessible, interoperable, and reusable
FCC	fluid catalytic cracking
FCIC	Feedstock-Conversion Interface Consortium
FDA	U.S. Food and Drug Administration
FD-CIC	Feedstock Carbon Intensity Calculator
Fe-B	iron-boride
FEM	finite element method
Fire MAPS	Fire Monitoring, Alerts, and Performance System
FMEA	failure mode and effect analysis
FOA	funding opportunity announcement
FOG	fats, oils, and greases
FPEAM	Feedstock Production Emissions to Air Model
FPO	fast pyrolysis oil
FTC	freeze tape casting
FTOT	Freight and Fuel Transportation Optimization Tool
FTS	Fischer-Tropsch synthesis
FY	fiscal year
GAI	Global Algae Innovations
GAMS	General Algebraic Modeling System
GCAM	Global Change Analysis Model
GDE	gas diffusion electrode
GGE	gasoline gallon equivalent
GHG	greenhouse gas
GMO	genetically modified organism
GREENSCOPE	Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a Multi-Objective Process Evaluator
GREET	Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies
GT	Global Thermostat

GTAP	Global Trade Analysis Project
GTI	Gas Technology Institute
GTL	gas to liquid
GWP	global warming potential
HBCU	historically Black college or university
HCU	hydrothermal cleanup
HDCJ	hydrotreated depolymerized cellulosic jet
HDO	hydrodeoxygenation
HEFA	hydroprocessed esters and fatty acids
HObT	Host Onboarding Tool
HOD	Host Onboarding & Development
HOG	high-octane gasoline
HPC	high-performance computing
HSI	hyperspectral imaging
HTL	hydrothermal liquefaction
IAA	indole-3-acetic acid
IAB	industry advisory board
IACMI	Institute for Advanced Composites Manufacturing Innovation
IBR	integrated biorefinery
IBRF	Integrated Biorefinery Research Facility
ICAO	International Civil Aviation Organization
IEO	Industry Engagement and Outreach
IFD	issued for design
IH^2	Integrated Hydropyrolysis and Hydroconversion
ILUC	induced land use change
INL	Idaho National Laboratory
InMAP	Intervention Model for Air Pollution
IP	intellectual property
IPA	isopropyl alcohol
IRR	internal rate of return
ISPR	in situ product recovery
JUST-R	Justice Underpinning Science and Technology Research
KDF	Knowledge Discovery Framework
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LCA	life cycle analysis
LCFS	low-carbon fuel standard
LCOE	levelized cost of energy
LIBS	laser-induced breakdown spectroscopy
LOUP	Lubricating Oils From Upcycled Plastics
LUC	land use change
MARINER	Macroalgae Research Inspiring Novel Energy Resources
MBL	alpha-methylene butyrolactone
MBSP	minimum biomass selling price
MEA	membrane electrode assembly
MEG	monoethylene glycol

MEK	methyl ethyl ketone
MES	microbial electrosynthesis
MESP	minimum ethanol selling price
MFSP	minimum fuel selling price
ML	machine learning
MLP	multilayer plastic
MMA	methyl methacrylate
MMT	million metric tons
MOOC	massive open online course
MOT	mild oxidative treatment
MPa	megapascals
MRF	materials recovery facility
MSI	minority-serving institution
MSP	minimum selling price
MSSP	minimum sugar selling price
MSU	Montana State University
MSW	municipal solid waste
MTO	methanol to olefins
MVL	methylene valerolactone
MYPP	Multi-Year Program Plan
NADH	nicotinamide adenine dinucleotide
NGO	nongovernmental organization
NIR	near-infrared
NMR	nuclear magnetic resonance
NMSW	nonrecyclable municipal solid waste
NPV	net present value
NRCS	Natural Resources Conservation Service
NREL	National Renewable Energy Laboratory
NSF	National Science Foundation
NTP	nonthermal plasma
NZTT	Net-Zero Carbon Fuels Technical Team
OEM	original equipment manufacturer
OFS	oleo-furan surfactant
OpEx	operating expenditures
ORNL	Oak Ridge National Laboratory
OSN	organic solvent nanofiltration
OSRO	organic solvent reverse osmosis
OSU	Oregon State University
P3-HP	poly(3-hydroxy)propionate
PA66	polyamide 66
PAA	polyacrylic acid
PABP	performance-advantaged bioproduct
PAM	polyacrylamide
P&O	progress and outcomes
PBAT	polybutylene adipate terephthalate
PBR	photobioreactor

PC	phycocyanin
PCA	principal component analysis
PCR	post-consumer recycled
PDO	pentanediol
PDU	process development unit
PE	polyethylene
PEM	polymer electrolyte membrane
PET	polyethylene terephthalate
PFAS	per- and polyfluoroalkyl substances
PFOS	perfluorooctane sulfonic acid
PGM	platinum group metal
PHA	polyhydroxyalkanoate
PHB	polyhydroxybutyrate
PHU	polyhydroxyurethane
PHW	post-hydrothermal liquefaction wastewater
PI	principal investigator
PISU	Process Integration and Scale-Up
PKS	polyketide synthase
PLA	polylactic acid
PM	particulate matter
pMBL	poly(alpha-methylene butyrolactone)
pMMA	polymethyl methacrylic acid
PNNL	Pacific Northwest National Laboratory
PO	polyolefin plastic
PolyID	Polymer Inverse Design
POLYSYS	Policy Analysis System Model
PP	polypropylene
PTS	phase-transition sorbent
PTU	polythiourethane
PU	polyurethane
PUP	polyurethane precursor
PVC	polyvinyl chloride
PVDF	polyvinylidene difluoride
QbD	quality by design
QEG	Quasar Energy Group
qPCR	quantitative polymerase chain reaction
R&D	research and development
RAB	Revolving Algal Biofilm
RABR	Rotating Algae Biofilm Reactor
RBEM	Regional BioEconomy Model
RCF	reductive catalytic fractionation
RCFP	reactive catalytic fast pyrolysis
RCR	Renewable Carbon Resources subprogram
RD&D	research, development, and demonstration
ReEDS	Regional Energy Deployment System
REMADE	Reducing Embodied Energy and Decreasing Emissions

ResIn	Responsible Innovation for Highly Recyclable Plastics
RFS	Renewable Fuel Standard
RIN	renewable identification number
RMP	risk management plan
RMPG	Risk Management Plan Guidance
RNG	renewable natural gas
RPO	residual pyrolysis oil
RTI	Research Triangle Institute
SAF	sustainable aviation fuel
SAFFiRE	Sustainable Aviation Fuel From [i] Renewable Ethanol
SAMPE	Society for the Advancement of Material and Process Engineering
SBI	Stove Builder International
scfm	standard cubic feet per minute
sCO_2	supercritical carbon dioxide
SCP	single-cell protein
SDI	Systems Development and Integration
SDSMT	South Dakota School of Mines and Technology
SE-CLG	sorption-enhanced chemical looping gasification
SepCon	Bioprocessing Separations Consortium
SMART	specific, measurable, achievable, relevant, and time-bound
SME	subject matter expert
SMR	steam methane reforming
SNL	Sandia National Laboratories
SNP	single nucleotide polymorphism
SOA	state of the art
SOC	soil organic carbon
SoCalGas	Southern California Gas Company
SOEC	solid oxide electrolysis cell
SOPO	statement of project objectives
SOT	state of technology
SPD	synthetic paraffinic diesel
SPERLU	Selective Process for Efficient Removal of Lignin and Upgrading
STH	syngas to hydrocarbons
STRAP	solvent-targeted recovery and precipitation
SUP	Scale-Up Portfolio
SUPERBEEST	Scaling Up PERennial Bioenergy Economics and Ecosystem Services Tool
SUPF	single-use flexible plastic film
SWAT-C	Soil and Water Assessment Tool – Carbon
SWIFT	Single-Pass, Weather Independent Fractionation Technology
TA	technical assistance
TAL	triacetic acid lactone
TCPDU	Thermal and Catalytic Process Development Unit
TD-NMR	time-domain nuclear magnetic resonance
TDO	thermal deoxygenation
TEA	techno-economic analysis

TEG	thermoelectric generator
TEM	techno-economic model
Tg	glass transition temperature
THP	thermal hydrolysis processing
Tm	melting temperature
TOS	time on stream
TPA	terephthalic acid
TPD	ton per day
TPU	thermoplastic polyurethane
TRL	technology readiness level
TRY	titer, rate, and yield
TuFF	Tailorable Universal Feedstock for Forming
Tv	vitrimer transition temperature
UD-CCM	University of Delaware Center for Composite Materials
UHS	unhydrolyzed solids
UIUC	University of Illinois Urbana-Champaign
UMaine	University of Maine
UNM	University of New Mexico
USDA	U.S. Department of Agriculture
U.S. DRIVE	Driving Research and Innovation for Vehicle Efficiency and Energy Sustainability
USFS	U.S. Forest Service
VFA	volatile fatty acid
VGO	vacuum gas oil
VOC	volatile organic compound
VolCat	volatile catalyst
W2X	waste to X
WATER	Water Analysis Tool for Energy Resources
WBS	Work Breakdown Structure
W-C	tungsten-carbide
WRRF	water resource recovery facility
WSU	Washington State University
WTE	waste-to-energy
WWTF	wastewater treatment facility
XANES	X-ray absorption near edge structure
XPS	X-ray photoelectron spectroscopy
XRF	X-ray fluorescent
ZSM-5	Zeolite Socony Mobil–5

CONTENTS

INTRODUCTION

The Project Peer Review meeting took place April 3–7, 2023, in Denver, Colorado. The Peer Review brought together reviewers, project performers, Bioenergy Technologies Office (BETO) staff, and stakeholders along the entire bioenergy supply chain. Projects were systematically reviewed by 69 external subject matter experts from industry, academia, nonprofits, and government. BETO's funding portfolio was presented in 12 technology areas:

- Advanced Algal Systems
- Agile BioFoundry
- Biochemical Conversion and Lignin Utilization
- Carbon Dioxide Utilization
- Catalytic Upgrading
- Data, Modeling, and Analysis
- Feedstock-Conversion Interface Consortium
- Feedstock Technologies
- Performance-Advantaged Bioproducts, Bioprocessing Separations, and Plastics
- Organic Waste Conversion
- Systems Development and Integration: Emerging and Supporting Technologies
- Systems Development and Integration: Scale-Up.

Each review session included a technology area overview presentation that linked the projects in the portfolio to the technology area challenges and the program strategy for measuring progress and managing deliverables toward outcomes. A panel of independent reviewers reviewed and scored individual projects within each session and provided recommendations regarding the strategy and progress of the technology area. Results of the 2023 BETO Peer Review may be used to help inform programmatic decision-making, modify or discontinue existing projects, guide future funding opportunities, and support other budget and strategic planning objectives.

The 303 project presentations reviewed represent a total U.S. Department of Energy (DOE) investment of more than $561 million and cover activities that incurred costs from fiscal years (FY) 2021–2023. Figures 2 and 3, respectively, depict the number of presentations reviewed by technology area session and the associated funding allocation.

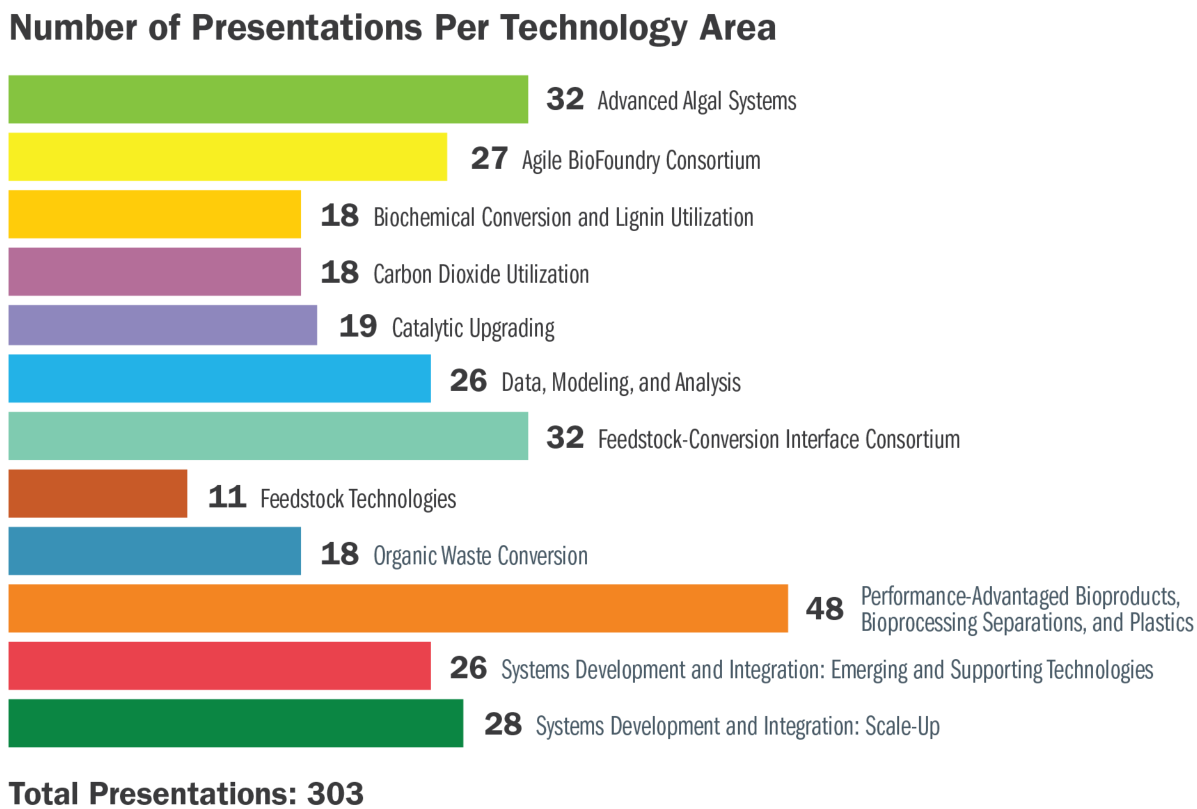


Figure 2. Number of presentations by technology area session

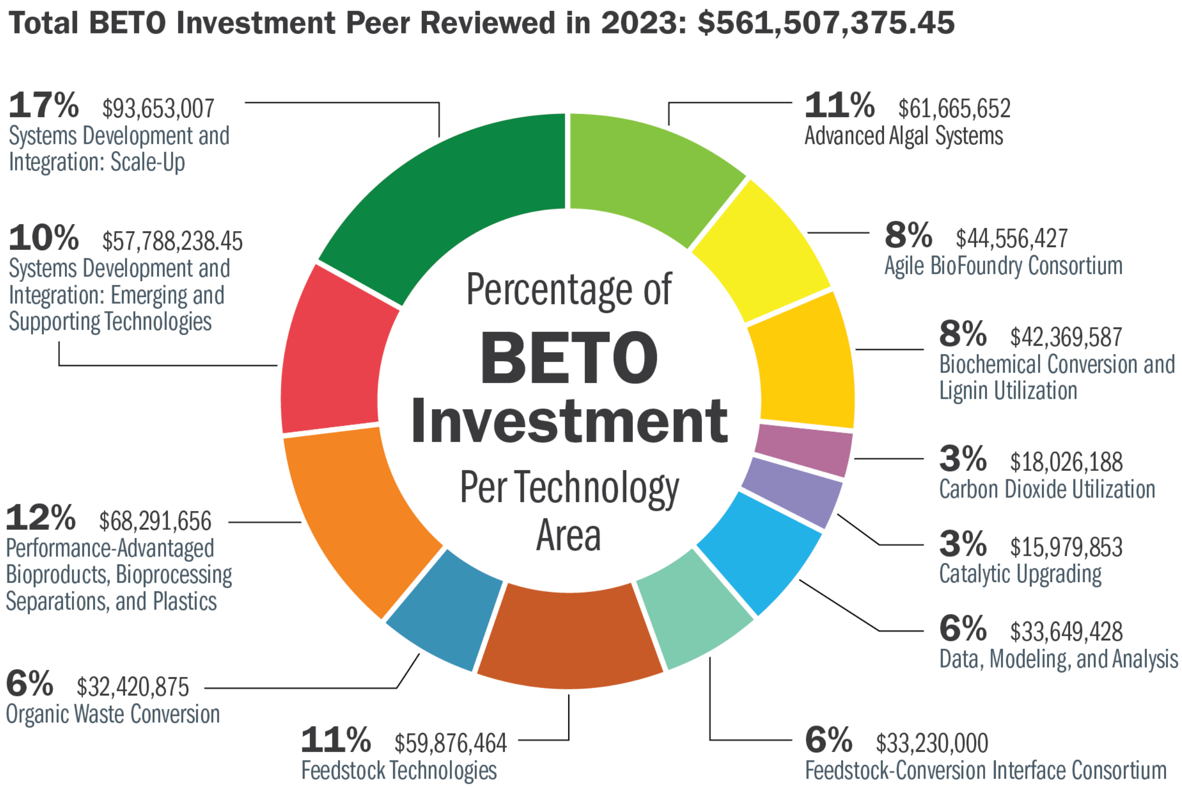


Figure 3. Total BETO funding of reviewed activities by technology area session

ROLES AND RESPONSIBILITIES

The BETO 2023 Peer Review was planned by an internal planning committee composed of BETO federal and contractor staff designated with the responsibility for developing and coordinating all aspects of the review process in compliance with EERE standards for conducting Project Peer Reviews. This committee included a federal lead and contractor support for each of the technology areas, as well as a federal Peer Review chair responsible for all aspects of the overall process, with a coordination and execution support team.

The reviews were conducted by individuals external to BETO with expertise in their fields and organized into review panels for each of the technology area sessions. The Advanced Algal Systems and Performance-Advantaged Bioproducts, Bioprocessing Separations, and Plastics technology areas hosted two sessions with separate panels due to their high number of projects. The review panels for each technology area consisted of four to seven external individuals selected based on technical expertise and professional qualifications in their designated technology area. Efforts were made to ensure experiential, institutional, and geographic diversity within each review panel by including a mix of reviewers from industry, academia, and federal agencies, with a range of expertise in relevant focus areas. Additionally, BETO proactively sought out expertise from outside of established networks with external calls for reviewers, and then made selections through a lens of improving diversity, equity, and inclusion in the makeup of the panels. Reviewers were required to sign legal agreements confirming an absence of a conflict of interest with the projects they reviewed. Final decisions on reviewer selection were made by the internal planning committee, with final approval by BETO’s director. In addition, one reviewer on each panel was designated as the lead reviewer. In most cases, lead reviewers had previous experience participating as a reviewer in a prior BETO Peer Review. The extra responsibilities of the lead reviewer included gathering the individual reviewer comments and scores and synthesizing them into a summary report for inclusion in this document.

Table 1 lists the members and affiliations of the lead reviewers of each panel. Members of each technology area review panel are listed within each technology area session summary.

Table 1. Lead Reviewers

Review Session	Name	Affiliation
Advanced Algal Systems	Lora Cameron-Landis	Lonza
Advanced Algal Systems	Tyler Johannes	University of Tulsa
Agile BioFoundry	Karen Draths	Michigan State University
Biochemical Conversion and Lignin Utilization	Lisette Tenlep Akers	LignoBio
Carbon Dioxide Utilization	Charles McCrory	University of Michigan
Catalytic Upgrading	Cory Phillips	Air Company
Data, Modeling & Analysis	Jason Jones	ICF
Feedstock Technologies	Jingxin Wang	West Virginia University
Feedstock-Conversion Interface Consortium	Phil Weathers	Weathers Associates Consulting
Organic Waste Conversion	Samantha MacBride	New York Department of Environmental Protection
Performance-Advantaged Bioproducts, Bioprocessing Separations, and Plastics	Sharon Haynie	Hypatia Technology Works
Performance-Advantaged Bioproducts, Bioprocessing Separations, and Plastics	Michael Mang	Danimer Scientific
Systems Development and Integration: Emerging and Supporting Technologies	Gene Petersen	Independent consultant
Systems Development and Integration: Scale-Up	Ray Miller	Verdecute Consulting

PROJECT EVALUATION CRITERIA

Reviewers evaluated each project on the following criteria: approach, progress and outcomes, and impact. Reviewers provided a numeric score per criterion, as well as written comments to support their scoring.

- **Approach**—Projects were evaluated on the degree to which:
  - The project performers have developed an approach with substantial merit to advance the state of the art, as relevant to the defined BETO program and technology area goals.
  - The project performers have developed an approach with significant potential for innovation in its application.
  - The project performers have a clear management plan and successful implementation strategy that includes risk identification and mitigation strategies.
  - The project provides routes for communication and collaboration with related projects and/or advisory boards, if appropriate.
  - If applicable, the project has an adequate approach to addressing diversity, equity, and inclusion in their project plan.

- **Progress and outcomes**—Projects were evaluated on the degree to which:
  - The project has made appropriate progress toward addressing the project goal(s).
  - The accomplishments have been achieved on schedule with the planned approach and, if relevant, the risk mitigation strategies have been employed to maintain project progress.
- **Impact**—Projects were evaluated on the degree to which:
  - The project demonstrated a clear connection of project approach to the potential for significant impact and outcomes.
  - The project has clear commercialization potential or has used or plans to use industry engagement to guide project deliverables, as relevant.

Scores ranged from 5 (outstanding) to 1 (unsatisfactory) per the rubric in Table 2.

Table 2. 2023 BETO Project Peer Review Scoring Rubric

Outstanding	Good	Satisfactory	Marginal	Unsatisfactory
5	4	3	2	1
All aspects of the criterion are comprehensively addressed. There are significant strengths and no more than a few—easily correctible—weaknesses.	All aspects of the criterion are adequately addressed. There are significant strengths and some weaknesses. The significance of the strengths outweighs most aspects of the weaknesses.	Most aspects of the criterion are adequately addressed. There are strengths and weaknesses. The significance of the strengths slightly outweighs aspects of the weaknesses.	Some aspects of the criterion are not adequately addressed. There are strengths and significant weaknesses. The significance of the weaknesses outweighs most aspects of the strengths.	Most aspects of the criterion are not adequately addressed. There may be strengths, but there are significant weaknesses. The significance of the weaknesses outweighs the strengths.

FORMAT OF THE REPORT

Information in this report has been compiled as follows and is based on the following sources:

1. **Peer review report introduction:** This section contains overview information on the Peer Review process, roles and responsibilities, and project evaluation criteria.
2. **Technology area summaries:** This section contains 12 chapters that represent the comprehensive evaluation for each technology area reviewed. Each chapter includes:
   A. **Introduction:** An overview of the technology area's project portfolio, including total funding of the projects reviewed and percentage of total BETO project portfolio.

   B. **Review panel members:** A list of names and affiliations of the independent subject matter experts who provided project evaluations and contributed to the review panel summary report.

   C. **Review panel summary report:** This summary of project evaluations provides insight regarding the technology area's overall strategy and progress. This section was drafted by the lead reviewer for each technology area in consultation with the full review panel. Consensus among the reviewers was not sought, and reviewers were asked to include any differences of opinion along with their recommendations.

   D. **Technology area programmatic response:** Represents the program's official response to the recommendations provided in the review panel summary report.

   E. **Project evaluations:** Includes the results of each project evaluation, including the following elements:

      i. **Project name and the lead project performer organization:** The full project name is listed as the heading, followed by the lead project performer's organization.

      ii. **Average project score per review criterion:** A bar chart depicts the average scores for each evaluation criterion, the range of scores per criterion given to the project by the individuals within the review panel, the average project score, and the average of all the projects in the technology area per criterion.

      iii. **Summary table:** Reference information about the project, which includes the recipient organization, principal investigator (PI), project dates, and total DOE funding.

      iv. **Project descriptions:** Project abstracts were submitted by each project performer.

      v. **Reviewer comments:** Verbatim comments made by the review panel, edited only for grammar and clarity. Each comment response represents the opinion of one reviewer. Reviewers were not asked to develop consensus remarks, and in most cases the reviewers did not discuss their overall comments on each project with one another. In a limited number of cases, reviewer remarks deemed inappropriate or irrelevant were excluded from the final report.

      vi. **PI response to reviewer comments:** The response to the reviewer comments provided by the project performers. Responding to reviewer comments was optional.

ADVANCED ALGAL SYSTEMS

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Advanced Algal Systems (AAS) Program is one of 12 technology areas that were reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 32 active projects were reviewed in the AAS sessions by two panels of four external reviewers. Of the 32 projects reviewed, 14 were reviewed by the Cultivation and Strain Development panel and 18 were reviewed by the Integration panel. For information about the structure, strategy, and implementation of the program and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks, which can be accessed at the Peer Review website: www.energy.gov/eere/bioenergy/2023-project-peer-review.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $61.7 million, which represents approximately 11% of the BETO portfolio reviewed during the 2023 Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Daniel Fishman as the Advanced Algal Systems Technology Area review lead, with contractor support from Jamie Meadows of Boston Government Services and Phillip Lee of Allegheny Science and Technology. In this capacity, Daniel Fishman was responsible for all aspects of review planning and implementation.

CULTIVATION AND STRAIN DEVELOPMENT PANEL

Name	Title and Affiliation
Dr. Tyler Johannes*	Professor at University of Tulsa
Dr. Laura Carney	Former Director of Ag Science at Heliae
Dr. Ify Iwuchukwu	Director, Pilot Plant at Oxford Biomedica Solutions LLC
Dr. Kalyani Maitra	Associate Professor at Fresno State University

* Lead Reviewer

INTEGRATION PANEL

Name	Title and Affiliation
Dr. Lora Cameron-Landis*	Associate Director of Upstream Process Development and Manufacturing at Eli Lilly
Valerie Harmon	President and CEO at Harmon Consulting Inc.
Dr. Mark Jones	Dow (retired)
Dr. Paul Roessler	Algenol (retired)

* Lead Reviewer

CULTIVATION AND STRAIN DEVELOPMENT REVIEW SUMMARY REPORTS

Prepared by the Advanced Algal Systems Review Panel – Cultivation and Strain Development

INTRODUCTION

The cultivation and strain development of algae have emerged as a promising avenue for addressing the challenges of sustainable energy and resource production. As the world seeks alternative sources of fuel and raw materials, BETO has taken a proactive role in supporting and funding research in this field. The 2023 BETO Peer Review of the AAS – Cultivation and Strain Development serves as a testament to DOE's commitment to driving innovation and remaining a global leader in this domain.

The AAS Program focuses on advancing the cultivation techniques and genetic engineering of algae to optimize biomass production and improve the efficiency of biofuel production. Through strategic partnerships with academia, national laboratories, and industry stakeholders, BETO aims to accelerate the development and deployment of sustainable and cost-effective algal production technologies. This Peer Review offers an opportunity to assess the progress made by the AAS Program, evaluate the effectiveness of the funded projects, and identify areas for further improvement.

The findings of the 2023 BETO Peer Review reflect BETO's unwavering dedication to advancing cultivation and strain development technologies. The review highlights the successful outcomes achieved by funded projects, such as the development of robust genetic tools, engineering systems for improved cultivation, and real-time monitoring toolkits for algal culture. These accomplishments demonstrate the efficacy of DOE's funding approach in driving meaningful advancements and bridging the gap between research and commercialization.

By reaffirming DOE's position as a global leader in funding cultivation and strain development technologies, the 2023 BETO Peer Review underscores the importance of ongoing research and development efforts in the algae cultivation sector. As the world transitions toward a greener and more sustainable future, BETO's continued support in this field will play a vital role in unlocking the full potential of algae as a renewable resource for biofuel production and other applications.

STRATEGY

The AAS Program's strategic goal is to develop technologies that enable the production of environmentally sustainable algal feedstocks that perform reliably in conversion processes to yield renewable fuel blendstocks, as well as bioproducts and chemical intermediates. The program structure encompasses cultivation and strain development, as well as integration, covering a wide range of research areas to achieve the goal using different approaches. The program has reflected on learnings, addressed gaps, and adjusted investments accordingly. It has successfully funded critical path technologies and filled known gaps. The funding mechanism, including innovative and high-risk seed projects, has been appropriate.

The recent lab calls align with the barriers and challenges to achieving BETO's goals. The program should ensure that successful approaches have potential for commercial deployment and consider closer collaboration with industry partners to harmonize efforts and attract continuous funding. The previous and ongoing funding announcements have been well designed and managed. Efforts to monitor portfolios for overlaps and consolidate efforts for better outcomes should continue. Encouraging and funding new principal investigators (PIs) with fresh ideas and approaches is recommended. The strategic objective of focusing on algae as a renewable resource for biofuels and byproducts is well defined, and the funding mechanisms have facilitated collaboration and progress. While the academic and national lab efforts seem to focus on pond crashes, industry perspectives should be considered to ensure alignment. Targeted funding for bioprospecting or genetic modification of extremophiles may be worth exploring. Productivity improvements are still needed, and research on strains tolerant to higher temperatures caused by climate change could be beneficial.

STRATEGY IMPLEMENTATION AND PROGRESS

The implementation of the strategy within the AAS Program has shown significant progress and successful management of funded projects. A broad range of disciplines, including strain development, carbon utilization technologies, wastewater integration, engineering systems, logistics, techno-economic analysis (TEA) and life cycle analysis (LCA) models, and system integration, have been funded, demonstrating a comprehensive approach toward achieving the goals and targets set forth by the AAS Program. Key accomplishments such as the EcoRecover™ process for wastewater treatment, the real-time monitoring toolkit for algal culture, genetic tool development, and productivity improvement highlight the advancements made in addressing the barriers and technical challenges identified in the program.

The AAS Program has effectively used BETO funding to address challenges related to the successful deployment of algal production technologies. The program's transparent platform has facilitated stakeholder engagement and provided a means to track progress for funded projects. The diverse range of institutions and locations represented in the funded projects demonstrates the program's ability to bring together national labs, industrial partners, and academic institutions to contribute to the development of renewable carbon resources using algae as feedstock.

While significant progress has been made in various aspects, including biomass forecast systems, harmonization of analysis data, and the production of resilient algal strains and toolkits, there is a need for further advancements in low-cost, sustainable biofuel production from algal oil. The AAS Program should continue to fund projects focusing on strain improvement and encourage diversification in strain selection criteria during bioprospecting. Additionally, combining projects on bioprospecting, strain evolution, and engineering with existing technologies and toolkits could lead to breakthroughs in biomass productivity. Consideration should also be given to the exploration of extremophiles and thermophiles, as they can contribute to contamination control, carbon utilization efficiency, and summer production.

Overall, the AAS Program has made substantial progress in implementing its strategy, managing projects effectively, and promoting collaboration among diverse stakeholders. Continued funding for critical areas such as strain development, engineering, and bioprospecting, along with a focus on commercialization and industry adoption, will contribute to the achievement of BETO's goals in biomass production and low-cost sustainable biofuel production from algal sources.

RECOMMENDATIONS

Based on the comments provided, the three most important recommendations to strengthen the portfolio in the near to medium term are:

1. **Address pond crashes and stability**: During the review, it was noted that two industrial teams expressed no concerns regarding pond contamination. Interestingly, both of these teams use extremophile algae cultivated at high pH levels. While there has been significant attention from academic and national lab efforts in addressing this issue, it is important for AAS to investigate the validity of these claims, considering that the current funding opportunity announcement (FOA) focuses on algae crop protection. If pond contamination is predominantly a challenge encountered in smaller-scale academic and national lab settings rather than in industry, allocating AAS funds towards pest management may not provide significant value. However, if there is indeed a genuine discrepancy, it highlights an inherent disconnect between academic/national lab efforts and industry, which BETO should actively work to resolve.

2. **Target efforts for high-pH- and heat-tolerant algae strains**: BETO should focus on identifying and/or engineering algae strains that are tolerant to high pH levels and heat. These traits are likely to be

important for improving biomass productivity and resilience in outdoor pond conditions. By prioritizing research in this area, the program might be able to address the recent slowdown in biomass productivity gains and work toward achieving higher biomass productivity targets.

3. **Engage industry partners and address scale-up challenges**: BETO should actively engage industry partners to identify gaps and barriers in scale-up efforts. Collaborating with industry stakeholders will provide valuable insights and help address challenges related to commercial deployment. Industry involvement should be encouraged to ensure the technologies developed through the program have a higher likelihood of adoption. Input from industry partners will also contribute to the TEA and LCA processes, improving the program's ability to assess the cost and energy effectiveness of biofuel production.

By implementing these suggestions, the AAS Program can strengthen its portfolio, accelerate progress toward achieving BETO's goals, and foster greater industry engagement in the algae sector.

INTEGRATION REVIEW PANEL SUMMARY REPORT

Prepared by the Integration Review Panel

INTRODUCTION

Integration projects—those focused on the technology development required to bring biofuel cultivation from lab-scale, proof-of-concept work to demonstration- and commercial-scale operations—are clearly necessary for the creation of an algal biofuels industry. Integration projects include pilot-scale operations, process analytics, dewatering, fractionation, and development of the algae fractions into fuel and valuable materials. The majority of the portfolio relies on coproducts to improve biofuel production economics. Some of the projects target only algal products with no fuel production. While the initial proof-of-concept work is centered around bioprospecting, strain development, genetic modifications, metabolic engineering, carbon capture and delivery, cultivation, and refinement of algae fractions into petrochemical substitutes, integration aims to bring these disparate projects together as a unified whole, resolve any incongruities, and promote access to the energy market for algae-based biofuels by creating fully developed drop-in solutions. The bottom-up approach supports the maximum amount of creativity in solving problems unique to scalability, results in more informed research directions, and allows for a deep understanding of the complexities of algae production and processing, while general top-down guidance is provided by the strategic requirements of each FOA.

Additionally, the integration projects are intended to provide collaboration between industry and academic research. By working with academic labs, customers for algae products and operators of commercial algae operations are connected to potential supplies of raw materials and opportunities for new product distribution and new market value propositions. Researchers in turn receive additional funding, collaboration opportunities, facility and material resources, and access to economic and operational expertise.

STRATEGY

Due to the nature of the integration work, spanning several fields and specialties, the integration technology area covers a wide range of technologies. The intent of the projects is to move technologies closer to commercialization, taking lab-scale discoveries and showing they are viable in the field at larger scale. Gaps are filled between lab projects to bring together technologies to create a whole, functional production operation capable of meeting BETO fuel production targets. The goal, regardless of the individual project, is to enable the creation of an economically viable set of products from algal raw materials. The department identified and implemented several strategies toward this end:

- Projects must be guided by an agreed-upon model of TEA to illustrate the relevance and cost effectiveness of the project plan relative to BETO goals.

- Projects must collaborate with at least one industry partner to better assess the commercial feasibility of the work.
- Projects must meet the applicable productivity and carbon capture requirements established by the FOA to achieve economic targets that enable sustainable production and compete on the world stage with petroleum-based products.
- Projects in the integration category must meet a minimum technology readiness level of 3, with the proof of concept already established at small scale.

Historically, moving algae cultivation from the lab into open ponds has encountered significant challenges: contamination, predation, transgenic organism control requirements, weather variability and climate disruption, the available hiring pool for staff, land costs, water availability, cost of goods, and the need for specialized process monitoring. All create meaningful barriers to entry for algae-based fuels and coproducts. The technical challenges of mixing, carbon capture, facility energy use, mass transfer, and strain development at large scale all must be overcome to create an algal biofuels industry. In order to better address these gaps, integration projects contribute to the overall goal of the program to create an economically viable path toward production of algae-based fuels and coproducts, which are not associated with any particular unit operation or specific technological advancement. They focus only on successful integration of largely known and developed technologies into an overall, workable system.

STRATEGY IMPLEMENTATION AND PROGRESS

The strategy execution addressed the following categories:

Algae batch growth and direct air capture (DAC) technologies: Due to the nature of integration, many of the projects had overlap with algae growth projects to demonstrate feasibility in the field and scale-up. There were several strategies for DAC of CO_2 at pilot or larger scales.

Montana State University used high-pH and high-alkalinity capture in raceway systems (1.3.4.002) to shift the equilibrium reaction toward bicarbonate generation rather than carbonic acid and demonstrated a new mixing method that used a moving belt with cleats rather than a paddlewheel to improve kLa in the raceway and thereby improve CO_2 transfer to the media. A proof-of-concept prototype was created to demonstrate the mixing concept overall. The energy balance, use in algae cultivation, and scale-up proof of concept to develop this mixing method further will be performed later in the project.

A collaboration between the National Renewable Energy Laboratory (NREL); University of California, San Diego; Algix; and Gross-Wen Technologies (1.3.4.004) leveraged *in silico* modeling of different carbon capture proteins to create a new carbonic anhydrase (CA) overexpression system, characterizing metabolic networks and signal peptides for extracellular secretion in the process and resulting in significantly improved biomass generation in a Revolving Algal Biofilm (RAB™) cultivation system. Supplementation of the RAB system with exogenous CA as a CO_2 capture method increased yields by approximately 25% over sparging, and doubled yields from the RAB system alone. The biomass produced was found to be suitable for plastics manufacturing. Large-scale testing of the carbonic-anhydrase-secreting strains will be completed in the future.

A MicroBio Engineering project (1.3.4.006) using high-pH algal "weed" strains from Cyanotech investigated the use of the pond itself as a carbon sink via high alkalinity, added CA, and improved buffering capacity to spread the CO_2 transfer to the algae over the course of the day more efficiently compared to limited peak daytime transfer. One of the strains achieved the baseline productivity requirements and is moving forward with further evaluation. Carbon flux modeling was used to identify critical parameters for pond depth; however, the DAC skid is currently under development by Global Thermostat (GT) and will be implemented later in the project.

Duke University is also working on a DAC skid (1.3.4.010) to deliver CO_2-enriched air to algae ponds and storing it in the pond as bicarbonate. The benefit of the DAC module being produced by MoleculeWorks was the ability to use thinner membranes that could be stacked tightly together, allowing for a small footprint. Additionally, they are also investigating marine strains that may have higher productivity, especially as it relates to protein-based products with increased economic value. Optimal inoculation density was modeled for batch cultivation and will be tested for various strains from the Marine Algae Industrialization Consortium (MAGIC) project in the future.

Arizona State University's AUDACity project (1.3.4.003) developed a new ion-exchange polymer capable of absorbing CO_2 from the air and delivering it to algae directly, and identified the operational parameters required for efficient CO_2 capture and delivery. Scale factors of the polymer were identified, and optimal parameters were characterized. Drying time required to reenable CO_2 absorption, nitrate competition for adsorption sites on the polymer, and an initial washing period to remove growth-inhibiting leachables were studied, and implementation strategies were developed. The novel polymer system performed similarly to an existing commercially available polymer, discharging the captured CO_2 efficiently to the algae pond, enabling a 2.2-fold increase in methyl laurate yield, and eliminating the losses normally observed during CO_2 sparging.

Los Alamos National Laboratory's (LANL's) work on media optimization and recycling of media components (1.3.4.205) using Bayesian machine-learning methods identified the most efficient way to use nitrogen and phosphate dosing and recycling at scale, lowering cultivation costs. The initial modeling and data set is promising, and it will be interesting to see how the model is validated against empirical testing; dosing methods and forms will need to be characterized, along with water quality and optimal temperature conditions.

Global Algae Innovations (GAI) (1.3.4.001) presented the challenge of growing algae outdoors during unusual rain conditions, responding to the events in a way that maintained high-productivity and high-value products. A large number of patents are in progress for downstream product development and unit operations, though step yields and product quality data for the various product streams remain to be seen. There were insufficient data from the rain event to sufficiently develop a mitigation strategy. Due to the patent strategy, the results will not be disseminated to industry until patent applications have been submitted or published.

An Arizona Center for Algae Technology and Innovation (AzCATI) project (1.3.5.287) provided further insight into culture failures and how they can be modeled, discovered early, treated if possible, and optimally managed in a facility to maintain productivity. The team encountered a challenging parasitoid infection during their work that necessitated a change in approach and risk mitigation measures to better understand and manage the pond dynamics. Resistance to fungicide was observed to develop quickly, which demonstrated one of the practical issues associated with open cultivation. Quantitative polymerase chain reaction (qPCR) identification of microbial contaminants and creation of a gene-based library for rapid diagnostics will be useful for moving the field forward, particularly with respect to developing best practices for cohesive contamination control.

University of Illinois at Urbana-Champaign's wastewater-grown algae demonstrated impressive 73% increases in oil productivity, a method for reducing ash content, and increased oil conversion (1.3.5.286); they also tested the benefit of media supplements and a method for recovering organics from hydrothermal treatment of wastewater. The use of wastewater-based rotating biofilm cultivation improves the economics of production. Demonstration-scale projects are planned for the future to show scalability of the improvements.

Finally, Colorado School of Mines developed a novel high-biomass, high-lipid-productivity strain using a novel mutagenesis technique and fluorescence-activated cell sorting to select the most productive clones, which demonstrated continued increased productivity in outdoor ponds (1.3.5.282) after enrichment for tolerance of stressful events. It will be important to see how it compares directly to control strains at scale, and how well the strains will maintain their productivity over time, especially *Nitzschia.*

Downstream algae fractionation and fraction refinement: The Combined Algal Processing for the Synthesis of Liquid Oleofuels and Products (CAPSLOC) project (1.3.4.204) developed a downstream biorefinery process (i.e., mild oxidative treatment [MOT] of acid-hydrolyzed biomass) that could accept starting materials from multiple feedstocks, yielding lipid, solid, and hydrolysate fractions to be further processed into fuels, fine chemicals, polymers, graphitic carbon, and protein. The development of a feedstock-agnostic biorefinery with multiple product lines is a critical contribution toward both renewable energy production and reduction of petrochemical use, and provides a pathway for supply chain debottlenecking of many of the products.

A Pacific Northwest National Laboratory (PNNL) project (1.3.4.102) to develop hydrothermal processing for multiple feedstocks identified several cost-advantaged feedstocks that could meet BETO's price target for algal biofuels, reducing the cost of fuel significantly, and used the method to process a worst-case scenario of high-ash wastewater-grown nuisance algae successfully into struvite fertilizer and fuel fractions. The flexibility of feedstocks is impressive and seems likely to be economically advantageous compared to dedicated single-source facilities.

Lumen Bioscience's Access Carbon project (1.3.4.008) expanded the downstream product offering into biotherapeutics, leveraging a recombinant spirulina platform to provide recombinant antibodies for intranasal delivery. Media optimization, pH, and alkalinity parameters were optimized by design of experiment and machine learning to minimize the range-finding experiments typically necessary for platform development and characterization.

Process analytics and diagnostics: Strain generational stability and trait drift, as well as contamination diagnostics, were characterized in the Optimizing Selection Pressures and Pest Management to Maximize Algal Biomass Yield (OSPREY) project (1.3.5.280), led by the New Mexico Consortium. Based on the observation that many lab strains fail catastrophically in field trials due to contamination and possible trait drift, the study developed field-ready pest detection techniques that provided results rapidly enough for pond management to respond to the infection and rescue the algae productivity. Loss of genetic stability in the field was significantly higher than observed in the laboratory strains due to outdoor selection pressures, and trait drift of pond cultures was identified as potentially having site-dependent phenotypes rather than being linked to genetic instability. The field-deployable qPCR method for diagnostics and monitoring may be helpful, especially over several seasons and when compared across different facilities, seasons, and scales.

A project from GAI (1.3.5.284) presented the use of rapid offline spectroscopy for protein, carbohydrate, and lipid content prediction using machine learning and neural networks to optimize the quantification of specific fractions. These methods allow for standardized materials handling and processing to improve the comparability of strain improvements and assess the efficacy of media supplementation, as well as the impact of environmental effects. Improvements to productivity were reported using both biotic and abiotic methods, which will be described in upcoming patent applications.

Techno-economic models: The major development in the techno-economic model field was the highly detailed Aspen Plus model developed by NREL (1.3.5.200), with an Excel version available to the public. The model was iteratively validated by 8 years of real-world data from the Development of Integrated Screening, Cultivar Optimization, and Verification Research (DISCOVR) project, integrating polyurethane (PU) and protein coproducts into the final analysis. This revised model demonstrated the criticality of coproducts toward the goal of making biofuels economically feasible. Adoption of the model framework by many other laboratories validates its usefulness and impact on the field as a whole, and the team has made excellent efforts to make the work publicly available. Keeping the model updated with current data, including product quality metrics, will provide even more value to the industry and the field.

This model was integrated with a PNNL model of the high-throughput hydrothermal liquefaction (HTL) unit operation (1.3.5.202) and downstream processing for hydrogen generation, naphtha and diesel production, sustainable aviation fuel (SAF) production, and a struvite fertilizer coproduct generated by PNNL from a mix of biomass sources. The critical result of the PNNL model demonstrated the importance of leveraging wastewater-grown algae and other waste materials as a source material to achieve a price of $2.61 per gasoline gallon equivalent (GGE). Further empirical testing of product quality will be required for validation; initial testing of oil products for jet fuel has supported the model.

Several projects incorporated updates to the harmonized TEA in their work, especially as it relates to increased productivity, reduced system input requirements, and additional coproducts with higher market prices than commodities.

Training: The Algae Technology Educational Consortium (ATEC) remains the centerpiece of training the current workforce for not only biofuels production, but also biotechnology jobs more generally (1.3.5.201). ATEC's outreach, especially during the COVID-19 pandemic, has expanded to 41 schools and served more than 190,000 students via their course offerings, which include in-person coursework at universities and community colleges, internships, K–12 STEM education, internships, and massive open online courses (MOOCs). Their outreach to historically Black colleges and universities, Hispanic-serving institutions, Asian American and Native American Pacific Islander-serving institutions, and Alaska Native and Native Hawaiian-serving institutions has made biotech education accessible even in regions without algae cultivation operations, enabling workforce development and thereby providing a scientifically trained labor pool for employers as well as job opportunities for historically underserved groups.

RECOMMENDATIONS

Overall, the reviewers feel that the projects reviewed were well aligned with BETO goals and are being well managed. In general, projects are making excellent progress in advancing the state of algae technology development. Projects are moving cultivation and processing technology forward toward contribution to the displacement of petroleum-based products in a cost-effective, economically competitive manner. Projects are monitored actively, and the interaction of staff with investigators appears to be working well. Projects were adjusted appropriately in response to new data. We commend the good work and see no major corrections to the program needed. That said, we do have some minor corrections and comments on individual projects:

1. The focus on DAC of CO_2 to minimize reliance on transported CO_2 and/or collocation with flue gas production will be critical for making algae production for commodities and fuel economically feasible, enabling the use of inexpensive land and reducing logistics and process piping requirements for commercial-scale facilities.

2. There remain a few critical gaps between academic research and industrial implementation: contamination response and culture rescue, downstream processing of the various algae components for commercial sale, and a clear scale-up characterization that would bring a shorter path between the $n = 1$ facility design and the n^{th}-plant optimized version.

3. With respect to the contamination response, we would like to see increased understanding of contamination and the microbial flora associated with algae cultivation generally, standardized contamination response methods (which are common in industry), and more nuanced definitions of what constitutes acceptable versus unacceptable contamination levels, "crashing," and conditions that more subtly limit productivity in an outdoor pond environment.

4. Downstream processing of the algae components should also be given more in-depth consideration: While high-priced coproducts contribute toward a more economically feasible TEA, the volumes of those coproducts relative to their market size, in comparison to the demand for fuel, is unbalanced.

Further, downstream product TEA standardization could benefit the field by providing a true comparison of the different methods and their feasibility. In order to meet economic requirements, oil fractions were often diverted to other products rather than fuel, reducing renewable fuel production. Product quality and comparability to the current market products needs to be characterized to validate the economic viability of the processing steps.

5. At the very large scales representative of the ponds needed for commodity chemical and fuel production, we feel that more work around characterizing mixing and kLa could inform the scale-down and pilot models being used to represent at-scale processes. While modular systems such as the rotating biofilm reactors should be relatively straightforward to scale up, novel DAC methods and large pond mixing systems are unlikely to scale linearly and require testing at scale. Industry could support better scale-down work by releasing monitoring data or allowing sensors to collect data during both successful and unsuccessful cultivation in order to better understand what parameters constitute successful batches as opposed to the effects of normal environmental flora and algae stress events.

6. Another concern is the number of process patents generated being used as a metric of success. Process patents are notoriously challenging to enforce, and the addition of multiple unit operations for material processing seems likely to add significant expense and risk of process failure. Due to the lack of enforceability and the existing prior art associated with seed oil processing and fermentation product fractionation and recovery, the value of process patent development may not be a significant outcome of the research.

BETO's clear, comprehensive, and industry-focused goal setting overall has been highly successful in guiding industrial and academic labs to focus on critical roadblocks toward at-scale commercial production. The stepwise advancement of the program has created impressive advancements in the implementation of real-world economics to hypothetical models, validation of the models with field trials and empirical evidence, and viable products that can be used as drop-in replacements for petroleum-based chemistries. Scalability has progressed significantly over the past several years, and the new goals for SAF will continue to address practical real-world challenges.

ADVANCED ALGAL SYSTEMS PROGRAMMATIC RESPONSE

The 2023 review of the AAS Program owes its success in large part to the excellence and dedication of the diverse group of eight individuals who agreed to serve as independent peer reviewers. The AAS Program, as it continuously strives to hone its strategy and improve on the outcomes of its investments, is deeply indebted to their service and values the highly relevant and actionable recommendations that resulted from their efforts. From all at the AAS Program and BETO: Thank you reviewers!

The AAS Program is deeply grateful to the reviewers for their acknowledgment of DOE's "unwavering dedication" to advancing the state of the art for advanced algal systems. It is very heartening to hear that the efforts of the AAS Program to craft relevant, aggressive strategies to accelerate the commercialization of "sustainable and cost-effective algal production technologies" are recognized by the reviewers as a globally leading approach. In the AAS Program, because of our strong mission focus, we constantly seek to improve through disciplined and continuous evaluation of strategic direction and execution. Thus, we cannot thank the reviewers enough for holding the AAS Program up as a "testament to DOE's commitment to driving innovation."

This review cycle is particularly valuable to BETO as it undergoes a realignment of how it manages its algae and feedstocks work. Beginning in fiscal year (FY) 2023, BETO embarked on changes to move the AAS Program into a new program area entitled Renewable Carbon Resources and to integrate the management of the formerly separate AAS Program activities with the former Feedstock Technologies Program. This was done in recognition of the suite of available carbon resources that BETO is focusing on to meet decarbonization targets. Continuing the realignment of its strategy, BETO shifted a significant amount of FY 2023 AAS budget resources to its Scale-Up Program (Systems Development and Integration) for pre-pilot work on algal systems.

In 2023, the AAS Program presented its portfolio of projects in two parallel tracks, split roughly between the development of individual technologies or approaches to strain and cultivation improvement and the integration of multiple systems to improve productivity and cultivation performance. These two tracks, "Cultivation and Strain Development" and "Integration," were reviewed by separate review panels even though the projects and strategy remain unified. This achieved the desired outcome of lessening the burden of the review on reviewers, staff, and presenters by shortening the in-person commitment from 5 days in 2019 to 2. Steps were taken to ensure that the separate panels of reviewers nonetheless received a complete picture of the AAS Program, its strategy, and management.

Although there are two separate Review Panel Summary Reports, the response here focuses on the top recommendations from each report in a unified response. The recommendations made by the panels serve as important guidance as BETO moves forward in its mission. Neither panel noted the need for major corrections to the AAS Program strategy or execution, but both did offer valuable recommendations for consideration going forward. The program offers a detailed response to the top recommendations here.

Recommendation 1: Further advancements in low-cost sustainable biofuel production from algal oil, including efforts on extremophile strains and increased focus on culture stability and contamination response

The recommendation to pursue further advancements in low-cost and sustainable algal biofuel production is one that the AAS Program is glad to take. While the AAS Program is pleased that the reviewers recognize the significant advancements in algal biofuel technology and progress in algae productivity made possible through the AAS Program's efforts, we recognize that further development must take place to accelerate the commercialization of algal biofuel technologies. We agree with this recommendation and feel that it validates our program strategy in that further advancements are not only needed but are attainable through the continued execution of the AAS Program strategy. An initial step in this direction was taken by issuing a call for national laboratory projects focused on "Carbon-Negative Algal Biofuels" using FY 2024 requested funding that seeks to understand analytically and experimentally the feasibility of pathways that can leverage low-carbon-intensity products and/or environmental services to provide low-cost and low-global-warming-potential algal biomass for conversion to SAF. The recommendations to focus on strain improvement and diversification of strain selection while combining efforts on bioprospecting, strain evolution, and engineering with existing technologies is a valuable one and can be considered as the program continues to pursue increases in productivity.

The suggestion to consider a more targeted investigation of extremophile strains aligns well with the direction that the DISCOVR consortium is taking to rescreen strain libraries at higher pH and to continue to implement efforts to grow strains at high pH, salinity, and temperature. To further this area of development, the AAS Program released an FY 2023 funding opportunity for algal crop protection technologies and looks forward to announcing the selections by the end of FY 2023.

Recommendation 2: More consideration to downstream processing and conversion of algae components

While the AAS Program has historically dedicated the bulk of its focus to algae strain development, biomass production, and cultivation improvements, there has been a dedicated focus area on the interface between algae biomass and conversion. These efforts—directed primarily through engagement with relevant centers of core capabilities at NREL and PNNL for the low-temperature fractionation of biomass into constituents for conversion and upgrading and the high-temperature deconstruction and upgrading of whole biomass—have informed critical developments in the state of technology (SOT) for converting algal biomass and often serve as the basis for scale-up considerations by industrial partners. However, this area has not been a primary focus of the AAS Program's efforts, largely due to the challenges of matching the conversion process requirements for both continuity and fidelity of biomass production to the downstream process. Consequently, the challenge in providing consistent and adequate supplies of representative algae biomass for conversion process development has been great. However, as both the pathways to algae-based products and the ability to produce biomass in the desired composition and formats become more attainable due to the steady progress achieved in strain development and cultivation improvement, we are excited to explore more opportunities in this space, particularly in ways that demonstrate the potential for low-carbon-intensity fuels enabled by advantaged products and/or services.

Recommendation 3: Engage industry partners and address scale-up challenges

This recommendation is especially valuable to the AAS Program, and we are glad that the reviewers see the need for continued engagement with industry stakeholders. The suggestion to incorporate industry inputs into TEA and LCA development is especially valuable and is something the program has long considered. Another consideration that the program made in FY 2023 that was not reviewed by this set of reviewers was the allocation of $15 million in the FY 2022 and FY 2023 budgets away from the Research and Development (R&D) Program and toward the Systems Development and Integration Program. This allowed the selection of five pre-pilot algae biofuel projects through the FY 2022 Scale-Up FOA. Scale-up projects, even at the pre-pilot scale, are an important progression from R&D activities because they allow for the construction and operation of unit operations that can begin to provide the necessary engineering data to de-risk further scale-up and integration of technologies. This suggestion is very aligned with BETO's commitment to continue seeking partners for pre-pilot, pilot, and demonstration projects for algal biofuels.

In conclusion, the AAS Program is grateful for the opportunity to work with the 2023 independent peer reviewers and appreciates the overall sentiment that the continued funding of the AAS Program strategy will contribute to BETO's overall goals for biomass production and conversion. With the recommendations summarized above in hand, BETO will continue to pursue strategies to move the state of the art forward for algal systems. BETO looks forward to presenting the results of its efforts to accelerate the advancement of algal system technology development and deployment to the public once again in the 2025 Peer Review.

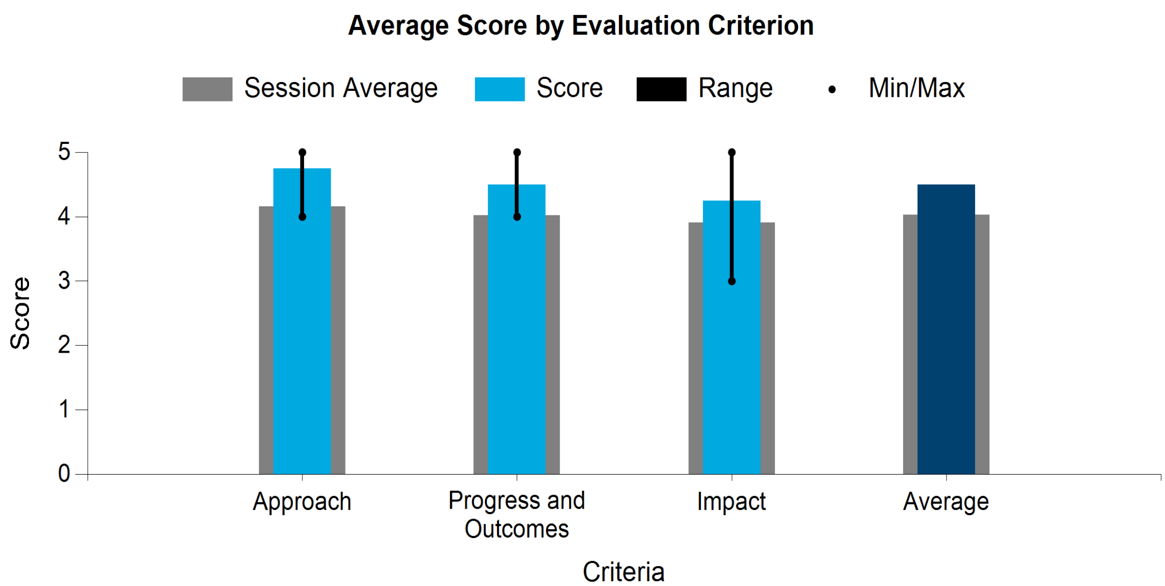
ALGAE BIOTECHNOLOGY PARTNERSHIP

National Renewable Energy Laboratory, Los Alamos National Laboratory

PROJECT DESCRIPTION

WBS:	1.3.1.131
Presenter(s):	Michael Guarnieri
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,550,000

Development of advanced genetic and phenotyping tools will be integral to achieving BETO algal biomass productivity, composition, and cost targets. However, despite recent advances, algal genetic engineering pursuits remain largely limited to "one gene at a time" targeting and analysis, and broad host-range tools are generally lacking, hindering the development timeline for newly emerging strains. Establishment of genome-scale, high-throughput genetic and phenotyping tools represents a key technical hurdle that must be overcome to realize the full potential of microalgae as an economically viable feedstock. To this end, the Algae Biotechnology Partnership proposes to develop high-throughput tools to generate and phenotype genome-scale libraries of an industrially relevant microalgae. The resultant pipeline will enable full characterization of the genetic basis of photosynthesis, carbon storage, and nitrogen metabolism to improve algal biomass composition and productivity. Key challenges currently being targeted include high-efficiency transformation and genome editing and high-throughput and automated adaptation of established phenotyping methodologies. To date, we have demonstrated tool transferability across multiple top-candidate deployment strains and initiated generation of a genome-scale *Picochlorum renovo* knockout library, laying the foundation for first-in-class tools for basic and applied research in deployment-relevant algae.



COMMENTS

- This project focuses on developing a high-throughput and automated pipeline for screening and genetic engineering tools to accelerate improvement in industrial strains of algae and cyanobacteria. The project is of clear relevance to BETO's Multi-Year Program Plan goals. An additional goal was to generate genome-scale libraries for *P. renovo* that will be publicly accessible.

- The project performers seem to have clear management plan while leveraging expertise from the different investigators. The team provided a project management, communication, and collaboration plan. Risk and challenges involved in the execution of this project were identified, and mitigation strategies were outlined as major milestones. The team also outlined an approach to addressing diversity, equity, and inclusion (DEI) in their project plan.

- The team has developed an optimized transformation and cryopreservation procedure for 96 well plate, next-gen barcode sequencing to enable library validation, as well as an established CRISPR system for targeted genome editing. These tools have also been used to enable platform expansion across multiple DOE offices. The team has made significant progress in 18 months and seems to be on track to achieving their goals. One area to be considered is ensuring that phenotyping and characterization methodologies are performed under simulated outdoor conditions to increase the chance of success. It's also unclear if these strategies will result in strains with improved biomass productivity that can be commercially deployed. Overall, the project seeks to address key research needs stated in BETO's Multi-Year Program Plan with the goal of developing strain improvement toolkits and technologies for improved biomass productivity.

- The project has made very good progress on strain engineering via high-throughput-capable genetic tool development, and it integrates well into BETO's goal for achieving strains with high mass productivity that are cost efficient and have carbon storage capacity. The team has established a partnership with three other national labs and an academic institution, all working together in a very cohesive environment with a high level of productivity. A major milestone has been reached for FY 2022 by achieving >5x transformation efficiency enhancement in *P. renovo*, exceeding 100 colony forming units (CFU)/µg DNA, as stated in the report. Another task focuses on delivering a publicly accessible, genome-scale mutagenic library of *Picochlorum* spp., and it has made significant progress despite some obstacles. The next task on phenotyping and characterization has been initiated by the team for *P. renovo* genome-scale mutant libraries. The team has addressed the DEI component in their project and remained on task, and one can only predict that the project will be successful to meet BETO's goal on producing sustainable, cost-effective algal biofuel. Data on how the engineered *P. renovo* is faring on open raceway ponds were not presented. Has any effort been made to design genetically engineered strains with resistance to predation? The team has effectively dispersed their research findings through several publications, patents, and presentations.

- This project appears to be managed well and involves teams with appropriate expertise and backgrounds to achieve the project goals. They have a DEI component even though it was not required at the time of funding. The project aims to develop/deliver a toolkit that can transform any algae strain. The work started with a top production strain (*Picochlorum* sp.), chosen due to its high productivity and doubling time. They have so far demonstrated the transformation toolkit on 12 strains, most of which are BETO relevant, but appear confident that it will work for any strain going forward (within 1–4-week turnaround time). Mutants are screened based on lipid and carbohydrate production but could include other targets like pigment production, supporting both fuel and coproduct pathways. Several mutants have already been grown outside at larger scale. The team appears to have met, and in some cases exceeded, their project goals.

- The project team is focused on delivering universal, high-throughput-capable genetic engineering tools. The approach uses the latest genetic engineering techniques to improve strains, and the project aligns well with helping BETO achieve biomass targets. The project appears to be on schedule, and appropriate risk mitigation strategies have been employed. Mutant libraries and high-throughput phenotyping methodologies for two *Picochlorum* strains have been successfully developed to date; thus, the team has made appropriate progress toward project goals. The wider impact of the work is difficult to assess given the focus on only *Picochlorum* strains; thus, it is recommended that the project team test the developed tools on other industrially relevant microalgae species before the end of the project. The project team has made the strains and DNA sequences publicly available, and the developed tools should aid microalgae commercialization efforts.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive and constructive feedback. The project team shares the reviewers' enthusiasm regarding progress to date; we have made substantial progress in strain engineering and phenotyping, achieving all project milestones to date, and we are on track to achieve end-project goals. Regarding performance under simulated outdoor conditions to increase the chance of success, we agree with the reviewer's suggestion; all strain validation will be performed under diel light and temperature cycling to reflect outdoor deployment at the AzCATI test bed. Regarding the likelihood that our proposed strategies will result in strains with improved biomass productivity that can be commercially deployed, we note that the overarching goal of the project is to establish enabling capabilities to rapidly generate and characterize strains with an array of phenotypes, including, but not limited to, altered carbon storage flux to lipids and/or carbohydrate, growth rate, and pigment content. It is our expectation that the resultant mutant library generated from our work scope will result in a subset of mutants with enhanced deployment properties. Importantly, the resultant tools emerging from this project will provide an invaluable resource to the algal R&D community, providing a blueprint for high-throughput strain engineering and phenotyping, as well as a *Picochlorum* genome-scale library, representing a first-in-class tool for a non-model, deployment-relevant microalga. Regarding strain performance outdoors, to date we have deployed our wild-type cultivar, which achieved >20-g/m^2/day outdoor productivity at the AzCATI test bed. Though deployment is outside the scope of the current project, we have a series of active complementary projects focused on strain deployment, including development of phosphite-mediated cultivation, which present a promising crop protection and predation resistance strategy. Regarding the wider impact of the work beyond *Picochlorum* strains, we note that we have demonstrated our genetic toolbox efficacy in a series of top-candidate BETO DISCOVR deployment strains. It is our expectation that the tools developed herein will be readily transferable to other industrially relevant cultivars as they come online. To this end, parallel efforts are already underway to incorporate *Scenedesmus* sp. 46B-D3, a representative industrial high-storage carbon strain, into our development pipeline. Efforts to date have established genetic transformation capabilities therein, using the genetic toolbox developed in our initial period of performance, and phenotyping during diel cycling, including ash-free fry weight, carbohydrate, lipid, and proteins.

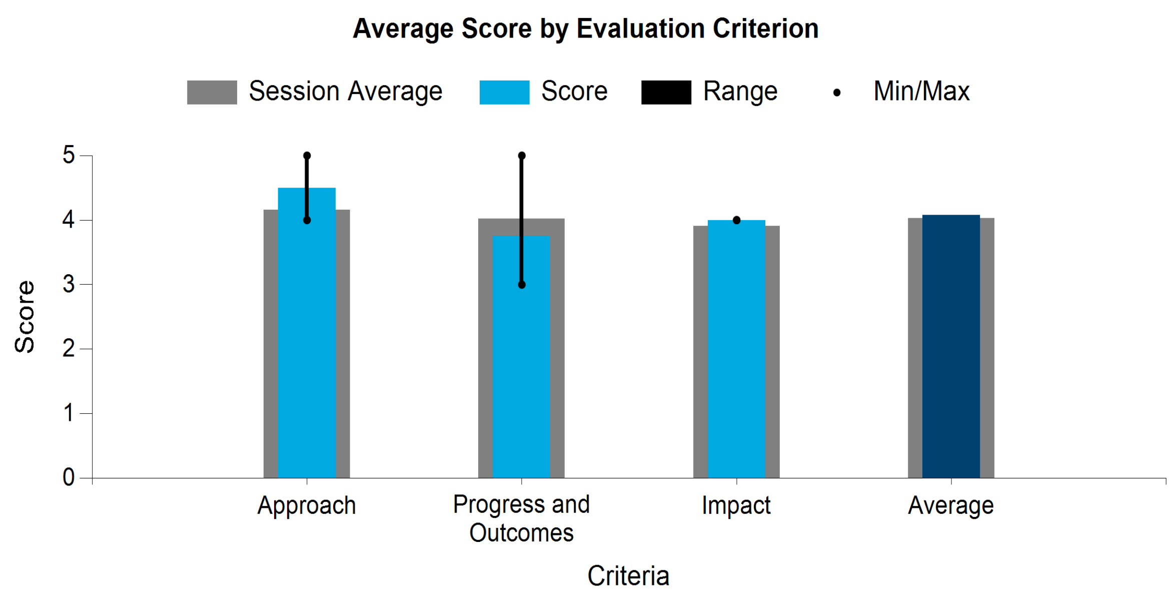
ALGAE DISCOVR

Pacific Northwest National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, National Renewable Energy Laboratory, Arizona State University, Colorado School of Mines

PROJECT DESCRIPTION

WBS:	1.3.1.501
Presenter(s):	Michael Huesemann
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2022
Total Funding:	$8,768,025

To meet the DOE 2030 annual productivity target of 25 g/m^2/day, the DISCOVR consortium—a collaboration between PNNL, LANL, NREL, Sandia National Laboratories, Colorado School of Mines, and the AzCATI test bed at Arizona State University—was tasked with identifying and testing new high-productivity algae strains and finding ways to further improve biomass productivity during cultivation, enhance biomass value, and increase crop protection and culture stability. Major accomplishments include successful utilization of the DISCOVR strain downselection pipeline, culminating in the top seven strains being deployed in outdoor growth trials at AzCATI. These were selected from a comparative study of temperature and salinity tolerance of 42 strains, followed by productivity assessment of 25 strains under climate-simulated conditions, leading to 13 strains cultivated in outdoor ponds. Adding growth-promoting molecules, reducing oxygen inhibition, and using luminostat control each increased productivity by >20% relative to baseline productivity. New methods were developed to simulate outdoor ponds in photobioreactors (PBRs) and to predict and prevent pond crashes using spectroradiometric monitoring and integrated pest management. A concerted effort in year-round cultivation trials led to a 60% increase in annual biomass productivity since 2018 (11.7 to 18.5 g/m^2/day) when strains from the DISCOVR pipeline started to be deployed in SOT trials, equivalent to a reduction in biomass selling price of 27%, from $824/ton to $602/ton.



COMMENTS

- This project focuses on reducing total microalgae biofuels production cost by applying an integrated screening platform to identify highly productive strains, testing new concepts to improve productivity and culture stability, and using TEA to identify economically feasible concepts to test out on ponds. The expected outcome is to reach the BETO 2030 target of $488/ton years ahead of schedule. Their goals and approach are reasonable.

- The team had a clear management plan with a well-defined task structure and leads. They identified risks and implemented mitigation strategies, as well as establishing channels of communication and collaboration among team members. The also outlined go/no-go decision points and milestones that were all met. The team is composed of six national labs and two institutions.

- The team was successful in selecting seven top strains for SOT trials that resulted in a 60% increase in the SOT productivity to 18.5 g/m^2/day and a 27% decrease in minimum biomass selling price (MBSP) to $600/ton. The project made significant progress toward increasing productivity and stability in outdoor ponds. The project had a good balance between lab-scale and outdoor testing, which is crucial to demonstrate the feasibility of the proposed technology and commercial deployment of the technology. From the strain selection pipeline, there seems to be no improvement in productivity since 2020. The project performers should consider diversifying their strain selection criteria and integrating strain improvement technologies and toolkits. For instance, the team should consider integrating previous projects that have demonstrated glycogen knockdown and deletion on a sucrose phosphate synthase enzyme that showed improved photosynthetic oxygen evolution and biomass productivity.

- The team demonstrated improved growth in flask and outdoor simulated environmental PBRs using indole-3-acetic acid (IAA) and suggest reduction in MBSP with IAA. It's unclear how stable IAA will be in outdoor conditions and the impact of contaminant and ecological diversity on the performance of IAA. If a higher concentration and multiple feeds of IAA are required for outdoor cultivation, the cost impact may be detrimental.

- OptiLum operations showed a significant improvement in biomass productivity and a reduction in cost of about 22%–38%. It's unclear if the hydraulic load and cost of pumping associated with a semicontinuous process was considered and if the project performers are considering recycling the water. Significant progress has also been made in the area of crop protection using fungicides and saline strains that have shown more than 60% improvement in productivity. The use of algal bacterial co-cultures showed promise, but concerns of bacteria overtaking the pond and competing with nutrients should be considered, as well as the overall impact on biomass productivity/quality and downstream processing.

- Plans for the next 3-year cycle include demonstrating 70% CO_2 utilization efficiency, achieving mean time before failure target of 20 days, and attaining annual biomass productivity of 20 g/m^2/day. It's not clear what approach the team intends to use to achieve the goals.

- Overall, significant progress has been made in selecting high-producing strains for the different seasons, deploying a biomass improvement and crop protection strategy. The team has demonstrated productivity improvement in the AzCATI outdoor algae cultivation and leveraged a TEA model to identify key cost drivers. One area the team can focus on is commercial deployment of these strategies and collaboration with industrial partners.

- The team has made significant progress in their effort to achieve the goals outlined in the DISCOVR project. Through uninterrupted cohesive interactions, communications, synergy, and productive coordination by employing a structured, tiered assessment process, the team has been successful in identifying seven algal strains that are currently under pond SOT trails at the AzCATI test bed. The DISCOVR project advanced through inputs and knowledge sharing with the community, as well as researchers in other BETO projects. The consortium uses their core capabilities to actively collaborate with algae industries, academia, and a culture collection center. They have successfully delivered their outputs in several areas involving data collection, SOT, and pest resilience of cultures, as well as to downstream projects related to genome sequencing, multi-omics, molecular toolboxes, biomass, and nutrient cycling. The stream of continuous feedback data facilitates DISCOVR team researchers adding in new strains to the pipeline as the project progresses. DISCOVR's productivity data seem to be on track and successful in keeping up with BETO's target 25-g/m^2/day annual average by 2030. The impact of the DISCOVR project is displayed by the product that the team has to offer to the community from their last 3-year effort. The team has made a remarkable contribution to addressing some of the major challenges and issues related to algae-derived biofuel cost, productivity, culture resilience, and biochemical composition. DISCOVR has been active in sharing their research findings through extensive publications in peer-reviewed journals and partnerships with industries and academia. The team has made a significant effort to diversify and democratize their gained knowledge about algae cultivation in every possible way that will benefit society and provide solutions to challenges. One aspect that seemed to be missing was the data for any specifically engineered pest repellent strain, which would be an important area to explore and consider for crop protection considering the vastness of expertise in the team. If one has been employed, the emphasis on it was not clearly mentioned in the report.

- As one of BETO's flagship projects, this consortium has generated many technologies and a huge amount of data useful to inform algal production. The management team seems well put together, and no communications issues are obvious. The work also benefits from a third-party advisory board that was recently reshuffled to be more scale-up focused. Importantly, DISCOVR has so many entities involved in the effort with a high degree of outreach to the academic and national lab sectors that there is high potential for future algae leaders to emerge from this effort. They also appear to have a DEI component even though this was not a requirement of the project. However, after 9 years of work, it is disappointing that more formal connections with industry have not been made or spun off from the project. The leveling off of MBSP over the last several years is also concerning, as there was a steady decrease over the first 5–6 years. The presenter stated that the initial decreases in MBSP were due to new strains coming on board that were highly robust and productive (namely *Picochlorum*). However, the conclusions were that they had exhausted the available strains and instead would address the leveling off with OptiLum technology and growth-promoting molecules. Neither of these have been validated enough to be confident of the economic feasibility or the magnitude of the effect on productivity. Growth-promoting molecules could be promising because they are used so widely in traditional agriculture, but work still needs to be done to make sure they remain stable in outside pond conditions and, if needed, multiple doses are still economically feasible. This poses a lackluster end to an otherwise strong effort. From the 2021 report, there seemed to be discussion of opening up the DISCOVR pipeline and outdoor testing to engineered strains, which could be an important tool to target MBSP, but that was not mentioned this year to my knowledge. Perhaps a stronger industry tie would uncover more strains (improved or otherwise) to test. Lastly, handoff of the technologies developed during this consortium would be more impactful to a future industry if the project included an outdoor validation step at multiple geographies, although this would be a much larger undertaking and likely outside the scope of BETO funding budgets.
- DISCOVR serves a valuable role in validating and testing collected strains in their strain pipeline for BETO. DISCOVR made impressive productivity and MBSP gains in 2019 and 2020; however, minimal gains have been realized over the last 2 years. The collection of additional *Picochlorum* strains from the Gulf of Mexico is encouraging, but increased efforts should be made to identify new strains to introduce into the DISCOVR pipeline. The management plan is clear, and the project team seems to communicate effectively, even given its large size. Future work might be directed to the isolation of high-lipid, alkali-tolerant strains for outdoor cultivation given the success of other projects in the BETO portfolio in regard to pond crashes.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' comments and the opportunity to present a brief response to the major points raised. Regarding the need to identify new strains for introduction into the DISCOVR pipeline: As the DISCOVR project is now shifting its focus on improving CO_2 utilization efficiency at a higher pH, we will "reopen" the strain screening pipeline to identify strains that meet the new requirements. Building on the success of previous BETO-funded projects, PNNL established a collection of strains that are promising for high-pH cultivation. All the strains will be evaluated and downselected following the original DISCOVR pipeline concept but with new criteria (e.g., high pH). Furthermore, we are evaluating additional novel unique species from bioprospecting efforts beyond the focus on *Picochlorum* species. Since February 2023, additional cultivars have been obtained from bioprospecting in the Gulf of Mexico. *Picochlorum* persistently dominates most grow-outs from this area, but several diatoms and an *Ostreococcus*-like alga have also been isolated, which may be added to the DISCOVR pipeline if warranted after additional productivity testing. Two separate sampling trips have also been conducted at high-pH and saline lakes across the Western United States, as well as on the Pacific Coast. We hypothesize that sampling from a geographically diverse set of locations with high-pH waters will yield alternative species or strains with higher pH tolerance for competitive carbon use efficiencies. In addition to improved growth at higher pH, we are targeting new strains with different biomass compositions relative to *Picochlorum* species, specifically strains with a higher lipid content, which will improve MBSP. These newly identified strains will be tested in parts or all of the DISCOVR pipeline. Finally, we are continuing to identify new strains from culture collections or from prior successful cultivation efforts in other projects. One genus that stands out is *Tetraselmis*, which is currently one of the marine SOT test bed strains. *Tetraselmis* is the only genus to have exceeded, on an extended cultivation basis, the outdoor pond productivity values obtained by *Picochlorum*. Importantly, many strains in this group are significantly easier to harvest than *Picochlorum*, with associated reductions in MBSP. Regarding commercial deployment of DISCOVR strains and concepts and collaboration with industrial partners: We agree with the reviewers that collaboration with industrial partners is highly beneficial and should be pursued to the maximum extent possible. In the past, we collaborated with ExxonMobil (they provided the top summer season strain *Picochlorum celeri*) and Algenol. As part of our DISCOVR call for collaboration, we evaluated several crop protection compounds from Aequor. Given that DISCOVR team members already have connections to other companies, such as Heliae, Qualitas, Viridos, GAI, and Chevron, we will build on these to create potential collaborations with the DISCOVR project. We are also leveraging the technical advisory board in quarterly all-hands review meetings of planned research. This is an established framework that we can build on to specifically solicit feedback on challenges experienced by industry that the R&D tasks could better align with. Although our technical advisory board has numerous members from industry (Lumen, Qualitas, Umaro Foods, and MicroBio Engineering) that we can reach out to for collaborative opportunities, we will consider adding several new industry members (e.g., Chevron) next year to facilitate the offtake of microalgal biomass to SAF. Finally, we will keep the "call for collaboration" open to engage with industry. Regarding the stability and cost of the growth-promoting molecule IAA: We agree with the reviewer's comment that we have not yet analyzed the stability of IAA in our experiments. However, IAA has been used successfully at scale under outdoor agriculture conditions and in our experiments with outdoor mimicking scripts (high light intensity). IAA is effective at very low concentrations (1 µM) and cost-effective (inexpensive) at bulk price. Also, to address the issue of cost-effective supply of IAA, we are developing an algae:bacteria co-culture system to supply bacteria-produced IAA and make IAA supplementation sustainable and cost-effective. Regarding the cost of pumping associated with OptiLum operations: Changes in water movement due to lower harvested densities using OptiLum-based cultivations are effectively captured by the NREL Algae Farm Model, which translates them to compatible variations in the costs of pumping and dewatering operations. Recycling the spent medium from dewatering operations back to cultivation ponds is a longstanding assumption of SOT assessments in the BETO portfolio and, while not actively researched in the DISCOVR consortium, this consideration could be revisited whenever further experimental data are available from partner BETO projects. Regarding the concern that bacteria could overtake the pond and reduce productivity when using algal bacterial co-cultures for crop protection: It should be noted that bacteria are already present in any and all open-pond production systems. Algae and bacteria have coexisted and influenced ecosystems with all modes of interactions—from mutualism to parasitism. The bacteria used in this project are derived from ponds where they were already present and were determined to have no negative impact on productivity prior to our use. Because outdoor ponds are being operated under photoautotrophic conditions, as opposed to mixotrophic conditions, there is very low risk of the bacteria overtaking production ponds or significantly competing for nutrients. Regarding the approach to meeting the next 3-year cycle goals for CO_2 utilization efficiency, mean time before failure, and annual biomass productivity: Although per BETO guidance, presenting plans for future research was not required, we provided 19 slides in the supplemental section outlining the objective, approach, expected outcomes, and impacts of 19 different subtasks that will be carried out during this 3-year cycle. Here is a short overview of the six different tasks that will be executed during the current 3-year cycle: Task 1 focuses on improving biomass productivities via (a) OptiLum and Turbidostat culture control, (b) addition of growth-promoting bacteria, and (c) evaluation of seaweed pond culture. Task 2 is aimed at improving CO_2 utilization efficiency by (a) minimizing CO_2 outgassing via cultivation at air/water equilibrium pH; (b) optimizing the medium water chemistry; (c) isolating high-lipid, alkali-tolerant strains; and (d) optimizing CO_2 utilization efficiency in large outdoor ponds. Task 3 centers around biomass quality tracking and optimization and addresses the development of (a) high-throughput biomass compositional analysis, (b) valorization of protein, and (c) preservation of biomass intrinsic value. Task 4 focuses on increasing crop protection and culture stability by evaluating (a) companion cultures, (b) radiospectrometric monitoring, (c) biomarker discovery and assay deployment, and (c) crowd-sourced agent characterization. Task 5 involves performing outdoor cultivation trials at the BETO SOT test bed at AzCATI. Task 6 focuses on carrying out techno-economic and life cycle analyses in support of DISCOVR tasks. Regarding missing data on specifically engineered pest-repellent strains for crop protection: Engineering of pest-resistant strains is dependent on *a priori* knowledge of mechanisms of resistance, including the genetic basis for those mechanisms. To date, very few resistance mechanisms have been characterized to the degree needed for precise engineering of algal strains of interest. At this point in the development of crop protection strategies, it is far more important to add to our knowledge base of resistance mechanisms than to focus our efforts on generation of new genetically modified strains. However, armed with sufficient understanding of pathogen resistance mechanisms, we do foresee our results providing fundamental knowledge that will guide informed biodesign of resistance engineering targets for algal production strains. Regarding the lack of validation of OptiLum operations and use of growth-promoting molecules: Because of limitations in budgets and resources, we had to carry out initial proof-of-concept OptiLum research in bench-scale indoor PBRs. We fully agree that further validation is necessary. Therefore, we have plans to evaluate the performance of OptiLum operations in indoor and outdoor raceway ponds, including at the SOT test bed at AzCATI. Regarding the validation of growth-promoting molecules, we are shifting toward algae:bacteria co-culture methods wherein the bacteria produce the growth-promoting molecules. We believe this will be a more sustainable and cost-effective approach than applying growth-promoting molecules directly. We plan to test this algae:bacteria co-culture approach in outdoor ponds in Year 3. While we may not expect the step change in productivity that we observed in early years, the focus of this current 3-year cycle is to establish a strong foundation in operational conditions (OptiLum, Turbidostat, growth-promoting molecules) to position us to help scale improved strains in a future effort. Regarding the lack of testing of genetically engineered strains: The evaluation of genetically modified strains was repeatedly discussed over the years. It was decided to evaluate only wild-type cultivars to simplify outdoor cultivation trials—i.e., avoid regulatory permitting for many different genetically modified strains. Instead of considering genetically modified strains as a solution to achieve higher productivity and stability, we are using a pond ecology and companion culture approach to achieve these goals in an environmentally compatible manner with extremely low or zero risk. Regarding outdoor testing at multiple geographies: We currently have two test bed sites (i.e., the PNNL Algae Testbed and the SOT Testbed at AzCATI) at different geographies, although both are located in Arizona due to favorable climatic conditions for outdoor pond cultivation. We agree that outdoor cultivation at multiple geographies, particularly in different climates, would be beneficial. Consequently, several years ago, we identified a potential second SOT test bed site at Texas AgriLife in Corpus Christi, Texas, located at the Gulf of Mexico. We also considered a potential test bed location in Miami, Florida. However, due to limited BETO funding, we have been unable so far to proceed with plans to conduct outdoor pond trials at additional geographies. We are investigating opportunities to bring additional test beds online in the future to cover a more diverse climate spectrum, provided funding is available for training and deployment.

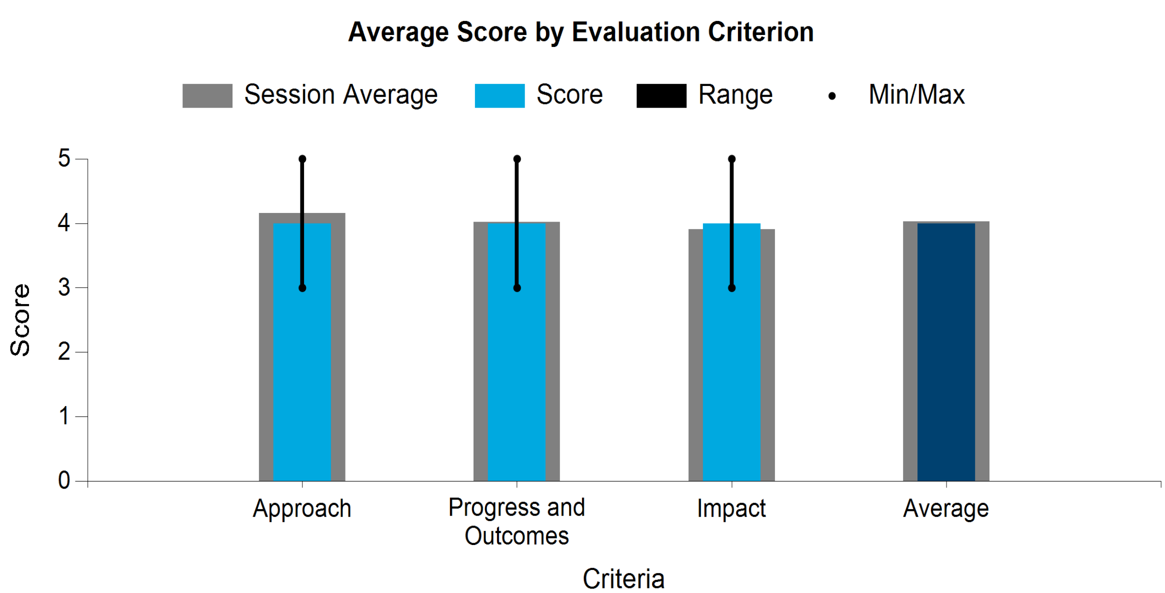
DIRECT AIR CAPTURE INTEGRATION WITH ALGAE CARBON BIOCATALYSIS

Arizona State University

PROJECT DESCRIPTION

WBS:	1.3.1.670
Presenter(s):	John McGowen
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$4,000,000

This project will deliver a full experimental integration of DAC technologies with novel algae strains—derived from the genetic engineering of *Scenedesmus* (or *Acutodesmus*) *obliquus* (UTEX393). Both of these are more resilient than the wild-type strain and increase annual productivity by at least 20% while maintaining the quality of the biomass for conversion to fuels and products. This novel project aims to open the field for DAC integration with increased photosynthetic carbon capture and storage biocatalysis by addressing key barriers that currently limit overall process efficiencies, accompanied by a cost and sustainability assessment. The collaborative team of scientists at Arizona State University and NREL, supported by DAC partner Silicon Kingdom Holdings, will build on years of research in both algae cultivation and central carbon metabolic engineering that have pushed the boundaries of increasing and controlling biomass productivity and quality. This team is uniquely positioned to both push the frontier of algae engineering and directly align new technologies with ongoing multiyear SOT outdoor production trials. This project presents opportunities for techno-economic and sustainability analysis for DAC technologies, supported by Silicon Kingdom Holdings partners. A critical contribution of this project is the proposed installation of a MechanicalTree™ at AzCATI, allowing for the unique and seamless integration of biological and chemical carbon capture technologies.



COMMENTS:

- This project proposes a technology that uncouples algae production from collocation with point sources of waste CO_2, opening options for siting of algae cultivation. The project performers allowed three approaches: (1) integration of passive DAC into algae cultivation using innovative carbon delivery and enzyme catalysis, (2) engineering of the UTEX393 strain for carbon flux control, and (3) pond design for improved time to failure and overall productivity. This goal is of clear relevance to BETO's mission and Multi-Year Program Plan goals. Successful execution will reduce the cost of production and eliminate the constraints of siting algal production systems close to industrial CO_2 supply.

- The team did not outline a management plan but had a well-defined task structure and leads. They identified risks and outlined mitigation strategies. The clearly defined their baselines for cultivation performance targets with go/no-go decision points.

- The team proposes to use a commercial-scale demo unit for passive DAC that will be integrated with the AzCATI test bed and novel membrane-based CO_2 delivery in combination with an enzymatic biocatalysis unit. It's unclear how the cost of this deployment will impact biomass production cost and whether the benefits outweigh the cost. The impact of environmental conditions such as wind and dust on passive DAC performance should be considered for cost analysis. The approach the project performers plan to use to engineer UTEX393 for carbon flux control is also unclear. Overall, not a lot of progress has been made toward the goals outlined due to delays in contracting.

- This proposal aims to design a modeled, integrated, passive DAC for outdoor algae cultivation that will encompass innovative carbon delivery and enzyme biocatalysis application by strain engineering to provide a sustainable and economical pond system. The team had the initial success of setting up the commercial-scale MechanicalTree, which is being tested to optimize its operation and shows promising results; it has achieved 50% carbon utilization efficiency with the coupling of the membrane technology. The operation of the membrane technology was not very well explained and was difficult to understand. The continuous monitoring of the pond health and the microbial profiling work have provided significant data for crop management, which is a challenge for open-pond production. The task of metabolic engineering of strain UTEX393 showed improved photosynthetic carbon assimilation. The AzCATI team has made good progress in all the defined areas as stated in their project goals and is currently on schedule.

- This project is led by a comprehensive team and plan. The management structure/communication appears to be clear and includes industry partner(s) involved in developing/deploying the technology. There is a high risk that the engineered strain will be more susceptible to pathogens, and in that case, the team will rely on mitigation strategies already in place or switch to a different strain in order to meet their goals. The technology being developed is very interesting and potentially highly valuable in utilizing DAC to grow algae. The tree technology raises concerns about being too complicated to operate long term, and it is hard to imagine it will be economically feasible at the scale needed for algae biofuel and in the environments where scale-up will be feasible (i.e., dusty non-arable land). Feasibility would be increased if the team had an algae producer interested in partnering, or at least demonstrating the technology at a small scale. It will be important to have a well-worked-out TEA for this technology that can be validated.

- The passive DAC technology seems innovative and avoids having to collocate the algae cultivation near a waste CO_2 source. Appropriate risk mitigation strategies have been identified. The project passed initial verification in January 2022, but the project wasn't awarded until October 2022. Some preliminary results have been achieved, and progress does seem to be accelerating. Some technical detail was provided for the mechanical tree that inspires more confidence in the project. Uncoupling algae farming from point source CO_2 with the novel DAC-sourced carbon would have a significant impact on large-scale algae cultivation.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their time, thoughtful comments, and constructive criticism. With respect to the perceived technology complexity for the mechanical tree, we feel the opposite is true, and this passive DAC has the potential for massive scaling. In fact, the targets for our partner Carbon Collect are scales of CO_2 removal necessary for sequestration, not just reuse. The main goal with respect to the modeled integration of this DAC technology with algae cultivation is to perform a thorough TEA and LCA at different farm scales to assess feasibility for algae cultivation and allow Carbon Collect to assess the commercial potential for algae cultivation as an early target market for their technology. To ensure maximum impact, we are talking with algae cultivation companies and are actively pursuing additional funding opportunities that would allow for the next stage of actual integration into an algae farm. Having access to a commercial-scale, technology readiness level 6 demonstrator of the passive DAC technology, operating outdoors in an arid, dusty environment, is to gain the necessary data and understand the actual performance. Different sorbents and operation modes are being developed to allow for multiple deployment environments, and Carbon Collect, outside the scope of this project, is working to understand how those factors affect performance.

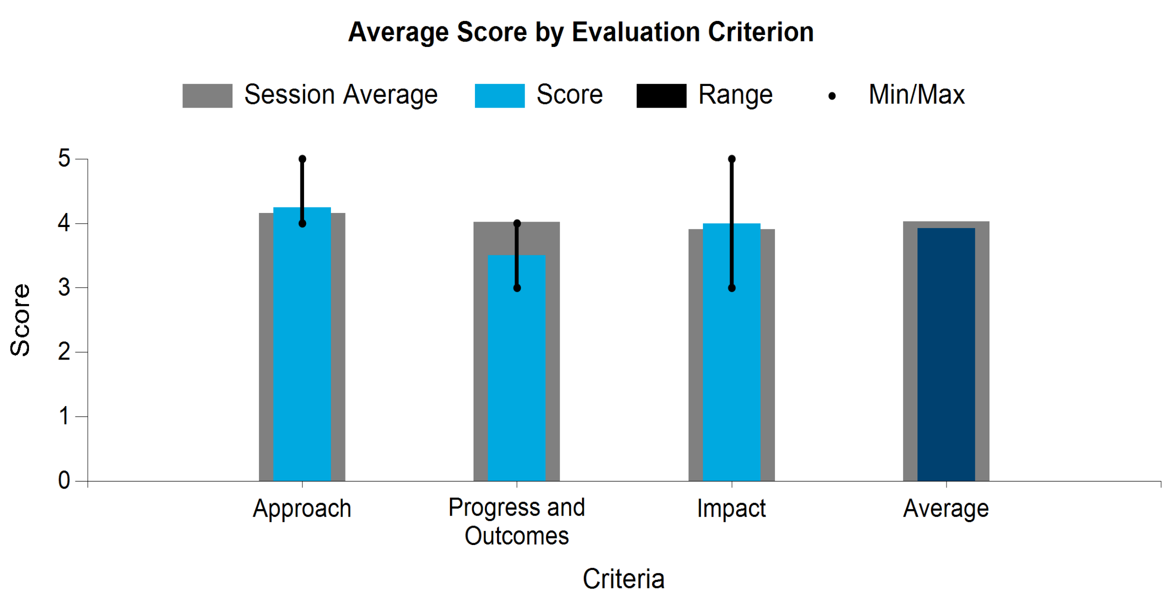
ENHANCED PRODUCTION OF ALGAE LIPIDS AND CARBOHYDRATES FOR FUEL AND POLYURETHANE PRECURSORS

University of California, San Diego

PROJECT DESCRIPTION

WBS:	1.3.1.672
Presenter(s):	Stephen Mayfield
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$4,000,000

In this project, we are combining genetic engineering, traditional breeding, and high-throughput screening to generate high-quality biomass for the production of fuels and high-value PU coproducts. We first identified extremophile strains of one green algae and one cyanobacteria and characterized these strains for the accumulation of naturally occurring polyurethane precursors (PUPs). We have translated an entire suite of previously developed genetic tools to these commercial strains and used *in vitro* evolution to evolve strains for improved biomass productivity in high-salt and high-pH media, as well as increased PUP production. We are now using synthetic biology to engineer metabolic pathways to optimize the production of fuels and PUPs in these strains. We have already started developing the chemical methods to convert these PUPs into fuels and PU monomers, including novel PUs containing aromatic polyols. In collaboration with our key industrial partner, Algenesis, we have used these novel polyols to make commercially relevant PU products and determined their physical specifications, including an ability to biodegrade. Finally, with the Kendall lab at the University of California, Davis, we have started TEA and LCA to model the impacts of producing high-value PU coproducts on the economics of fuel production in algae.



COMMENTS

- The goal of this project is to increase productivity by 20% over their baseline productivity using strain and/or cultivation improvement approaches under environmentally simulated and outdoor conditions. The proposed production of high-value PUP as a coproduct will drive biomass production cost down. This is in line with BETO's goals of increasing productivity, reducing biomass production cost, and developing strain improvement toolkits. The use of highly productive extremophiles will enable cultivation under high pH and high salt concentration.

- The team seems to be a good mix of research and industry partners. The team had a well-defined task structure that will ensure success of the proposed work; however, they did not address any risk or mitigation strategies. The team management did not demonstrate a well-established channel of communication and collaboration among team members.

- Progress has been made in the team's multipronged approach to strain improvement and culturing in high salinity to reduce contamination. They have demonstrated their ability to cultivate and genetically modify extremophilic cyanobacteria and green algae, which is incredibly valuable across the industry. It's unclear whether there are impacts of genetic modification on biomass productivity and what the project performers are doing to address this. The project performers should also consider outdoor performance of PCC 11901 in the spring and fall, when temperature and light are not optimal for growth and productivity.

- The project has explored in depth the usefulness of extremophile algae with strong reasoning and has been successful in identifying a halotolerant species that was genetically transformed, bred, and produced a robust strain with improved characteristics. The project has delivered PUPs from this extremophile algae via chemical means that have been used to produce algae-based novel PU foam products. This is highly commendable. The PI mentioned very abruptly that the rest of the biomass left after PUP extraction will contribute to biofuel production, and not much information was given in this regard, indicating a probable shift of focus for the project. There are two project partners, and how often the team meets to plan and discuss progress was not mentioned. How the concept of DEI will be addressed in the project was also not mentioned.

- This project aims to demonstrate the use of an engineered extremophile alga (*Chlamydomonas*) for fuel and coproducts. The major focus presented was for PUPs, which can be converted to fuels and/or bioplastics. This project has an industry partnership with Algenesis, which specializes in biodegradable plastics. Although this is an exciting and promising space for algae, this does not appear to be geared toward fuel production, and no algae grow-out demonstrations are involved in the project. The presenter does make a compelling case for growing extremophile algae for coproducts in terms of the media facilitating reduced pests and increased DAC potential. This begs the question of why extremophiles are not more prevalent in the industry, another reason why a grow-out component would be highly beneficial for this project. The team's genetic engineering work is also very exciting. However, this project does not appear to include an effort to advance scale-up/cultivation technologies, and it is unclear how it advances the BETO goals for this funding cycle. Otherwise, the technologies described here are poised to add considerable value to commercializing algae.

- The approach of focusing on high-pH extremophiles and high salt tolerance seems appropriate. Furthermore, the production of high-value coproducts such as PUP is also worthwhile; however, the current project plan seems to lack a credible effort to produce some type of fuel. The project team is making good progress according to their project workplan and seems to be on track to complete project objectives. The genetic tool development in this project is strong and should be useful for engineering other extremophiles. The impact of the high-value PU coproduct would be significant; however, it is not clear if the remaining biomass could convert into useful fuels to meet BETO targets.

PI RESPONSE TO REVIEWER COMMENTS

- Response to reviewer comments (response after reviewer comment): The project performers should also consider outdoor performance of PCC 11901 in the spring and fall, when temperature and light are not optimal for growth and productivity. We are downselecting to the extremophile algae strain for continued optimization, and for that strain, we will examine growth rates in the fall and spring.

- The PI mentioned very abruptly that the rest of the biomass left after PUP extraction will contribute to biofuel production, and not much information was given in this regard, indicating a probable shift of focus for the project. After PUP extraction (starch and 3HP), we will do a complete lipid extraction and use that material to make SAF.
- There are two project partners, and how often the team meets to plan and discuss progress was not mentioned. We meet every week with Algenesis, and once a month with BASF.
- Although this is an exciting and promising space for algae, this does not appear to be geared toward fuel production, and no algae grow-out demonstrations are involved in the project. We will have algae grow-out this spring and summer at our Biological Field Station; we will use three 300-liter indoor ponds to produce sufficient algae biomass to extract at least 1 kg of PUP. We also have sixteen 800-liter small ponds and two 15,000-liter larger ponds, but these are outdoors, so are not allowed for transgenic algae grow-outs.
- This begs the question of why extremophiles are not more prevalent in the industry, another reason why a grow-out component would be highly beneficial for this project. As stated previously, we will have a grow-out to obtain the data required for the LCA and TEA. As far as extremophile algae under industrial use, extremophiles are grown at Cyanotech in Hawaii and EarthRise in Imperial Valley under continuous growth. All other large-scale algae production is short batch mode, like at Qualitas in New Mexico. So extremophiles are used by industry, they are just not used by university and national lab researchers—which are not part of the algae industry!
- However, this project does not appear to include an effort to advance scale-up/cultivation technologies, and it is unclear how it advances the BETO goals for this funding cycle. We did not propose to develop new cultivation technologies in this project; we leave that to projects with the appropriate chemical engineering approaches that we do not have. We will, however, most certainly test our genetically engineered strain in a grow-out to provide the proof of concept that our engineered strain is biologically superior to the baseline native strains we started with.
- It is not clear if the remaining biomass could be converted into useful fuels to meet BETO targets. In Phase II, we will extract the residual lipids and demonstrate that they are suitable for conversion into SAF, per the BETO requirement.

ADVANCING ALGAL PRODUCTIVITY THROUGH INNOVATION IN CULTIVATION OPERATION AND STRAIN TRAITS (ADAPT-COST)

Colorado State University

PROJECT DESCRIPTION

WBS:	1.3.1.673
Presenter(s):	Ken Reardon
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$4,001,133

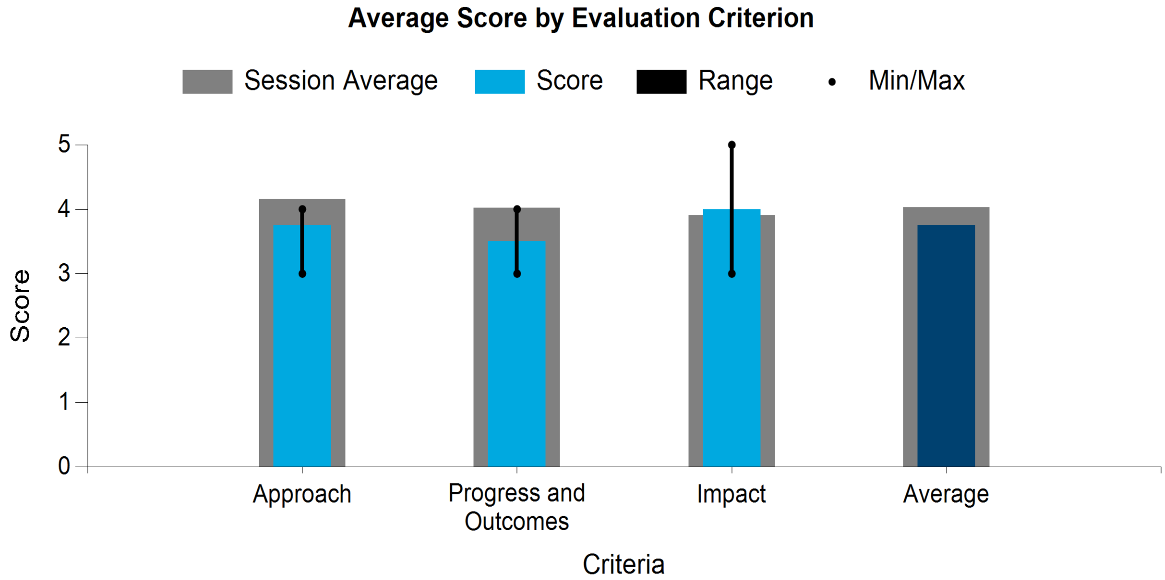
Current algal productivity levels remain insufficient to achieve BETO's goal of $2.50/GGE for algal biofuels. In this project, a set of strain improvement strategies will be linked with novel approaches to improve cultivation operations based on traditional CO_2 supply (Subtopic 2a). The overall result will be a 20% increase in areal productivity, with biomass quality improved to achieve a fuel yield of more than 85 GGE per ton of biomass.

The project uses the microalga *Nannochloropsis oceanica* CCAP84910, closely related to the strain used by Qualitas Health in their Imperial, Texas, facility. *N. oceanica* was chosen because Qualitas has a substantial track record with this organism at industrial scale and because Colorado State University, LANL, and Qualitas have experience with *N. oceanica*, including genetic modification, genome assembly/annotation, and cultivation in an industrially relevant saline medium. *N. oceanica* is stable under real environmental conditions, and Qualitas has developed solutions to minimize pest pressures. This project focuses on cultivation in spring, with outdoor tests at Qualitas and AzCATI.

The strain improvements to be performed are chosen to improve the ability of cells to use both photons and carbon. Photosynthetic carbon assimilation and biomass productivity are limited by ribulose-bisphosphate carboxylase-oxygenase (RuBisCO) inefficiencies. Algae have developed RuBisCO isoforms with modestly enhanced CO_2 affinity or a variety of carbon-concentrating mechanisms. We will engineer an advanced carbon-concentrating mechanism into *N. oceanica* to increase CO_2 assimilation efficiency, resulting in improved biomass yields and productivity.

The cultivation improvements are designed to overcome the limitations of traditional sequencing batch operation, manual offline measurements of biomass and nutrients, and poor prediction of large-scale cultivation performance from pilot cultivations. In this project, we will develop a strategy for continuous/near-continuous cultivation. This advanced cultivation mode will be supported by novel sensors of biomass and nutrients. A computational fluid dynamics model will translate results from mini- to full-scale ponds and guide the advanced cultivation operation, as well as the location of sensors. The cost of supplied CO_2 will be reduced by delivering it to ponds without sparging, either using the CA membrane technology currently being developed in a BETO project or a simpler abiotic membrane.

The combination of strain and cultivation improvement technologies will lead to a 20% increase, indoors and outdoors, in areal biomass productivity and biomass quality, yielding more than 85 GGE/ton of biomass. These technologies can be translated to other algae and other seasons, supporting the BETO productivity goals throughout the year and across the industry.



COMMENTS

- This project focuses on improving the productivity and biomass quality of *N. oceanica* in the spring through genetic modifications to enhance photon and carbon use efficiencies, developing sensors and strategies for effective cultivation operation, and integrating both strategies for deployment. This is of clear relevance to the BETO Multi-Year Program Plan goals. The project's goals are innovative and ambitious, but reasonable.

- The project performers seem to have a clear approach while leveraging expertise from the different investigators. Task structure was proposed with quantifiable go/no-go decision points. However, the team needs to provide more clarity on channels of communication and collaboration. Some risks involved in the execution of this project were identified and mitigation strategies outlined. Other risks, like fouling sensors and saturation of biomass probes, were not addressed.

- Overall, not a lot of progress has been made toward the goals outlined due to the late start of the project, but successful deployment of an improved strain and implementation of continuous cultivation with biomass and nutrient sensors will improve understanding and increase biomass productivity. It's unclear what impact hydraulic load will have on cultivation due to semicontinuous operations, and the project team should consider media recycle for the proposed strategy.

- The project focuses on implementing molecular biology techniques for genetic modification of *N. oceanica* to form pyrenoids that will potentially increase the efficiency of CO_2 fixation by the RuBisCO enzyme. In this realm, the project also emphasizes the deployment of sensors to monitor effective cultivation operations addressing nutrients and environmental factors for pilot-scale outdoor raceway pond systems. Despite having subcontracting issues, the project has made significant progress in specific areas defined in the project. A low-cost nutrient sensor, cQUBE, for ammonia and iron has been developed and will be in operation shortly. The particular need or reason for determining only iron and ammonia (and not other dissolved ions) is not articulated in the project. It would be helpful to know if it is a marker for any event prediction in the pond. The team has multipronged approaches for robust strain development and good mitigation strategies laid out for different challenges. The question comes up for the strain engineering effort—did the team explore the idea underlying the role of carbonic anhydrase CAH1 and RuBisCO's activity relationship in carbon fixation for these mutated strains? Similar work is reported on the *N. oceanica* CCMP1779 strain from Lawrence Berkeley National Laboratory in the literature. It would be good to know if some work was conducted on *Nannochloropsis oceanica* CCAP84910. How the project partners coordinate the workflow and how the DEI component will be incorporated into the project has not been discussed.

- This project aims to improve the productivity of *Nannochloropsis* by genetically engineering pyrenoid formation, improve carbon fixation, and improve biomass sensor technology during cultivation. Multiple entities are involved in this project, and communication between them was not made clear. The technology approach is very comprehensive, focusing on one strain, and could deliver valuable toolkits for future biofuel production. All permits are already in place for grow-out demonstration at AzCATI and at Qualitas in Texas. Although stated as stretch goals, having two different locations for outdoor validation and having an industry partner (Qualitas) is an advantage for this project, making it stand out in the BETO funding portfolio. Outdoor growth would be done in continuous culture, using contamination mitigation practices already in place; however, contamination during continuous cultivation poses a significant risk. The presenter did not think switching to batch culture, if continuous fails, would hinder them achieving their goals. The project did have a delayed start but appears to be on track to complete in time.

- The strain improvement approach of modifying *N. oceanica* to form pyrenoids is high risk, high reward, but if successful might have a significant impact by increasing carbon fixation at ambient CO_2 levels. The risk mitigation strategy identified if the pyrenoid strain improvement strategy is unsuccessful is vague and needs to be more clearly articulated. The project was delayed due to subcontracting issues and started in January 2023. Appropriate go/no-go milestones have been identified. The impact of the work is difficult to assess based on the delayed start of the project.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments, and we appreciate that they have recognized the innovation of our project. In the paragraphs below, we provide responses to these reviewer comments. Team collaboration and communication: The project is designed to be very collaborative, with data, materials, technology, and samples being shared across tasks and team members. Examples include the testing at AzCATI of strains developed at Colorado State University and LANL, the application of sensors developed at Colorado State University and QBI at AzCATI and Qualitas Health, and the use of data from all experimental work in the TEA and LCA modeling. The main channels of communication are team meetings (currently monthly but transitioning soon to biweekly) and a shared data site (Box). This has proven successful in other similar projects. Sensor development risks: We are aware of the potential for fouling and for optical signals beyond the linear range, and have mitigation plans to address these should they be observed in our testing. Chemical sensor selection: A reviewer asks why sensors are being developed only for iron and urea. The answer is that QBI has already developed sensors for nitrate, nitrite, ammonium, and phosphate. The two new sensors will complete the platform for the major nutrients in microalgal cultivation. Strain engineering and CA: A reviewer asks whether we have explored the “underlying role of carbonic anhydrase CAH1 and RuBisCO’s activity relationship in carbon fixation.” We are aware of the publication mentioned by the reviewer and appreciate the suggestion to include the role of CAH1 in our research. Our hypothesis remains that including a functional pyrenoid in *N. oceanica* will have benefits for cell growth and carbon efficiency. As noted in the cited publication, the CAH1 system appears to result in leakage of CO_2 to the surroundings. With a functional pyrenoid, that leakage could be reduced or eliminated. DEI: We appreciate the suggestions for enhancing the diversity and inclusion aspects of our project. While the FOA under which our project was funded did not have a DEI requirement, our team is committed to the principles of DEI. We make efforts to recruit a diverse set of students, especially undergraduates, to participate in this project, and plan to conduct outreach events at Colorado State University’s Spur campus in Denver, with the goal of reaching students from communities underrepresented in STEM fields. Contamination during continuous cultivations: A reviewer notes a concern that contamination during continuous culture could pose a risk. While we are not aware of data for continuous cultivation, there is a report on the effects of semicontinuous harvesting in which more frequent harvesting resulted in *lower* contamination rates. This was only one study, of course, and we will soon learn from our research whether the same trend is observed.

METABOLIC CARBON FLUXOMICS DURING COMPOSITIONAL SHIFTS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

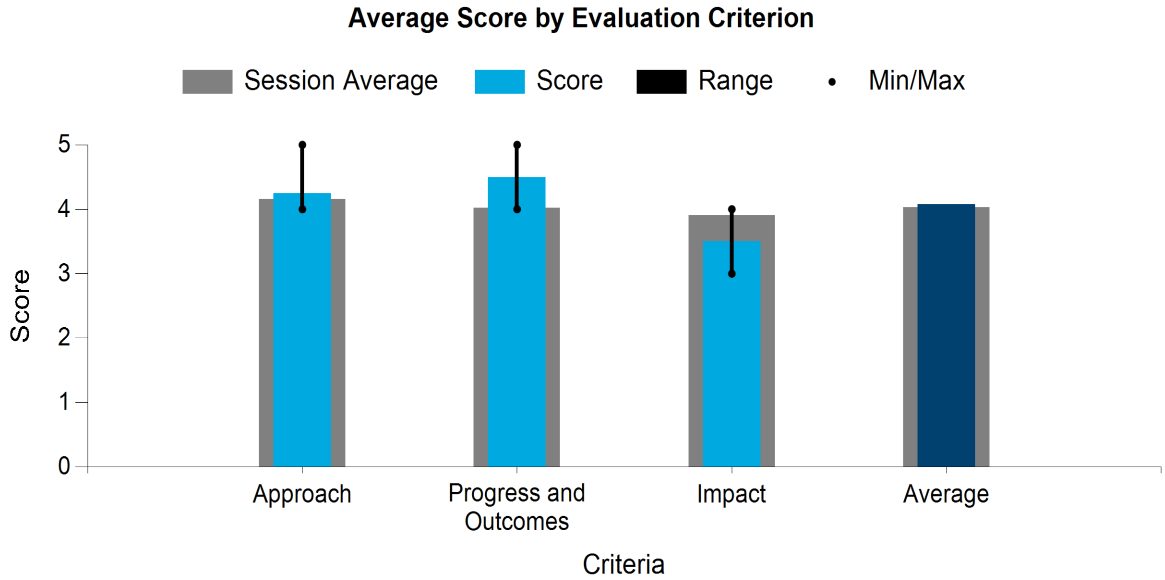
WBS:	1.3.2.005
Presenter(s):	Lieve Laurens
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$750,000

This project aims to pursue the identification of biomass compositional shift metabolic markers for multiple DISCOVR-relevant species of algae through the utilization of quantitative targeted and untargeted metabolomics, coupled with machine learning. This will allow for mapping and manipulating the shifts when algae cells are exposed to a wide array of environmental stressors. The goal is to identify parameters that are under the control of the future algae farmer to tune algal biomass composition toward selective applications, at minimal cost to the production and/or fuel cost.

Sharing this project's findings with industry and collaborative test bed operations to identify scenarios to implement to achieve compositional improvements, this project alone will not directly become commercialization-ready with an open-source dissemination strategy of the approach, algorithms, and methods associated with this work toward collaborators and partner projects.

This in-depth metabolomics approach to understand the respective metabolic signatures and dynamics has largely been missing from the quest to understand the primary drivers behind shifting biomass composition toward more conversion-friendly carbon sources (lipids and carbohydrates). To specifically understand the primary carbon storage rates in different biochemical sinks, it is necessary to present a more holistic metabolomics profile for all metabolites along the carbon assimilation pathways, including the Calvin–Benson–Basham cycle, known to be at the basis of the careful orchestration of the fate of carbon in photosynthetic cells.

We have collected a physiologically diverse set of metabolomics data sets for multiple strains by varying the light, temperature, nutrients, and diel light conditions, each leading to a distinct compositional profile of the biomass. The application of an unsupervised learning approach to reduce the dimensionality of the data has already indicated a set of metabolites that are correlated with compositional shifts for *Scenedesmus* biomass and will be extended to achieve a more quantitative prediction by this project's interim decision point in FY 2023.



COMMENTS

- The project focuses on identifying metabolic predictors of compositional shifts in algal outdoor production. Their approach is to identify nutrient conditions that enable a shift in composition without impacting biomass productivity and then propose metabolic engineering targets/pathways that are implicated in the composition shift. This is an innovative approach, and if successful, can provide information that will improve the productivity of algal strains by metabolic engineering.

- The team had a clear management plan with a well-defined task structure and leads. They identified risks and implemented mitigation strategies, as well as established channels of communication and collaboration among team members. The team also outlined an approach to addressing DEI in their project plan.

- The project performers have made significant progress in developing a high-throughput physiological testing environment, as well as optimizing a workflow for high-performance liquid chromatography–mass spectrometry. They have developed a data set for two strains under 28 different growth and media conditions. This could be a useful tool for metabolic engineering of high-producing strains if heatmaps for metabolite upregulation at different time points can be correlated to the different growth conditions, biomass productivity, and composition shifts. The project performers should also consider the risk of doing all the work indoors, where contaminants and outdoor conditions can change the metabolic profile. The end goal of the project is the selection of implementable physiological strategies to shift biomass compositional quality and value with minimal impact on biomass productivity. It's unclear from the presentation how the project performers intend to achieve the end goal.

- The project aims to increase the opportunity for algal biomass productivity to meet BETO's SAF targets. The main objectives for the project are to identify metabolic predictors for composition shift of outdoor algae pond cultures based on nutrient conditions (phosphate and ammonium) without affecting the biomass production and advancing the knowledge for metabolic engineering targeting this shift. The team envisions that this metabolomics predictor toolkit coupled to machine learning will enable them to contribute to BETO's goal of producing high-SAF feedstock for biofuel production. This is a very ambitious goal, and the project has made significant progress by building synergy between different national labs to conduct several simulated experiments while addressing several risk factors and subsequent mitigation strategies. The project has demonstrated some unique relationships between metabolites/pathways and compositional profiles and claims to have implemented a workflow for strain-agnostic metabolomics fingerprinting. The team has a well-defined workflow structure, and the DEI component has been incorporated in the project. There is no mention of patents/publications, except about presenting at one of the upcoming international conferences.

- This project aims to develop a toolkit to predict the composition dynamics of algae biomass in order to steer a crop toward specific coproducts, thereby increasing the value of algae biomass in general. This project has a clear management structure and benefits from being tied into other efforts at the national labs. The team appears to have made a strong effort toward the BETO DEI targets, even though this particular project was not required to do so. The team has valuable expertise and access to sophisticated equipment and has generated some very nice data using PBRs. There is no targeted outdoor component to this project specifically; however, the learnings will have to be validated in outdoor reactors before any strategies become readily implementable by industry, etc. Contamination pressure and an unpredictable outdoor environment could make key learnings in PBRs irrelevant. The presentation given by the DISCOVR consortium described how the compositional analysis will be used by them, and it seems there is some validation planned in outdoor ponds that will be beneficial. This project approach and impact would have been stronger if the validation was directly built into their goal structure.
- This project is focused on unraveling the metabolic predictors to control the fate of carbon allocation, has sustainable merit, and is an important part of aiding BETO in achieving more carbon-efficient SAF production. The management plan seems appropriate, and risk mitigation strategies are in place. Collaborations with DISCOVR and the Algae Biomass Organization are appropriate. The project is halfway through the funding period and seems to be making good progress. The project team has developed and implemented a workflow for strain-agnostic metabolomics fingerprinting, built a data set with 28 different physiological conditions, and identified some unique relationships between metabolites and compositional profiles. The impact of the work is clear and has identified correlations that indicate a strong relation to high carbohydrate and lipid content in biomass as value drivers.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' thoughtful and complimentary comments on the project presentation. A couple of the points raised focused on the connection between indoor and outdoor relevance of the approach and ultimately the application space tested. This work is a focused effort on controlled-environment probing of predictive factors for shifting biomass composition to become more amenable to bioconversion. Specifically, the implementable strategies that could achieve the goal of shifting the biomass quality can be nutrient formulation and cultivation operations (e.g., N:P ratios, pH, and adding signaling metabolites to alter carbon allocation in the cells), as well as metabolic engineering targets for synthetic biologists manipulating particular critical metabolic pathways. For all the work presented, we use an indoor bioreactor system that has been validated as climate-simulating outdoor cultivation (of the algae test bed at AzCATI), both in terms of growth and biomass composition (work that was briefly presented as part of the DISCOVR consortium presentation), which gives us confidence that some of the identified metabolic and physiological responses to abiotic perturbations are translatable to at least the outdoor environments. One important factor that is not included in these simulations is the biotic impact of microbial ecology on biomass composition. This is a nascent research area that makes developing and simulating relevant conditions much more complex, and is outside the scope of this work. Outdoor biotic contaminants are likely to be variable parameters, and replicating these indoors can convolute metabolomics results and make it impossible to dial in on predictors of composition shift. With the successful validation of the predictive metabolic signatures, a future trajectory of this work may include the translation to outdoor test bed confirmation, which would include biotic and abiotic influences. The interaction between metabolic predictors under pressure from contaminants is unclear and will need to be tested outdoors. However, if successful, the implementable strategies will still improve the valuable biomass component (carbohydrate/lipid) productivity of the strain. In this initial project, we want to first identify (and deconvolute) the metabolomics response of composition shift for the strain in axenic cultures to guide metabolic engineering. We are currently focused on quantifying the carbon flux parameters under selected physiological conditions for a select set of species, and we are preparing a manuscript that describes the unique contribution of the unbiased carbon allocation study that we have completed. The overarching deliverable of this work is to not only understand but also make carbon allocation metabolomics more broadly accessible and comparable, and we will make methodologies and reports openly available.

BROAD SPECTRUM ANTIFUNGAL POND PROTECTION

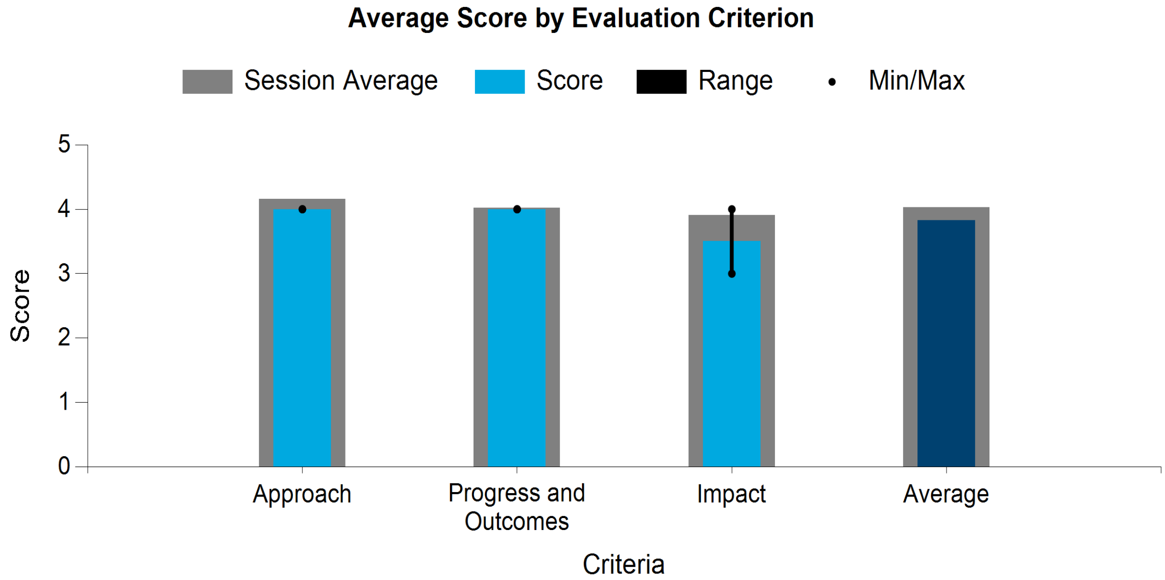
Sandia National Laboratories

WBS:	1.3.2.044
Presenter(s):	Todd Lane
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,000,000

Project Description

The economic production of algal biomass for biofuels and coproducts is dependent on the development of crop protection strategies and technologies that are both cost effective and broad spectrum—offering projection from the greatest diversity of deleterious species. In previous work at Sandia National Laboratories, we isolated multiple independent microbial consortia that are capable of protecting *Michrochloropsis salina* from grazing by the rotifer *Brachionus plicatilis.* These consortia were shown to be persistent, with protective effects enduring for more than 30 days in outdoor cultivation trials. They also have no deleterious effect on algal production and, in fact, appear to enhance the growth rate of the algae. They can be readily maintained in co-culture with algae, not requiring a separate cultivation and inoculation system. Thus, crop protection systems based on biological control by selected bacterial consortia add essentially no additional cost to algal production.

In the current project, we are extending such consortia-based systems to the protection of a diversity of algal strains against a variety of fungal parasites. We have screened and selected multiple independently derived microbial consortia that protect algal strains from a diversity of fungal species. These consortia have been shown to increase the time to failure in standard fungal infection assays by 70%–100%. Each independent consortia is being cross-evaluated with a range of algae and fungal combinations to identify the isolates or consortia that display the greatest breadth of protection. The microbial community structures of these consortia are being determined via second-generation sequencing. We are identifying the organisms that are most strongly correlated with the protective activity and specificity of each consortia. In future work, we will combine consortia to create novel consortia with expanded protective capabilities. These second-generation consortia will be tested for persistence and range of protection (both algae and fungal pathogen) and stability in outdoor culture systems. This project is designed to develop cost-effective crop protection strategies and technologies that are broadly applicable to a variety of production algae and deleterious species. By reducing the frequency of pond crashes due to biocontamination, this technology will increase annualized yields and thus reduce the overall cost of algal biomass production.



COMMENTS

- The project proposes to develop a microbial consortium that will reduce pond crashes from fungal infection. Their approach is to co-cultivate these protective strains or consortia with algae, allowing for a cost-effective method of prophylaxis. If successful, the project will advance BETO goals of minimizing pond crashes that will increase annualized yields and thus reduce the overall cost of algal biomass production.

- The team had a clear management plan. They identified risks and outlined mitigation strategies, as well as established channels of communication and collaboration among team members. The team also outlined an approach to addressing DEI in their project plan.

- Overall, the team has made significant progress toward their goal. Successful demonstration of this pond protection approach on an outdoor trial will enable commercial deployment. The team developed standard crash assays for all their agents. The project performers should consider nutrient availability, stability of consortia during the run, competition when increasing consortia concentrations to extend the life of the production pond, and overall impact on biomass productivity. The impact of revived biomass from rotifer on biomass quality and downstream purification should also be considered. It is also unclear how this strategy will be commercially deployed considering the robustness of consortia pond control for different algal strains and environmental conditions.

- The goal of the project focuses on selection of microbial consortia that can be co-cultivated with algae, thus preventing fungal infection leading to pond crash. This will provide a zero-cost method for prophylactic treatment by avoiding the use of biocides. This project at Sandia National Laboratories has been able to establish a panel of six fungal pathogens for algae and six different sources of bacteria with prophylactic effect that assisted in 36 indoor laboratory-scale experiments. Sandia National Laboratories has been successful in demonstrating through several experiments that multiple protective strains or consortia can prevent fungal pathogenesis and hence effectively prevent pond crashes. The risks and mitigations have been addressed, which seems to be adequate considering the broadness of this area, especially when considering open-pond crashes. Algae test bed demonstration is in progress to check the stability of both pond and protective consortia over a greater period of time. Although the progress has been decent, there is no mention of the biomass productivity, which is an important aspect for BETO's mission. The major question is: How will this bacterial protection affect biofuel and bioproduct quality of the algal mass downstream? This project has embraced the DEI component, and the PI is enthusiastic about communication and collaboration with other labs and stakeholders to increase the breadth of the project.

- The specific management/communication structure was not made clear in the presentation. The approach to fungal pest management is novel and poses a low-cost (to no-cost) strategy using biological control from a beneficial consortium. The approach was validated with rotifers and had good results. Consortia data for fungal pests look promising so far, and it will be interesting to see these validated in outside cultures. For the 9/30/22 milestone data shown (Slide 14), sampling intervals were not consistent, and details may have been obscured. Any future testing, especially outdoors, should include daily sampling so as not to miss important inflection points of these complicated interactions. For the same milestone, Slide 15 shows the consortia only being effective after a reinfection event and not for the first 20 days of cultivation. This lag may not be feasible at scale unless it is built into the preproduction phase. The presenter reported that the consortia can be freeze-dried for storage/transport, which will be important for adoption by industry. No industry partner was identified, and although this was not a requirement of the BETO funds, it is unknown how open industry would be to using a pest control method like this versus chemical, unless the consortia are proven to be stable and/or maintain efficacy after the preproduction phase.

- The approach focuses on developing a low- to zero-cost prophylactic treatment to prevent pond crashes due to fungal infections. Risks and appropriate mitigation strategies have been addressed. The project appears to be on schedule, and project milestones are being successfully achieved. Current industrial efforts seem to be focusing on microalgae strains that tolerate high pH (>10). Most fungi seem to grow well only in the pH range of 4.0–8.0; thus, it's not clear how impactful this work will be if current industrial efforts continue to focus on extremophilic microalgae. The project team noted that temperature seems to be a driver of fungal infections; thus, it would be interesting to know what effect pH has on the rates of fungal infections in growing microalgae cultures.

PI RESPONSE TO REVIEWER COMMENTS

- Comment: "The project performers should consider nutrient availability, stability of consortia during the run, competition when increasing consortia concentrations to extend the life of the production pond, and overall impact on biomass productivity. It is also unclear how this strategy will be commercially deployed considering the robustness of consortia pond control for different algal strains and environmental conditions." Comment: "It is unknown how open industry would be to using a pest control method like this versus chemical, unless the consortia are proven to be stable and/or maintain efficacy after the preproduction phase." Response: Determining the stability of the consortia under production conditions is the focus of the second half of this project. We have already demonstrated that the consortia are stable for at least 30 days and retain full activity under laboratory culture conditions. As part of the current work, we are already evaluating the robustness of each consortium in the presence of multiple algal species. It is currently in the work plan for the remaining half of the project to test the consortia at pilot scale at both simulated outdoor conditions and in outdoor production systems with an appropriate partner. This testing will allow us to evaluate the robustness of the consortia under differing environmental conditions and with different strains. Our current evidence indicates that it is not necessary to increase the consortia concentration to increase stability and activity, as the consortia are stable and active at the concentrations that occur "naturally" in co-culture with each algal species.

- Comment: "Although the progress has been decent, there is no mention of the biomass productivity, which is an important aspect for BETO's mission. The major question is: How will this bacterial protection affect biofuel and bioproduct quality of the algal mass downstream?" Response: It is important to keep in mind that all open production systems already contain bacterial/algal co-cultures and that many of the consortia that we are testing are derived from outdoor algal cultivation systems. All consortia were initially screened for their impact on algal growth rate and biomass yield. Consortia that demonstrated a negative impact on either parameter were removed from consideration. We will be further investigating the impact of the consortia on biomass quality as part of the work plan for the second half of the project.

- Comment: “The team had a clear management plan.” Comment: “The specific management/communication structure was not made clear in the presentation.” Response: This is currently a relatively simple project from a management perspective, as it currently is a single-PI project at a single national lab, and all workers on the project report directly to the PI. In the event that we decide to collaborate with an outside institution for field trials, this effort will be mediated through a procurement agreement with that institution and Sandia National Labs, and will include a defined statement of work and reporting requirements.
- Comment: “For the same milestone, Slide 15 shows the consortia only being effective after a reinfection event and not for the first 20 days of cultivation. This lag may not be feasible at scale unless it is built into the preproduction phase.” Response: This lag in protection was due to the nature of the assay, where we infected at a very high multiplicity of infection. Infection with an initial high concentration of agents would not be the case in a natural infection. We have evidence that under a lower multiplicity of infection, such that is present in the early phases of a natural infection, the consortia will be able to interdict the infection and prevent biomass loss before the agent overruns the culture. In addition, we believe that the experiments, carried out at high multiplicity of infection, have resulted in a more protective consortium that that will be protective throughout cultivation and not just after the first round. Such evolution of the protective consortia is an intentional and integral component of our consortia development process, and we are currently evaluating the resulting consortia from these high-multiplicity-of-infection trials.
- Comment: “Current industrial efforts seem to be focusing on microalgae strains that tolerate high pH (>10). Most fungi seem to grow well only in the pH range of 4.0–8.0; thus, it’s not clear how impactful this work will be if current industrial efforts continue to focus on extremophilic microalgae.” Response: The overall strategy of development of microbial consortia for protection against deleterious species has been demonstrated to be effective against both grazer species and parasitoid fungi. There is every reason to believe that the strategy would be effective against other biocontaminants.

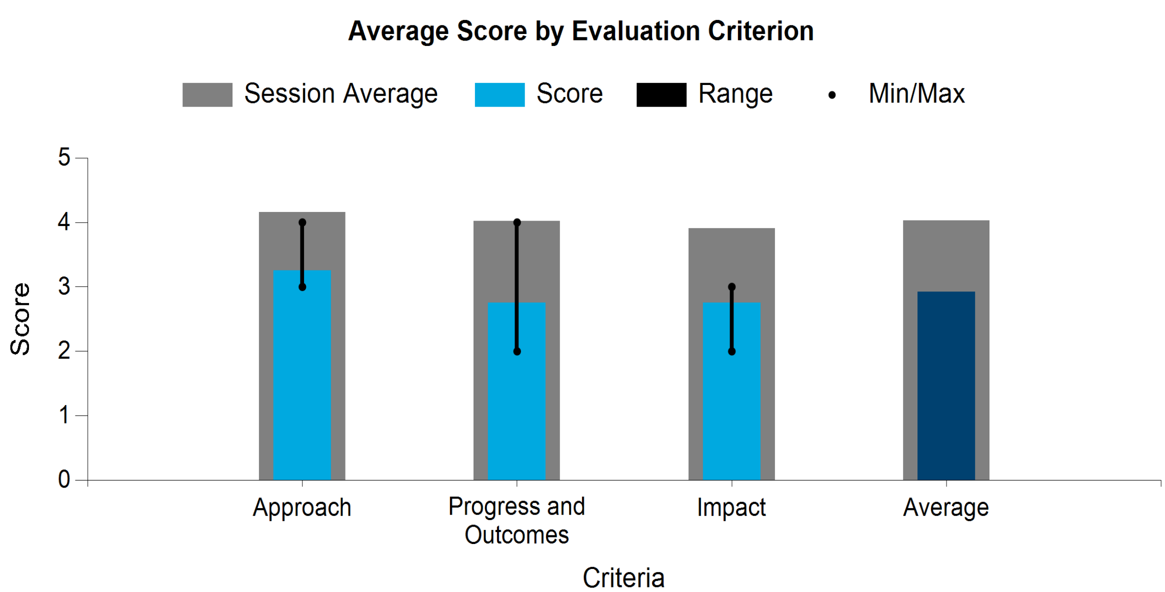
CARBON UTILIZATION EFFICIENCY IN MARINE ALGAE BIOFUEL PRODUCTION SYSTEMS THROUGH LOSS MINIMIZATION AND CARBONATE CHEMISTRY MODIFICATION

Duke University

PROJECT DESCRIPTION

WBS:	1.3.2.440
Presenter(s):	Zackary Johnson
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2023
Total Funding:	$1,928,295

High productivity and yields of microalgae grown in open-air raceway ponds for biofuel production require active inorganic carbon delivery to the water medium. In most research (and commercial) operations, this carbon is supplied in excess from external, often limiting, CO_2 sources. However, TEA/LCAs show that this approach can dramatically limit the broader application of algae-based biofuels. To address this gap, our team is using top biofuel algae strain candidates to (1) identify the minimum concentration of dissolved inorganic carbon (DIC) that can support baseline and target productivities and yields to improve CO_2 use efficiency, (2) test the enhancement of productivity and yields of candidate algae by supplying "CO_2" in the form of bicarbonate, (3) test a patented CO_2-based conversion technology as an improved carbon source on open raceway ponds at an established algae facility, and (4) test this technology on scalable sources (waste streams) of CO_2 using open raceway ponds. To date, we have made substantial progress on all of these goals, including transitioning to larger-scale trials and integration with industry.



COMMENTS

- The goal of this project is to demonstrate enhanced algal growth with overall reduced CO_2 requirement at an industrially relevant scale. If successful, the proposed work will have benefits to the algal industry and is well aligned with BETO's mission and Multi-Year Program Plan goals of reducing the cost of production.

- The management plan was not outlined, although team expertise and previous experiences are leveraged in this project. Risk and mitigation strategies were identified. The task structure was proposed, but quantifiable go/no-go decision points were not clearly outlined.

- Progress has been made toward the goals outlined. The project performers did not highlight outcomes of the strain assessment. It would have been helpful to see how strains with reduced pCO_2 threshold for growth and strains with growth enhancement on converted DIC waters compare to their baseline or current SOT. The team has done tremendous work testing the proposed approach in outdoor race ponds and showed improvement with DIC, but they did not outline the baseline and show improvement over the baseline. Progress has been made with TEA/LCA to assess commercial deployment of the technology, but the discussion would benefit from more specifics on how the strain's use of calcium carbonate ($CaCO_3$) and integration with the brewery will drive the production cost down, given that the use of limestone is not sustainable. Additional work is likely needed to achieve the end-of-project milestone of enhanced algal growth on high-DIC water at an industrially relevant scale.

- The team mentions the use of DAC coupled with DIC to produce high-performance outdoor algae cultivation for biofuels on developing approaches to minimize CO_2 use and losses to enhance overall algae productivity. It will deliver TEA data generated from the R&D to demonstrate lower potential costs for algal biomass and increased potential revenue from the incorporation of DAC with production of valuable algae products. The main mission of BETO is to generate substantial algal biomass, and this project aims to modulate the carbon input into the algal pond to maximize the production of algae biomass and bioproducts by avoiding undue excess use of the carbon source. Numerous strains have been assessed, and a few have been identified that show a growth stimulation in converted DIC water. The team mentions demonstrating the reduced capital and operating expenses for algae-derived biofuels being more economically feasible, but more data collection may be necessary to establish a higher confidence level and robustness of the system. The outdoor 1-liter ponds with the calcium carbonate/bicarbonate chemistry have shown promising results. More outdoor trails need to be counted to provide a consistent data set. It may still need some optimization to avoid precipitation of carbonate with the algae biomass. The plan for coupling the system with the local brewery for inorganic carbon has produced better results and reduced the use of carbon dioxide. The team has successfully published their research findings in peer-reviewed journals, making them available to the public. The PI of the project has received the Algae Biomass Organization Mid-Career Award, which is highly commended.

- This project targets increased productivity of algae using reduced CO_2 use and loss via DIC addition and incorporates a TEA/LCA. They planned to target two strains known to have good growth in benchtop bioreactors. It is certainly important and aligned with BETO goals to identify strains and conditions that allow for reduced CO_2 use, and lab-scale results looked promising. The presenter acknowledged that using a mined resource like limestone to increase DIC is not sustainable at larger scales; thus, this project appears largely academic in nature and may not help BETO get closer to their goal targets. The industry partner for this project is a commercial brewery, but due to the COVID-19 pandemic, they were not able to work with them, and instead simulated brewery inputs from a homebrew kit. The presenter listed various next steps, including doing replicate testing of their initial small-scale outdoor testing, doing outdoor testing at a larger industrially relevant scale, and working with the brewery directly. These are all critical steps to their objectives, which appear will not be completed, as the project officially ended last month. This level of completion is concerning, considering the project has been funded by BETO since 2018.

- This project seeks to demonstrate enhanced algal growth with an overall reduced CO_2 requirement at an industrially relevant scale. Risk mitigation strategies are identified; however, their implementation and effects weren't clearly communicated. Although the CO_2 conversion technology seemed intriguing, it seems likely that the work will not advance the state of the art. The high-carbon water seems to improve growth and yield at the cost of producing a precipitate, which could complicate downstream processing of fuels and coproducts. The project team prototyped a "femtoscale brewery" in an effort to satisfy Task 4, which focused on integration with industry. The principal outcomes from this small-scale prototype seem to be the quantification of CO_2 release and mass balance closure. The results from this prototype system do not give confidence that the technology could be scaled to a commercial brewery. The overall impact of this work seems minimal based on scalability issues and the current lack of industrial engagement.

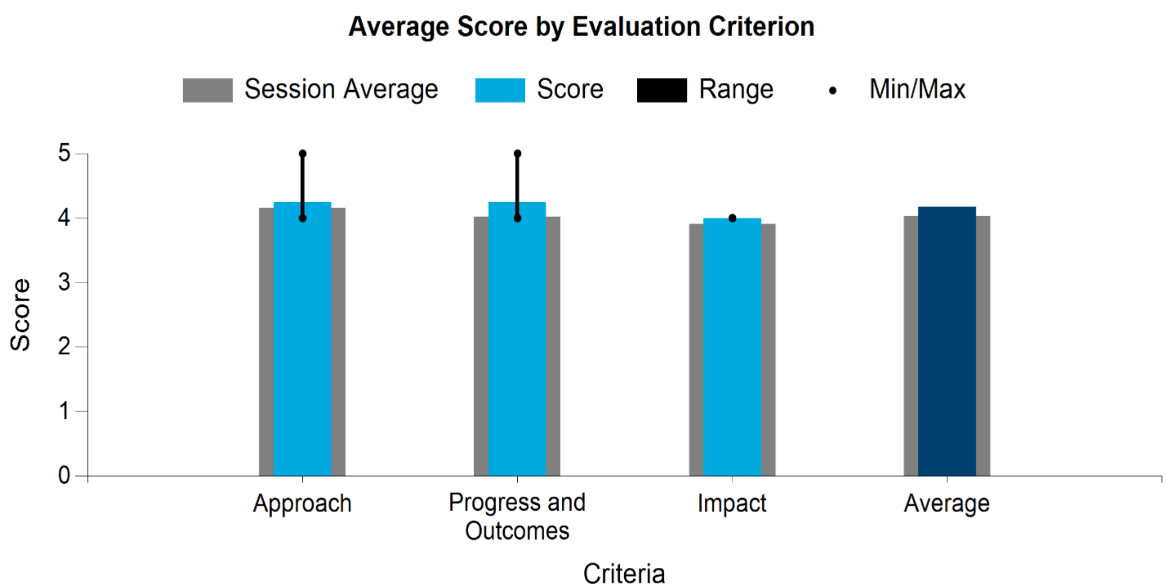
ECOLOGICAL MONITORING TECHNOLOGIES TO ENHANCE LARGE-SCALE MICROALGAE CULTIVATION, STABILITY, AND PRODUCTIVITY

Scripps Institution of Oceanography at the University of California, San Diego

PROJECT DESCRIPTION

WBS:	1.3.2.670
Presenter(s):	Lisa Zeigler
Project Start Date:	10/01/2021
Planned Project End Date:	08/31/2025
Total Funding:	$3,451,632

A critical component of any commercial-scale cultivation system is the challenge of ecological processes that can decimate or limit productivity of the target strain. Limitations may arise from interactions with contaminating negative biota (pests) or lack of algal adaptation to mixed communities—for example, axenic monocultures and closed-culture situations (engineered or natural strains) that result in reduced strain fitness among complex consortia. This project will bypass standard approaches of detecting and tracking single organisms using qPCR or Loop-mediated isothermal amplification (LAMP) assays to develop and employ affordable real-time monitoring using third-generation long-read sequencing. The Oxford Nanopore Technology is comparable to classical assay costs but has the advantage of providing real-time information about the physiological state of the algae and the associated microvirome, consisting of both microbes (bacteria, archaea, other algae, fungi, and protists) and viruses. Controlled laboratory-scale experiments will simulate diurnal raceway conditions and mimic current commercial-scale cultivation methods for pond transfer and scale-up, thus integrating across a lab-to-field model. In addition, prior and ongoing efforts on identifying positive ecological relationships now make it possible to engineer polymicrobial systems (designed ecosystems) aiming to promote optimal growth of algae pond ecosystems. Successful completion of tasks will result in the improvement of high-performance cultivation stability and reproducibility through advanced monitoring on an actionable time scale and biocontrol of field-scale campaigns.



COMMENTS

- This project focuses on developing and deploying real-time monitoring of algal cultures using third-generation long-read sequencing. The information generated will be used to build a database that will allow understanding of traits like stress and help drive mitigation strategy. This is in line with BETO's algae crop protection goals of developing crop protection methods and strategies to maintain robust productivity of algal cultivation systems and is part of Topic Area 2: APEX.
- The team seems to be a good mix of research and industry partners. The team had a well-defined task structure that will ensure the success of the proposed work and addressed any risk and mitigation strategies. The team management did not demonstrate a well-established channel of communication and collaboration among team members.
- The team has made significant progress in developing and implementing a method for real-time evaluation of a GAI pond-associated microbiome. A sample-to-sequence workflow with less than 12-hour turnaround time will accelerate understanding of microbiomes during periods of high performance and crash. It's unclear from this work how the project performers intend to use this information to correlate algal culture pond performance and stability. Also, more clarity is needed on how the use of this approach can inform the team running algal ponds about imminent problems with pond health so they can react accordingly given the technical expertise and hardware required for genome assembly and analysis of the resulting data.
- The project aims to develop a robust toolkit for outdoor algal cultivation that will facilitate and integrate lab-to-field easy transfer technology with the capacity to provide a curated algal microbiome database, perform systematic workflow analysis, detect ecological perturbation, evaluate stresses, and provide a collection of mitigation strategies. The team made good progress and transferred their lab-to-field trail in July 2022. There was no mention of how the initial ongoing stress and microbiome data are responding to the field protocol. Any projected information regarding the reduction of time and cost as an example would raise the level of confidence in the system. Some data or a mention of how successfully a simulated in-lab stress system was able to recover from the initial stress testing situation with application of any of the mitigating tools was absent. The team should plan to incorporate the DEI component into their project in the upcoming years.
- This project aims to deliver real-time pond composition monitoring, analysis workflows, and a decision tree for mitigation strategies for cultivation of elite algae strains. While still early in the project, the team has exceeded their real-time monitoring goals and reduced their sample-to-sequence workflow below target. The project appears well organized, but the management and communication structure was unclear. The technology will be validated at scale by an industry partner (GAI), which makes this project stand out among many in the portfolio. Standard operating procedure development for industry handoff is built into their goals, adding value to the project impact. The work is focused on the elite algae strain, *Nitzschia*, and it was unclear if/when the tools will be validated for application to additional strains.
- The approach of using real-time monitoring to analyze the ponds seems good. The project management plan is clear, and risk mitigation strategies are identified. The project is 1 year into the project timeline and seems to be on track. The technology will have a greater impact if the final version of the technology has an open framework such that anyone could use it.

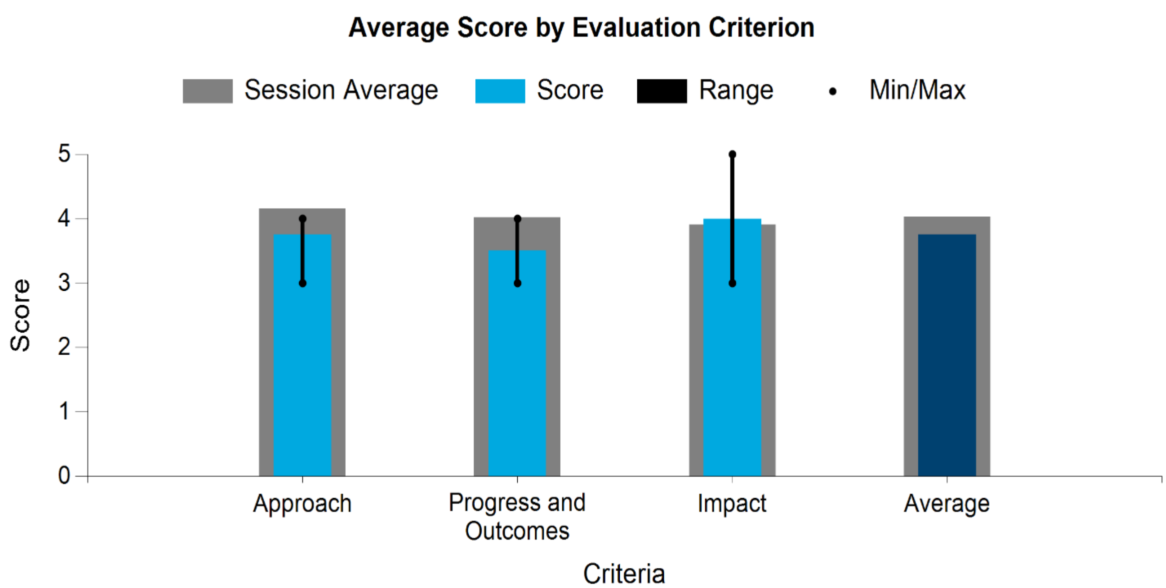
ENHANCED ALGAE PRODUCTIVITY IN CO_2 DIRECT AIR CAPTURE CULTIVATION

Global Algae Innovations

PROJECT DESCRIPTION

WBS:	1.3.2.671
Presenter(s):	David Hazlebeck
Project Start Date:	10/01/2021
Planned Project End Date:	03/31/2025
Total Funding:	$4,000,000

GAI was founded in 2013 to harness the unparalleled productivity of algae to provide food and fuel for the world, dramatically improving the environment, economy, and quality of life for all people. Our approach is to produce algae oil and algae protein meal coproducts that are economically competitive with current commodities. In this project, CO_2 is directly absorbed from the atmosphere into the open raceways so that no separate CO_2 concentrating or distribution system is needed. The main objective of the project is to increase productivity while maintaining a high lipid content. This objective will be achieved through application of a novel directed evolution approach to improve our elite biofuel strain of *Nitzschia inconspicua*, as well as a modification to the cultivation approach to leverage the characteristics of this strain to increase the overall productivity. The project has just started with facility improvements, and experimental work is anticipated to start in summer 2023.



COMMENTS

- This project focuses on developing improved strains and cultivation methods that increase productivity by at least 20% and lipid content by at least 35%, with all CO_2 supplied by DAC. This has clear relevance to BETO's mission and Multi-Year Program Plan goals. If successful, this will decrease the cost of CO_2 capture and delivery.

- The project performers did not map out a clear management plan or well-defined task structure. They identified technical challenges and risks and proposed some mitigation strategies.

- The team's approach to evolve three strains for high- and low-temperature weather will allow all-year cultivation. It's unclear how the project performers intend to improve the strain to tolerate a wide range of pH, temperature, salinity, and dissolved oxygen while still maintaining high productivity. This project will also benefit from the discussion of cultivation strategies proposed to improve productivity. Not a lot of progress has been made toward their goal.
- The focus of this project is on developing improved algal strains that will be cultivated in open raceway ponds with DAC and supplying CO_2 to the growing culture. GAI has worked on multiple similar projects with academic institutions and has expertise in indoor PBR productivity. GAI's project is on track and has made good progress, and production will be initiated soon. The company has about 20 patent applications filed from projects related to advances in algae cultivation. The system has been 90% installed, with the project currently in the equipment installation and checkout phase. Productivity of biomass and lipid content in Kauai was adjusted to 14.8 g/m^2/d. The PI should mention and provide some indoor bioreactor data/achievements where GAI has established high confidence levels. There is no mention of the DEI component in the project.
- The team structure is unclear but appears to be just GAI and Hamilton Robotics. The goal of this project is to increase algae productivity and lipid production for several improved *Nitzschia* strains while using DAC for CO_2, and a range of tolerances for pH, salinity, and dissolved O_2. The team uses a directed evolution approach and thinks they have a fix allowing engineered strains to perform better in open ponds than wild-type, a serious challenge for the industry historically. One major advantage of this project is the ability to do larger-scale outdoor testing at two GAI locations (in Hawaii and California). There were very few details given about the DAC piece to this project, but presumably it was presented previously or is non-disclosable due to intellectual property (IP) applications. In fact, the approach was not very detailed for most areas of the work, so it was hard to review. However, given that GAI is working toward commercial scale (presenter mentioned next 5 years), they do appear to be focused on their goals, self-constrained/guided by TEA, and have clearly made a lot of progress. Their efforts appear to fit well within the BETO portfolio.
- The project team seeks to develop improved strains through directed evolution and cultivation methods for open raceways with all CO_2 supplied via DAC. The method for supplying CO_2 via DAC does not seem to be clearly described in the presentation. The project team has passed initial verification and is currently working on installing equipment (90% installed and partially checked out). Some results were shown for a TEA, and the PI indicated that many production costs have recently increased significantly. The impact of the proposed work is difficult to assess given the content in the information provided. Future BETO updates should provide the reviewers with more technical information about the process and more detail about the proposed innovations.

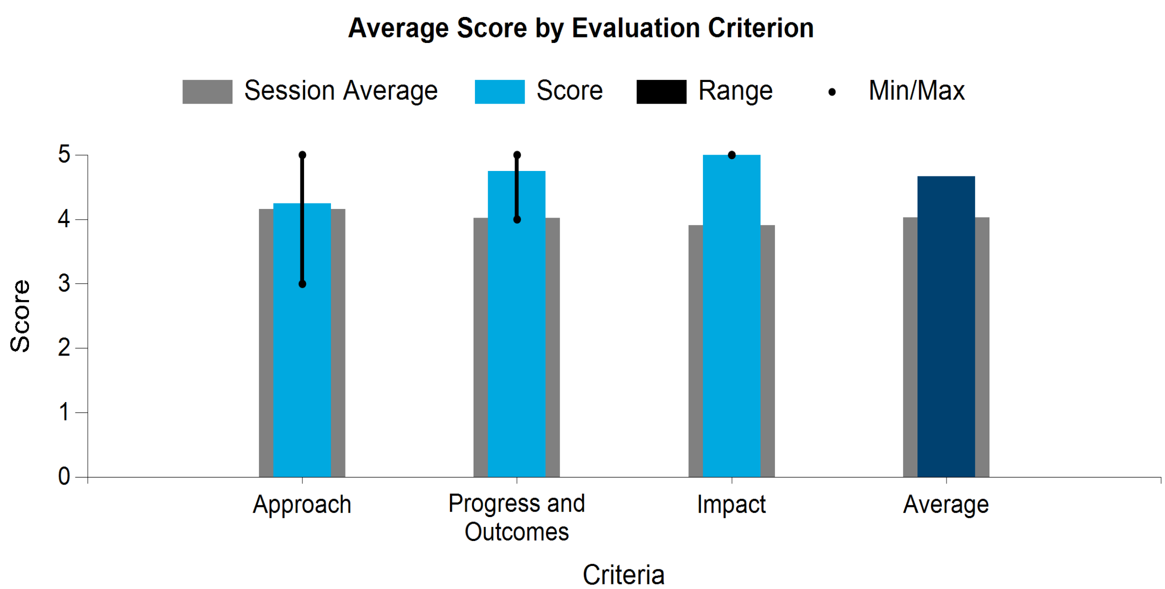
PROCESS OPTIMIZATION AND REAL-TIME CONTROL OF SYNERGISTIC MICROALGAE CULTIVATION AND WASTEWATER TREATMENT

University of Illinois at Urbana-Champaign

PROJECT DESCRIPTION

WBS:	1.3.3.001
Presenter(s):	Jeremy Guest
Project Start Date:	10/01/2020
Planned Project End Date:	12/31/2023
Total Funding:	$2,509,062

The goal of this work is to accelerate the commercialization of a high-productivity, mixed-community microalgal cultivation technology to synergistically recover phosphorus from wastewater and produce a biofuel feedstock. This project seeks to overcome challenges associated with the design and operation of high-rate processes that reliably achieve performance targets despite fluctuations in wastewater composition, climate, and microbial communities. The objectives of this work are to (1) develop a process simulator to predict process performance and sustainability, (2) develop a low-cost system for real-time monitoring of microbial community structure, and (3) leverage the simulator and monitoring system to advance the financial viability and environmental sustainability of algal cultivation on wastewater. These objectives are being accomplished through long-term characterization of a full-scale EcoRecover system installed at a wastewater treatment plant in Wisconsin, comprehensive characterization of microbial community structure and function, real-time microbial monitoring, process modeling, and sustainable design. This work has (1) identified indicators of stable system performance and impending process upset, (2) produced an open-source process simulator that predicts average effluent phosphorus within 0.01 mg P/L, and (3) yielded a novel, autonomous imaging technology achieving 86% accuracy for genus-level classification of industrially relevant microalgae.



COMMENTS

- The team proposes to integrate biomass technologies with municipal wastewater treatment to increase energy efficiency and reduce cost while still maintaining consistent biomass productivity. This is in line with Topic 2C's objective. The team approach to achieving the goals includes (1) advancing the current EcoRecover process, (2) deploying a low-cost microscope for real-time monitoring of cultivation ecology, and (3) validating an open-source process simulator for the cultivation of mixed communities. The current limitation of the technology is a lack of understanding of mixed community crashes, which will be addressed with the proposed work.

- The team had a clear management plan with a well-defined task structure and leads. They did not identify risks or proposed mitigation strategies.

- The project performers have made significant progress in demonstrating phosphorous removal using the EcoRecover process, using microscopy data to inform stable or variable performance and validate their process simulator. The impact of the wastewater treatment on biomass productivity and the consistency of yields given changes in feed stream for mixed communities are unclear. The team should consider the impact imbalance between ammonia-oxidizing bacteria/nitrite-oxidizing bacteria and the loss of *Scenedesmus* sp. on biomass productivity and the end use of the biomass. Overall, successful deployment of these technologies will not only be a huge benefit to wastewater treatment, but will also provide low-cost algal biomass.

- The project aligns with BETO's mission to support lowering the cost of biofuels through low-cost feedstocks while reducing the greenhouse gas (GHG) emissions of biofuels by offsetting the cost incurred during wastewater treatment for municipal water. The team aimed to develop a simulated open-source model following its calibration and validation, and well as assess the TEA and LCA success of cultivating several mixed microalgal communities. The second objective was real-life tracking of the structure of the microbial community via the use of low-cost microscopy, and finally, optimizing the EcoRecover process validation, locality-specific design optimization, and real-time monitoring of the system. The permanent EcoRecover installation was completed and is currently functional in the Village of Roberts, Wisconsin, and the construction of two more systems is in progress in the same state. The team has been successful in addressing their objectives in a very rational and efficient manner. The first system is in operation, and through organized teamwork and synergy, several areas—including online monitoring, on-site analyses, autonomous microscopy, biomass and omics characterization, TEA, and LCA for the cultivation of mixed microalgal communities—have been made operational systemwide. Through implementation of online sensors and analyzers, systemwide long-term monitoring and characterization have made this project greatly successful by achieving the goal of having effluent phosphorus.

- This project stands out from many in the portfolio in that there is a clear connection to an industry partner who is already using the base algae growth system to capture organic P from wastewater. The system is in operation at one small wastewater facility and under construction at two more in the same state. The project appears to have increased the reliability of this system with real-time monitoring of the community composition and environmental conditions. The team has gained knowledge on how to tweak the system if they see evidence of an imminent crash such that they can favor the target algae species. Project management was well laid out and is split between four teams, spanning a wide range of expertise. They appear well equipped to reach the project goals. The presenter explained that since the wastewater industry is highly risk averse, they have many industry and municipal advisors giving oversight to ensure they end up with a system that can be expanded nationally once it proves reliable. The project has exceeded its goals to date.

- The approach of developing real-time tracking of the microbial community and system control has substantial merit and significant potential to reduce phosphorus effluent in municipal wastewater. The project team has been working for 1.5 years on the project and seems to have made excellent progress in addressing project goals. The project team has met their go/no-go milestone for predicting effluent phosphorus, energy consumption, and biomass yield (i.e., amount of algae produced). The software developed in this project has allowed the ARTiMiS to approach 86% accuracy for species-level classification of industrially relevant microalgae, which is impressive. The overall potential impact of the project on other high-phosphorus-level areas seems significant, and it seems likely that the developed technology will be deployed to other wastewater treatment sites.

PI RESPONSE TO REVIEWER COMMENTS

- Response to Comment 1. We thank the reviewers for their supportive comments. With regard to risk management, two of the core risks are (1) if the system were to demonstrate completely stable performance with no variability or upset events (we cannot cause failure or intentionally undermine performance at an operating wastewater treatment plant) or (2) if we are unable to implement proposed process controls (due to perceived risk or inability to change at the Village of Roberts wastewater treatment facility). With regard to the first risk, the variability in performance of the upstream system has already resulted in adequate performance variability (and significant microbial community structure dynamics) that is enabling robust model calibration/validation, autonomous microscopy system development, and meaningful insight into full system functioning. With regard to the second risk, we have observed that executable process controls (e.g., increasing alkalinity, doubling the single-pass retention time in PBRs) have resulted in significant improvements in process performance and stability, as evidenced by the recent 3 months of winter performance with effluent total phosphorus below 0.03 mg P/L. Given these achievements to date, we are confident the existing system in the Village of Roberts provides adequate flexibility to mitigate these risks. Areal productivity over time is influenced by both the performance of the system and the influent phosphorus concentration. Although cultivation is phosphorus limited, phosphorus in significant excess can also undermine performance because it eliminates the selective pressure that drives stable system performance (i.e., P-available conditions in the mix tank and P-limited conditions in the PBRs). As recommended, we will more clearly link areal productivity to wastewater composition and two of the key drivers that have been identified—ratio of ammonia-oxidizing bacteria to nitrite-oxidizing bacteria and the loss of *Scenedesmus* sp. We will also link these events with the biochemical composition of the harvested biomass and its implications for downstream end uses.

- Response to Comment 2. We thank the reviewers for their positive comments. Moving forward, we will more clearly link operating data to BETO's goals for algal biofuel production. As a starting point, we will more clearly report areal productivities (e.g., we achieved high-performance periods with >40 $g/m^2/d$), and we will include conversion to biofuels and bioproducts in our TEA and LCA.

- Response to Comment 3. We thank the reviewers for their positive comments.

- Response to Comment 4. We thank the reviewers for their positive comments.

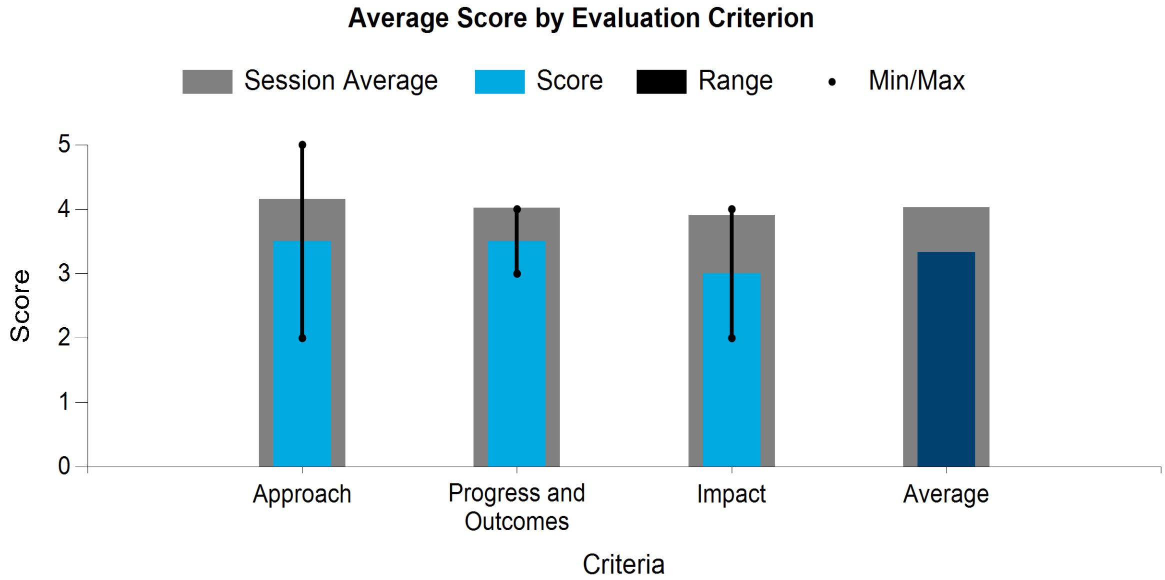
SYNERGISTIC MUNICIPAL WASTEWATER TREATMENT USING A ROTATING ALGAE BIOFILM REACTOR

Utah State University

PROJECT DESCRIPTION

WBS:	1.3.3.002
Presenter(s):	Ronald Sims
Project Start Date:	10/01/2020
Planned Project End Date:	05/31/2024
Total Funding:	$1,947,175

This project is a partnership among three industries, PNNL, and Utah State University to test a pilot-scale (1,100-gallon) algae biofilm platform—the Rotating Algae Biofilm Reactor (RABR)—at the largest municipal reclamation facility in the state of Utah (Central Valley Water Reclamation Facility [CVWRF]), treating anaerobic digester effluent to remove nutrients through cultivation of biofilm microalgae and to transform the harvested biofilm into biofuels and bioplastic. WesTech Inc. manufactured the RABR, and Algix will transform the feedstock biofilm into bioplastic. The six objectives of the project are to (1) increase the energy efficiency for total phosphorus and nitrogen removal, (2) improve the yield of biofilm indoor/outdoor tests, (3) improve the cost of total phosphorus and nitrogen removal, (4) meet the total phosphorus target after remediation, (5) produce bioplastic and TEA/LCA data, and (6) produce a TEA with three pathways for conversion of biofilm algae to bioproducts, including biocrude with HTL, bioplastic, and biofuels and bioplastic, and produce an LCA. The project approach includes four elements: (1) contribute to DOE's long-term vision of expanding the domestic resource potential of the bioeconomy by utilizing existing infrastructure to create a low-cost supply of algae biomass at water reclamation facilities nationwide; (2) produce renewable biofuels and bioproducts from biofilm algae using anaerobic digester effluent at CVWRF; (3) reduce the concentrations of phosphorus and nitrogen in the anaerobic digestate; and (4) apply the RABR technology for both cultivating and separating polyculture microalgae biomass from anaerobic digester effluent. Results from the first two budget periods that span from 10/1/2020 through 2/28/2023 include the 15 milestones in the statement of project objectives (Budget Period 3 is scheduled from 3/1/2023 through 5/31/2024 to address the remining 15 milestones). Results show that 14 milestones achieved target values that addressed biofilm yield and energy and cost reductions compared with baseline values for struvite formation and characterizations of the feedstock and RABR biofilms using microscopy and genetic testing. Milestone 5.1, producing 20 pounds of pilot RABR biomass (dry weight) has been delayed for 2 months (from February to April 2023) due to scheduling of the implementation of the mechanical infrastructure of the pilot RABR. This adjustment of the schedule for Milestone 5.1 does not impact the ability to achieve any of the other milestones of the project, including Budget Period 3. All of the targets identified for the go/no-go decision (Milestones 2.5, 3.1, 4.1, and 7.1) and the review meeting for the intermediate verification held on 1/26/2023 at the host site were achieved.



COMMENTS

- The goal of the project is to test a field-scale outdoor pilot RABR to remove total phosphorous and nitrogen from an effluent treating municipal wastewater and produce biofilm biomass for biofuels and bioplastics. The outcome of the project is to reduce phosphorus concentration by 70% and obtain a biomass yield of 2.4 tons per million gallons of treated water while lowering treatment costs.

- A management plan was outlined while leveraging the team's previous experiences in this project. Risk and mitigation strategies were identified. A task structure was proposed with quantifiable go/no-go decision points.

- The team has made progress in demonstrating productivity that exceeds their target of 7.5 g/m^2/day and proposes to implement TEA and LCA to help guide their work. The project performer should clarify the robustness of the harvest and seeding process, the impact on nutrient uptake, and how this technology can be scaled up. It is also unclear from this work what results in low nutrient uptake, given that contamination is not a challenge with biofilms. Overall, successful deployment of these types of technologies will not only be a huge benefit to wastewater treatment, but will also provide low-cost algal biomass if the cost of heating and raw materials are optimized.

- This project aims to utilize a RABR to remove nutrients, mainly phosphorus and nitrogen in the effluent water coming from the anaerobic digester of the municipal wastewater reclamation facility. The project aims to utilize the biomass from the algal biofilm for biofuel and bioplastic production in the downstream process, but not much information or data was provided related to how much initial progress has been made with the HTL process at Utah State University or Algix in the past 1.5-year time period that addresses BETO's goal for sustainable biofuel. The team has been quite successful on lowering the total phosphorus concentration in the effluent from the digestor by 47% and reducing the energy or power consumption cost for the RABR technology, as well as producing a significant amount of algal biomass. The optimization for biomass productivity needs to be closely addressed, as the current setup seems to be very susceptible to technical hiccups such as condensation and other related issues. A concern here is the use of plastic covers that can make the operational system more susceptible to microbial infestation and challenges as opposed to having a metal shed. This would bring up the cost for the setup but would provide sustenance through the different seasons. The genomic and taxonomic analyses for determining the composition and structure of the active algae-bacteria biofilm have made good progress for identifying the most dominant species at both lab-scale and outdoor experiments. Sharing and discussing data on establishing this co-relationship and parity between the outdoor and indoor RABR setup will be critical to understand the robustness of the system. There was information on how the team coordinates the work with student researchers, but mentioning how the work synergy is maintained with outside units and partners would provide the complete idea on workflow.

- This project demonstrates a RABR to capture nutrients from a wastewater facility in Utah. The idea behind the technology is very promising: a unique algal growth platform that, if done right, could bypass some of the risks associated with open raceways. The source algae for this project were collected on-site from a biofilm naturally forming on vent surfaces adjacent to the RABR. The algae community that populates the reactor appears to be quite robust to environmental and biotic contamination. Pest management was not an issue according to the presenter. Algae harvested could be used for various products, and an industry partner (Algix) is online for using it for bioplastics. It is unclear what the management structure is. The system does not appear to be scalable as is and would need to have harvest become automated, but it was unclear what stage of development this is. One limitation to this is that it has only been demonstrated in one location, but if it is expanded to other geographies, a local algae source would be used. The risk is that some of the knowledge gained in this project would not apply elsewhere. This project appears to be making good progress toward its quantifiable goals. Several risks were identified, mostly around engineering issues, and it is unclear how economic the proposed mitigation strategies are, especially if this system is scaled up.

- In its current form, the proposed RABR technology does not seem to advance the state of the art in municipal wastewater treatment. The project is on schedule and seems to have met targets on productivity, energy consumption, and removal of phosphorus. The risk mitigation strategies involving the plastic polycarbonate cover to control for temperature and wind effects and the use of electric heaters to control for condensation on the cover would seem to be impractical when scaling the RABR technology. The overall impact on the wastewater industry would seem to be minimal given the current method of scraping algae biomass off the rotating platforms. Other more scalable solutions should be explored for removing the biomass from the rotating platforms.

PI RESPONSE TO REVIEWER COMMENTS

- Our team would like to thank the reviewers for the engaged feedback regarding the project. As noted, the project met the interim go/no-go decision points for phosphorus removal and biomass productivity for the intermediate verification and will focus on robustness of harvest and the seeding process in the next phase of the project. Robustness of harvest is directly related to the sustainability of the cultivation surface, which is recycled post-consumer pop bottle plastic, and which has remained robust through the first 8 months of continuous pilot-scale operation using simple mechanical scraping of the surface layer of biofilm, leaving a residual layer of biofilm for continuous nutrient uptake. Robustness of seeding has been very good and was only required for the initial inoculum, which was sourced from the operating trickling filters at the host site, CVWRF. Because a residual biofilm remains on the cultivation material after harvest, nutrient uptake is also a continuous process. Regarding scale-up strategy, a full-scale RABR system for the treatment of a 0.6-million gallon per day side stream from CVWRF has been designed and was presented in a milestone report submitted to BETO with the diagram shown here. The design of the full-scale RABR system is based on discussion with project experts with CVWRF and WesTech. Project personnel also worked together to develop an economic analysis for this full-scale system, which was presented at the intermediate verification on-site meeting at CVWRF held on Jan. 26, 2023. While contamination was not a problem for the biofilm design, nutrient uptake observed and reported was low due to the low-temperature operations during late fall and winter in northern Utah, which is approximately 12°C–15°C. This temperature limitation will be eliminated at full scale because CVWRF will install temperature controls in 2024 as part of the upgrade to the entire facility that will maintain a minimum temperature of 25°C for optimizing other processes. The project staff will evaluate the anticipated improvement in operation and performance during the next phase of testing. The next phase (three) of the project aims to utilize the biomass to produce biofuel, through HTL, to address BETO's goal for sustainable biofuel and bioplastic production. The project team is addressing the technical hiccups, including temperature, through the upgrade to the full-scale CVWRF and condensation on the roof through construction of an improved greenhouse at full scale that will include a concrete base with improved ventilation and temperature control to provide sustainability through seasonal changes. The project will continue to evaluate genomic and taxonomic characteristics of the biofilm to understand the biofilm community structure and function. Work synergy is maintained through regularly scheduled weekly meetings, including a combination of Zoom for remote partners and in-person participation for local partners. Work synergy is also accomplished through both Zoom and on-site meetings among subgroups of partners; for example, coordination for genetic characterization between experts at PNNL and Utah State University; experts for HTL testing between PNNL and Utah State University; experts for wastewater treatment that include WesTech Inc., CVWRF, and Utah State University; and bioplastic production between Algix and Utah State University. This promising RABR technology project has demonstrated that pest management is not an issue due to the robust biofilm platform that can bypass some risks associated with open raceway contamination, as noted in the review comments, and limitations of light penetration through wastewater. Therefore, the scalability of the technology is the focus for the next phase of testing. The structural and functional components of bays, sections within bays, and cultivation shelves within sections, which were not discussed in detail, were developed as part of the initial RABR design with the end in mind for scalability and economy of operation. Determination of the full-scale size aspects, including physical components, automated harvesting, and cost of operation of a RABR system, is being undertaken during Phase 3, and is part of the TEA component. Based on the current pilot-scale unit, a full-scale RABR system has been designed based on discussion with project partner industrial experts, CVWRF, and WesTech Inc. Compared to the pilot-scale unit, the full-scale RABR system has a larger size for algae growth substratum, more frames per section, and supports for each rotating bay, which enables it to continuously treat 0.6-million gallon per day side stream water from CVWRF. Regarding applicability of the technology and RABR system to other sites, common characteristics of anaerobic digester effluent, which include high phosphorus concentration (50 mg/L) and high nitrogen concentration (500 mg/L), as well as warm temperatures (77°F), are typical and relatively independent of geographic location. The exception is the variable concentration of magnesium, which is necessary for struvite precipitation. Therefore, the host site (CVWRF) system is typical of municipal wastewater treatment facilities across the United Staes and provided the rationale for conducting the testing of the RABR system there. The economic aspects of a full-scale system are a focus of Phase 3, which includes a TEA. The current pilot-scale system treating 1,100 gallons of anaerobic digester effluent has provided insights with regard to temperature, wind, and harvesting challenges that are objectives for Phase 3 of the project, which is to develop solutions to these challenges. Temperature will be controlled at full scale with the plant for upgrade at CVWRF for other processes that will benefit the RABR technology, and therefore will not be an added cost. Wind will be addressed with greenhouse plans for the facility that will contain a RABR of 1.2 million gallons volume to treat a flow of 0.6 million gallons per day, which is considered viable for CVWRF and applicable to other water resource recovery facilities. Harvesting automatically remains the greatest challenge, and the project partner that manufactured the RABR, WesTech Inc., is working with Utah State University to identify solutions for testing and scale-up in terms of processes and costs. All of these factors potentially impacting scale-up are being incorporated into the TEA and LCA for a full-scale system. The comments of all four reviewers were very valuable and insightful and are currently being addressed and evaluated in Phase 3 of this project.

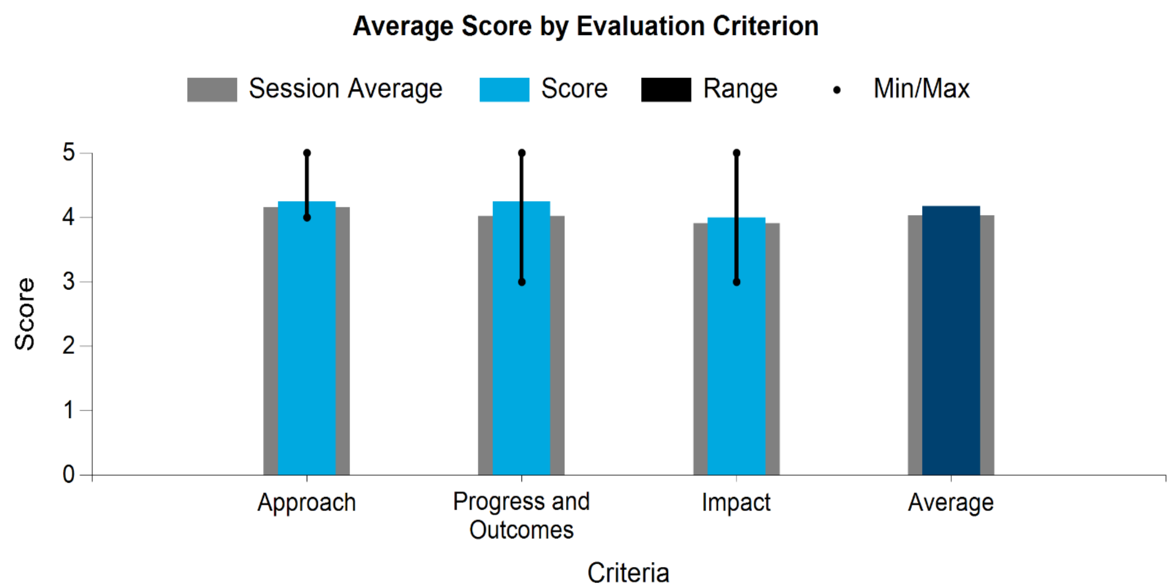
PRODUCTION OF ALGAE BIOFUEL WITH CO_2 DIRECT AIR CAPTURE

Global Algae Innovations

PROJECT DESCRIPTION

WBS:	1.3.4.001
Presenter(s):	David Hazlebeck
Project Start Date:	10/01/2020
Planned Project End Date:	12/31/2023
Total Funding:	$2,500,000

GAI has developed low-cost algae production technologies aimed at achieving commercially viable production of biofuel and high-protein meal. Radical advances have been designed and implemented throughout the entire process, resulting in many industry breakthroughs for large-scale algae cultivation, harvesting, and processing. In this project, CO_2 is directly absorbed from the atmosphere into the open raceways so that no separate CO_2 concentrating or distribution system is needed. The main objective of the project is to improve the economics of algal biofuel production by increasing the value of coproducts through improved separations and product development. A product spectrum was developed that doubles the value of the coproducts and has a market size commensurate with the biofuel market. The products are algae oil for fuel, PUs, and omega-3 oil; protein meal ingredients for food and feed; and nutrients recycled within the process. Many novel unit operations were developed for separation of the products. The focus of the remainder of the project will be on refinement of the downselected process flow and production of sample products for testing.



COMMENTS

- I agree with the author that there are a lot of unit operations to test and optimize, making the system quite complex. The complexity makes it more challenging to tech transfer the methods.
- There is excellent progress on the unit operation development.
- The outputs appear to include water in recycle nutrients. The mass balance does not sum up due to ash residues.

- The TEA looks very good at a net $226/metric tonne; the financial assumptions for cost of capital are reasonable. An unlevered internal rate of return of 20% is still quite good, depending on the underlying assumptions about land use (i.e., the land cannot otherwise be used for agricultural purposes, the land requires no utility from the local grid and can use solar power). Water rights may be quite complex to model depending on the location and could throw a real wrench into the TEA.
- More information on the new unit operations would be interesting.
- This project is aligned with the goals and is delivering against those goals. Concerns do exist, especially with product value. The claim that economics get better if higher-value products are made is hardly a revolutionary realization. Getting paid more for your products is always a plus.
- It is concerning that more products are the solution. Numbers of added unit operations add to complexity and capital cost. The fuel is the minor product by value. The data presented did not indicate careful examination of return on investment and thought about the complexity of marketing multiple products.
- The process patent count is big, but there must be a question about the true value created. The number of process patent applications was held up as a sign of progress. It does not come across as a compelling example of progress. One positive outcome of a patent is that it eventually becomes public information. It is concerning that these advances cannot be talked about for fear of wrecking a patent, making it impossible for us to review the novelty or impact. There are negatives. The biggest one is that process patents are difficult to police and frequently easy to circumvent. The patents were described as being in oil purification. This is a well-populated area due to the history of seed oil purification. It seems unlikely that there is an area of huge novelty remaining.
- Approach: The primary objective for this project is to develop a TEA-guided integrated process based on various novel unit operations that serve to lower the overall algal biofuel selling price by increasing the value of recoverable coproducts. This objective is in line with BETO goals. The project partners represent a good mix of companies for testing the coproducts for quality and marketability, but such testing has not yet commenced.
- Progress and Outcomes: The team indicated that an integrated process with 26 patentable steps has been developed that allows for the production of multiple coproducts (biofuel, plastic polymers, omega-3 oils plus glycerol, and protein [both concentrate and meal]), and which also claims credit for nutrient recycle. The combined value of these products was double the overall value of the original mix of biofuel plus protein meal. The presentation did not indicate a comparison of the combined cost of manufacture for the new suite of products versus that of the original products, so it's not really possible to say how much the net profit potential increased as a result of the new process, which is a more important metric than total selling price of the coproducts. In addition, it looks like the team is assuming that no substantial losses of material occur during this complex processing scheme, which is not realistic when the quality requirements for most of these products will dictate relative high purity levels.
- The coproduct suite shows that biofuel represents 17% of the biomass ash-free dry weight, and the mass balance indicates that the oil content of the harvested biomass is 50% of the ash-free dry weight (and fractionated oil was 40% of the ash-free dry weight after processing). Thus, the process as outlined does not appear to achieve the end-of-project milestone specifying that 50% of the oil should go to biofuel.
- Although favorable numbers were presented with respect to the enhanced economic value of the overall process, it is difficult to assess actual progress toward a favorable commercial outcome without a better understanding of the claimed unit operation enhancements and whether the higher-value products that contribute the most to the favorable economics have the characteristics, quality, and cost of manufacturing that would truly enable market entry. Although it is recognized that product testing can be

a long and expensive process and is planned in the remaining time of the project, it would have been highly desirable for the project team to present more information on the basic chemical nature of the multiple product streams and how those compare to existing products on the market.

- Information was not provided on one of the stated goals of the project, i.e., the mitigation of losses in DAC-maintained ponds after a rainfall event.
- Impact: The project team has developed a process that they feel would improve the economics for producing biofuels at large scale (reaching the selling price target of $2.50/GGE), primarily through coproduction of higher-value products. This will be an important outcome if the overall process is in fact economical and the markets for the resulting coproducts are robust. Currently, it is difficult to assess the real impact since the claimed improvements were not described due to patent applications that are expected to be filed.
- Approach: Good plan, good goals; not working with collaborators yet; risks were identified and the plan to address them is good. Outcomes: Lots of outcomes reported, but no data were shown, so it is difficult to know what has been accomplished. Impact: No plan for dissemination to industry weakens the impact.

HIGH-PH/HIGH-ALKALINITY CULTIVATION FOR DIRECT ATMOSPHERIC AIR CAPTURE AND ALGAE BIOPRODUCTS

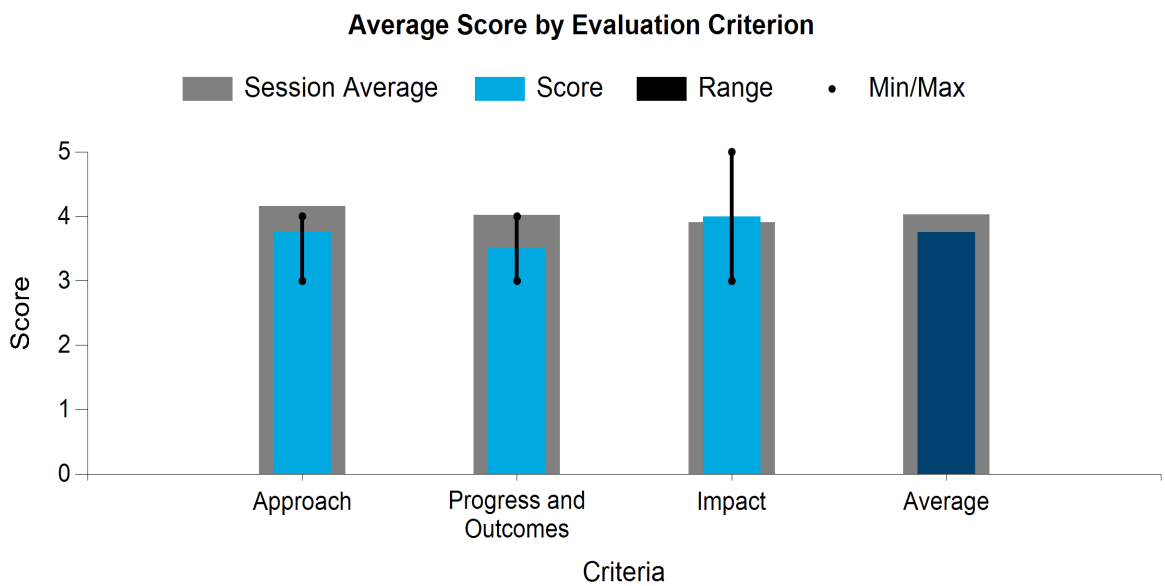
Montana State University

PROJECT DESCRIPTION

WBS:	1.3.4.002
Presenter(s):	Robin Gerlach
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2024
Total Funding:	$2,530,300

For algal biofuels to replace fossil fuels, it is imperative that cultivation systems are not constrained by the proximate availability of flue gas or other high-concentration CO_2 sources or the energy and infrastructure burden to deliver CO_2 over long distances. This project builds on our significant prior experience of cultivating algae in high-pH and high-alkalinity environments with enhanced DAC to produce fuels and high-value products. This project intends to test and improve a novel open-pond reactor design and facility operations to enhance CO_2 mass transfer from the atmosphere, as well as to improve cultivation-based strategies (nutrient supply, media recycling, and microbiome control) to optimize biomass productivities, biomass quality, and culture stability. The resulting biomass is being converted by pyrolytic fractionation into fuels and algae-based materials for the automotive and packaging industries, as well as for energy storage applications. Integrated TEAs provide feedback and forecast scenarios for different design and operation scenarios of prospective algal biorefineries.

This work contributes to eliminating the need for costly, external CO_2 supply, thus allowing for more flexible siting of algal production facilities capable of generating high-value coproducts using novel conversion pathways to improve the revenue potential of algal biorefineries.



COMMENTS

- Thank you for the org chart and communication slides; they are very helpful in understanding the management structure and function. The risk mitigation slides didn't clearly identify any risks or strategies.

- The bacterial oxidative stress hypothesis is interesting; it would be helpful to know iron levels in the media versus in bacterial transferrins to determine the feasibility of this hypothesis.
- The timeline was not provided for comparison.
- The engagement with Sonoco would be helpful to have more details on, as it is critical to the impact analysis.
- A useful experiment to demonstrate the actual contribution of the bacterial populations would be to individually add back isolates; even at shake flask scale, this would be a fairly simple factorial. Is it part of the plan?
- Power draw should be straightforward to measure and compare to the paddlewheel design.
- The team addressed all stated goals except the last presented, which is in the next phase.
- The power for the belt mixer and the advantages it creates were not well described. Just because something is different doesn't automatically mean it is better. The lack of clear metrics around why some changes were being made is a bit troubling. Additionally, the impact on capital cost and reliability was not even mentioned. It is different, but it is not clear what optimization variable drives adoption.
- Approach: The approach being taken to increase productivity while using DAC of CO_2 seems reasonable and is aligned with BETO goals. The multisite and multidisciplinary project team is well suited for conducting the different aspects of the project, although the interrelatedness of the subprojects is not always obvious. Communication and coordination between team members appears to be set up appropriately.
- Progress and Outcomes: The combination of a new pond mixing system and media carbonization/recarbonization with DAC shows promise, although the potentially higher energy requirements for the belt-and-cleat system need to be better understood because the increases in productivity and carbonization rate are not large.
- Very little information was provided regarding pyrolysis of algal biomass and PU foam production from algal biomass/oil. It would have been useful to show the chemical composition of the pyrolysis oil, as well as a comparison of the properties of foams made from polyols derived from algal oil, cottonseed oil (previous work from this lab), and petroleum.
- The TEA/LCA slide was not well explained; it was quite generic, and it wasn't clear whether it was showing past work based on typical growth systems or on the system under development in this project.
- Some academically interesting results regarding microbiome population dynamics were presented, although the connection of this work to the rest of the project was not obvious.
- Impact: It remains to be seen whether the belt-and-cleat system provides an advantage over typical paddlewheel-mixed ponds, but it is worth exploring in order to see if there are significant productivity increases and associated cost reductions.
- Although academically interesting and solid work, it is not obvious that significant value is being added to the overall project through the various analyses of the culture microbiome (e.g., metabolic modeling, population dynamics), especially because a clear benefit attributable to the microbiome has not been demonstrated in their system.

- Approach: Seems reasonable; however, I'm not sure how far this is moving the needle due to low technology readiness level. Outcomes: Goals have been met; it would be a good addition to the project to address the energy needed for mixing. Impact: The ponds are too small to have any relevance as far as the impact of a new design.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their comments and questions. Regarding the identification of risks, it became clear that the two major risks identified were not stated explicitly. The risks were (1) a loss of expertise in a key area, and (2) the possibility that the belt-and-cleat ponds will not result in increased recarbonization efficiency and/or biomass productivity. We agree that while the risks were not stated explicitly, the mitigation strategies were presented. The mitigation strategies are (1) "overlapping (and redundant) expertise and capabilities" and (2) "multiple strategies to achieve improvements in productivity" (which could each, separately, lead to the desired productivity improvements), including multiple possible recarbonization strategies (see below for details). The iron levels in the media are initially 0.018 mmol/L. The pH increases to 10.3 during cultivation, which will lower the solubility of Fe. Hence, we add chelated iron, and while we do not know whether the chelation holds at high pH, we have never seen an indication of iron limitation. Both Montana State University and the University of Toledo have, over the years, performed multiple iron add-back experiments with different iron sources but have not seen any growth enhancement, indicating that the cultures are not limited in iron. We have also tried to limit iron levels for work with microbiomes, but it has been difficult to achieve conditions in which iron is the limiting nutrient. The hypothesis regarding reduced oxidative stress was based on the observation that higher carbohydrate levels were detected in SLA-04 grown at high-pH and high-alkalinity conditions. Additionally, the metabolic modeling indicates that some of the bacteria in the microbiome might be involved in the mitigation of oxygen stress during the daytime and during glycolate degradation. Regarding the engagement with Sonoco: The team is in communication with Sonoco. We are still working toward generating appropriate size foam structures that Sonoco can test for thermal conductivity. However, we did test the small sample for density, and we are getting closer to the metrics provided by Sonoco. Regarding the noted usefulness of "add-back" experiments, the team has indeed conducted such experiments and has not observed any negative effects. We have had an occasional indication of a positive (i.e., growth-promoting) effect, but the effect has not been reproduced consistently. We are considering additional experiments to reproduce these results and scale up the size of cultivation systems as appropriate. Detailed results so far are available in the quarterly reports. Work is continuing, and a probiotics-based growth enhancement strategy is still being pursued for our SLA-04 cultures. We are planning to continue research in this area throughout the duration of this project and will report on this as appropriate in quarterly reports. The comments regarding the belt-and-cleat ponds are appreciated, and as indicated above and detailed below, we have multiple strategies outlined to potentially improve recarbonization efficiency in this project. The belt-and-cleat technology is just one of the approaches being evaluated as a promising alternative to the paddlewheel technology. The belt-and-cleat technology is new (project start: technology readiness level 3; expected project end: technology readiness level 5), and the principle is conceptually sound based on computational fluid dynamics modeling. Hence, the belt-and-cleat mixing technology has been a focus in this project so far. Distributed mixing with the angled cleats should increase surface renewal and thus CO_2 mass transfer from the atmosphere into CO_2-depleted cultivation medium. Our current comparisons are based on small-scale ~30-L raceways. While simply measuring power usage is indeed straightforward, the fact that we are using small (~30-L) raceways with oversized paddlewheels and cleats relative to what will be necessary in larger-scale production ponds complicates scalable comparisons between the belt-and-cleat design and the paddlewheel design. In general, the motors are also oversized for the raceway paddlewheels and belt-and-cleat system. We are discussing with the belt-and-cleat patent holder whether we can use his larger-scale prototypes (~10-m^2 surface area, ~2,500-L volume) for comparison tests, which would also include power consumption measurements. The metrics for the project are to compare the efficiency of belt-and-cleat versus paddlewheel ponds at equivalent power usage, and we are working toward a valid and defensible experimental comparison. Furthermore, as a measure of potential risk mitigation, the evaluation of alternative recarbonization strategies is built into the project if the belt-and-cleat technology does not prove to be an improvement for the high-pH, DAC algal cultivation approach. These alternative recarbonization strategies include designated recarbonization ponds (with paddlewheel, belt-and-cleat, or other mixing technology), membrane-based recarbonization, the use of absorber columns, and cascading flow. It is indeed a goal of the project to estimate the costs (both capital and operating costs) and compare them to paddlewheel-based pond designs. We appreciate the comment regarding the interrelatedness of the tasks and want to remark that each strategy we are pursuing has the potential to be implemented independently into the overall process of algal growth and post-processing of algal biomass. Each of the strategies pursued can result in an improvement in overall economics. Hence, the team we have assembled with its diverse backgrounds and areas of expertise is pursuing research independently, yet in a coordinated and complementary fashion, with the goal of providing more than an incremental step change as an overall outcome of this project. We are aware that only little information was provided regarding the details of the pyrolysis of algal biomass and PU foam production. Work on these tasks is ongoing. Information regarding the chemical composition of the pyrolysis oil and comparisons of the properties of foams made from polyols derived from different sources will be forthcoming. We have met our milestones and reported our progress in detail in the quarterly reports. More detailed information will be forthcoming in future quarterly reports, as well as during the next Peer Review meeting. Reviewers commented that the one TEA/LCA slide was perceived as generic, but we would suggest that this is a function of the need for brevity in these very short presentations. The LCA/TEA framework developed in this project is actually quite unique in that it involves a stochastic simulation that incorporates variability in weather conditions (temperature, solar irradiance, wind, and humidity) and market prices (using biodiesel prices as a proxy for algal biofuels) and does so at a daily time step. This allows for a more highly resolved characterization of variability in algal and algal biofuel production, as well as the corresponding impact on revenues, that then lead to an improved understanding of the financial risk that variable weather and market conditions can impose—an important criterion for investors and one that is garnering increased attention. Further research will involve the development of strategies for managing this financial risk via a combination of reserves and a novel index insurance product, with the latter being particularly interesting given the U.S. Department of Agriculture's recent designation of algae as a "crop" for the purposes of their subsidized crop insurance program. The stochastic nature of this LCA-TEA modeling platform and its focus on financial risk (both characterization and management) make it quite distinct within the biofuel space and should produce results that are both novel and of practical use to algae producers.

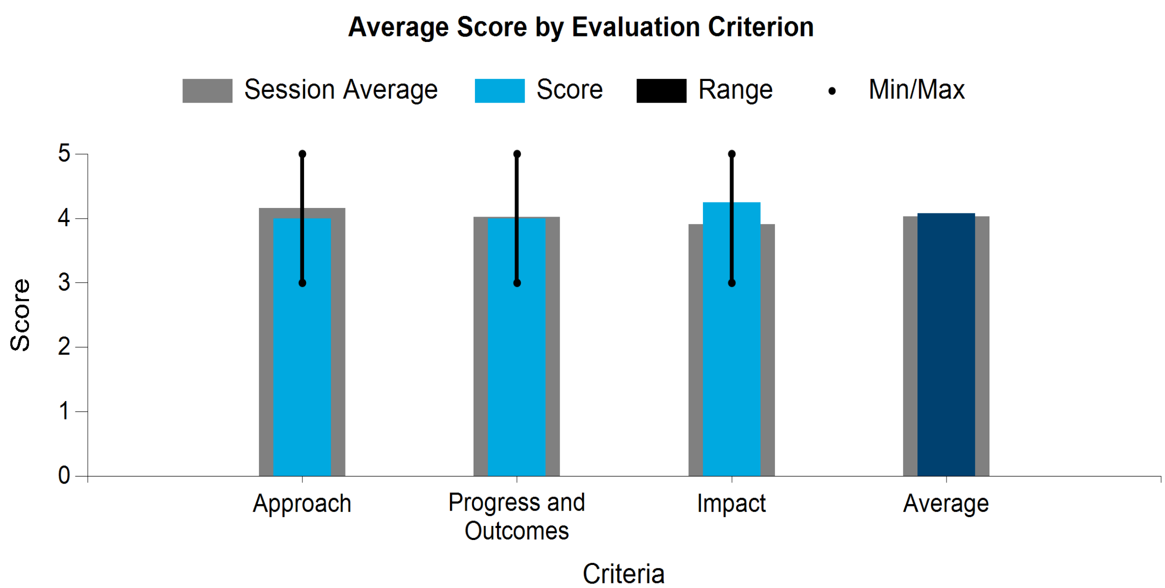
ARIZONA STATE UNIVERSITY'S DAC POLYMER-ENHANCED CYANOBACTERIAL BIOPRODUCTIVITY (AUDACITY)

Arizona State University

PROJECT DESCRIPTION

WBS:	1.3.4.003
Presenter(s):	Willem Vermaas
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$2,505,394

This project develops the AUDACity system, which efficiently delivers DAC CO_2 directly to cyanobacteria using moisture-driven sorbents and will demonstrate it in outdoor raceway ponds. AUDACity is used to cultivate *Synechocystis* sp. PCC 6803 strains developed at Arizona State University that have been engineered to excrete laurate or methyl laurate ($1/kg) and that contain phycocyanin (PC), a high-value natural dye for food and cosmetics ($1–$200/kg). The TEA of AUDACity shows that *in situ* methyl laurate harvesting can increase the fuel yield 2.2-fold over green algae, and fuel can be produced for $2.50/GGE when selling a coproduct valued at $6.30/kg, equivalent to whey protein. PC can be extracted in high yield and purity and was found to be stable at 100°C when dry. Synthesized and commercial DAC polymers have been shown to capture and rapidly deliver 90% of their CO_2 capacity in less than 1 hour. AUDACity was used to cultivate *Synechocystis* at lab scale using synthesized and commercial sorbents with productivities of 115–120 mg/L/d. Challenges include developing DAC polymers that rapidly capture and release CO_2 and that are biocompatible. Biocompatibility has been mitigated in part through adaptive laboratory evolution to select for strains that better tolerate the polymers. AUDACity impacts include reducing cost (projected <$50/tonne CO_2), reducing carbon intensity (from DAC CO_2), and eliminating ~70% CO_2 losses from sparging.



COMMENTS

- Communication with related projects or within the project is unclear.
- The scientific progress looks great. The team next needs to address extractables/leachables from the polymer due to the toxicity observed in the first immersion, as the fate of the extractable/leachable

material could have an impact on nutrient recycling and product adsorption of the material. For this reason, it may make more sense to stick with commercial anion exchange resins.

- There is no mention of whether the end product yields increased linearly with optical density in 96-h cultivation.
- The market size for blue dye should utilize current market size and make standard consumer product assumptions for market penetration unless there is an explicit reason to justify a different number.
- I have some reservations about PC carrying such huge value. That said, the project delivered against the stated goals, finding, perhaps, the proverbial "goose that lays the golden eggs," or at least an algae that lays blue eggs.
- PC is already a material of commerce. The presented economics are not overly compelling. A high-value coproduct will always improve economics. I remain skeptical simply because the disparity in cost and scale are so great between fuel and PC. I certainly believe an analysis with PC as the main product and fuel as a coproduct is warranted. This could be a good steppingstone to grow cultivation provided the market is truly underserved.
- Approach: The team is working to develop a CO_2 delivery system for algal ponds based on DAC that comprises polymer sorbents that capture CO_2 when dry and release the bound CO_2 when wet. A belt system that enters and exits the pond allows the polymer wetting and drying phases. This goal aligns with BETO goals to reduce the cost of algal biomass and biofuel production.
- Progress and Outcomes: A methacrylate-based polymer was synthesized and tested for CO_2 absorption and release kinetics. This was then tested (along with Excellion commercially available CO_2 sorbent sheets) to measure the growth of algae supplied with CO_2 in this manner. Although both materials supported growth of *Synechocystis*, growth proceeded for a longer time with the commercial sorbent.
- The methacrylate polymers were shown to be inhibitory to cyanobacterial growth, so effort was put into adapting the strains to the polymers using adaptive lab evolution. The mechanism of toxicity is not known; it would be useful to know if the polymers themselves were toxic or whether unpolymerized monomers or crosslinkers or other polymerization additives were the problem. For strains that appeared to develop a tolerance, it would be important to know whether the reported tolerance was a stable genetic change or simply a transient adaptation.
- Testing of the AUDACity system indicated that it is important for the sorbent belt to dry completely in order to reabsorb additional CO_2, requiring a longer belt. Problems were also encountered with nitrate in the medium binding to the sorbent instead of CO_2; it was not discussed whether other anions (e.g., chloride) would render this system unusable for saline or brackish waters, but this may be an important consideration. These issues would need to be resolved in an economically feasible manner before it could be deployed in commercial systems. (It is noted that a mitigation strategy is outlined to overcome DAC polymer fouling but has not been tested yet.)
- PC was examined as a higher-value coproduct to support biofuel production economics. Notably, the TEA and LCA indicate PC production of 40.5 tons/day, or >12,000 t/year. This amount greatly exceeds all forecasts for the PC market size over the coming decade, so the suitability of PC as a coproduct at the scale used in these calculations is questionable. (Note that the output values on the TEA/LCA slide also seem off, in that it reports 12,000,000 GGE/year of methyl laurate, but less than 10 GGE/year of biodiesel and naphtha.) Additionally, some of the energy or mass inputs are marked as 0, which also may be errors.

- Impact: Development of a low-cost CO_2 DAC system is certainly well aligned with BETO goals for reducing the cost of algal cultivation via lowering the cost of supplied CO_2. On the surface, however, the AUDACity system looks like it might be expensive to construct and implement, but the TEA slide presented didn't break out capital and operating costs for the system, so it's hard to assess. Considering the issues that have been seen in this project and the small amount of time remaining for the project, it will be difficult for the investigators to fully accomplish the most important goals of the project.

- Approach: Good project plan, good risk identification and mitigation plan, no management plan presented. It is not the correct approach to adapt an algae to a toxic substrate instead of switching to a nontoxic substrate, since one is available. Outcomes: The team is meeting goals, and research is going well. PC extraction is being done commercially, so this technology development is not a great addition to the project. Impact: If the technology works to catch CO_2 and supply it to the cultures, that is going to have a large impact. It seems like this technology would not be hard to implement. As part of project outcomes, I would like to see more on dissemination of information and how the CO_2 absorbent could be sourced (if it can). The PC work is not impactful as this is commercialized already; however, it is a great coproduct to increase value from the biomass.

PI RESPONSE TO REVIEWER COMMENTS

- We kindly thank the reviewers for their time and feedback on this project. We apologize for not covering team management due to time constraints, but we do have a very interactive and complementary team. Coproduct PC value and market size: The PC value and market (12,000 tonnes per year) used in the TEA was the value for whey protein, which has a much larger market ($6/kg; market size: 173,000 tonnes per year), so it is independent of PC as a coloring agent. Despite the disparity in cost and scale between fuel and PC, PC production is a great economic incentive for a pilot-scale facility or first-of-a-kind plant. However, the differentiator between AUDACity and commercial PC suppliers is that we have filed IP on a method to increase PC thermostability (100°C), which may greatly increase its food coloring market. Also, no PC cultivator is currently converting spent biomass to fuels. We have conducted an analysis with PC as the main product and fuel as the coproduct. We based the value and market size for PC on that for brilliant blue FCF (blue #1), which is ~5,000 tonnes per year, valued at $10/kg. PC largely scales linearly with biomass. Coproduct methyl laurate: There are typos in Slide 16. All fuel outputs should be in million GGE per year. AUDACity uses genetically modified strains that excrete laurate and/or methyl laurate into the cultivation medium during growth. Zero energy is required for methyl laurate extraction because it is a passive sedimentation and coalescence process. Once the biomass is harvested and high-value products are removed, residual biomass can be converted to fuels using HTL. Methyl laurate production is higher than that of HTL-generated fuels. Methacrylate polymer toxicity and strain adaptation: We initially were unsure of why the methacrylate polymers were toxic, so adaptive laboratory evolution was used to select for strains that grew well in their presence. Sequencing and continued growth without the polymer (followed by polymer exposure) are being performed to distinguish between stable genetic changes or a transient adaptation. Strains selected by adaptive laboratory evolution may have enhanced tolerance to quaternary ammonium compounds, which will benefit cell performance with all DAC polymers. Subsequent nuclear magnetic resonance analysis indicated that the polymers degraded under alkaline conditions due to Hofmann elimination and hydrolysis, which may release toxic oligomers into the medium. Suitability for AUDACity in brackish water or seawater: Cyanobacteria can be acclimated to grow well in brackish water or seawater. While our CO_2 capture principles rely on ions on the sorbent, which could exchange with inactive anions in high-salt medium, coatings or polymer materials that repel water and salt can be used to minimize ion exchange during brief (10–40-minute) exposures to the cultivation medium during CO_2 delivery, where CO_2(g) and H_2O(g) can still exchange during capture and release. Achieving goals with remaining time: The team continues to evaluate the top-performing sorbents for cultivation at the scale of 1 g CO_2/day and is gearing up for an outdoor cultivation trial (Aug.–Sept. 2023) at the scale of 100 g CO_2/day. We will apply for a no-cost extension to perform a second cultivation trial.

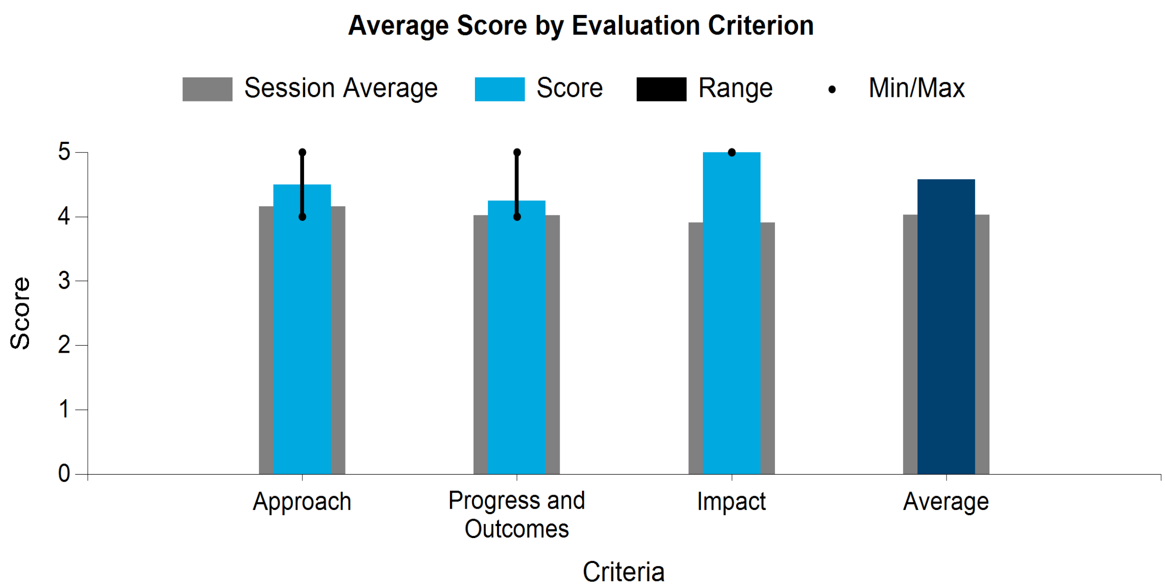
BIOMOLECULAR FILMS FOR DIRECT AIR CAPTURE OF CO_2

University of California, San Diego

PROJECT DESCRIPTION

WBS:	1.3.4.004
Presenter(s):	Michael Guarnieri
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,950,000

CO_2 delivery costs represent approximately 20% of the final biomass selling price in algal mass cultivation systems. Technologies that enable DAC of atmospheric CO_2 to decouple algae cultivation from CO_2 point sources thus present an opportunity to improve the economics and resource potential of algal biomass. Current DAC technologies typically employ amine- or caustic-based absorption, demanding significant water and/or energy inputs and incurring substantial capital expenditures. Conversely, bio-based approaches to DAC offer a means to bypass conventional techno-economic and sustainability hurdles. To this end, we propose to integrate recent advances in computational metabolic modeling, algal genetic engineering, algal cultivation, and algal biomass upgrading to enable secretion of CA for enhanced CO_2 capture and conversion in immobilized algal biofilms. Key challenges include genetic engineering of non-model microalgae for CA secretion and sustained, high biomass productivity in an immobilized biofilm. If successful, the resultant technology will present a first-in-class, no capital expenditure, renewable, bio-based approach to DAC and will ultimately increase the delivery and utilization of CO_2 by >20% relative to the current SOT. To date, we have achieved >50-g/m^2/day areal productivity from atmospheric CO_2, exceeding end-project goals and establishing a first-in-class, high-efficiency algal production system.



COMMENTS

- The approach using metabolic modeling to identify which proteins to target for redesign is good. *In silico* modeling is important.
- Densitometry is not a good quantitative measurement; it's better to use ELISA or an activity assay. The milestones are clearly identified and appropriate.

- Model first, then get data to validate the model. Task 6 should be earlier.
- Good job on the CA expression; the authors have a nice cassette system that is working well. I would have liked to see some molecular modeling to explain the decision of which CA to express and how to benchmark it against the bovine version they started with.
- There is no mention of risk mitigation strategies or whether they had to be deployed to stay on track. There was no mention of communication management.
- There is a clear connection to outcomes, particularly with polymer products and the DAC improvements and their financial impact.
- I wish the pond outcomes were more linearly scalable, but this is a known issue of transitioning to pond culture.
- What are you using for contamination control?
- A sensitivity analysis in the TEA to define the cost difference due to outdoor cultivation permitting processes would have been helpful to understand the applicability to other projects.
- Recent go/no-go review strongly indicates progress is being made against goals. Efforts are in line with stated goals and are showing progress. The project is early but has made commendable progress. Several positive results in different project areas show that the team is working well together across geographies.
- Approach: This project combines specific expertise and complementary knowledge and capabilities from several companies and institutions to address a number of important questions and objectives regarding algal biofuel production and DAC of CO_2. The activities of the different labs and companies seem to be well coordinated, and the interactions between the labs appear to be robust and productive. The TEA indicates that the team is on the right track to lower fuel production costs significantly via this approach, which is a key BETO goal.
- Progress and Outcomes: The metabolic model that was generated for *Picochlorum* has provided useful information on the presence of various biochemical pathways, and has also identified specific signal peptides that target native proteins to various locations in the cell, including extracellular secretion. This information will inform not only construct engineering for CA secretion, an immediate goal of this project, but also future metabolic engineering approaches for enhanced growth and product formation.
- Use of a common yeast expression system allowed rapid production and testing of numerous CAs from various sources under typical growth conditions associated with algal cultivation. This provided a shortcut for selecting and designing a heterologous gene for expression in *Picochlorum*. The summary slide indicates that the NREL researchers successfully engineered *Picochlorum* to secrete CA, but data were only presented for GFP secretion, so perhaps the CA expression results were still considered too preliminary to present.
- The team demonstrated an impressive increase in productivity in the RAB system when CA was added. This is an important outcome, assuming that the amount added was similar to what can reasonably be achieved via secretion of a heterologously expressed CA by an algal production strain. The activity and stability of the secreted CA in an open system will be critical information to understand, which will help to define the proper expression level needed (i.e., high enough for maximal ambient CO_2 use efficiency, but not so high that overall cell growth potential is limited).

- Finally, algal biomass from the RAB system was shown by Algix in preliminary testing to have promise as a feedstock for plastic composite production. Such coproduct formation will be important to lower the overall costs associated with algal biofuel production.
- Impact: The project team is making very good progress on enhancing atmospheric CO_2 update by algae in a commercially relevant production system. Successful completion of the project will advance the field and help BETO meet their current goals.
- Approach: Missing risk identification and mitigation. Are there any collaborations? Outcomes: Seem to be on or exceeding targets. The work on product quality is important, and increases impact. Impact: Seems relevant and impactful.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their time and constructive feedback. We agree with the reviewers' assessment that metabolic modeling presents a powerful approach to identify rational strain and protein engineering targets, and we will continue to refine and validate our models in the year ahead. Regarding protein quantitation, we agree that densitometric analyses are insufficient; we have completed activity assays and complementary mass spectral analyses in Budget Period 2 to quantify secreted protein concentration more accurately. Regarding CA downselection, we designed over 20 CA variants; top candidates demonstrating activity in seawater were transformed into a *Pichia pastoris* expression and secretion system to rapidly assess eukaryotic secretion capacity, followed by activity assays of culture supernatants. CA variants that retained activity in media and displayed active secretion capacity in *P. pastoris* were then incorporated into *P. renovo*. Growth assays under limiting CO_2 and CA activity assays on cell lysates served as a final downselection metric. Predictive modeling of protein secretion networks is currently being leveraged to further enhance the secretion capacity of three top-candidate variants. Regarding contamination control, this is outside the scope of the current proposal. However, we note that we have achieved biofilms comprising >90% of our target cultivar (as assessed via quantitative phylogenomic sequence analyses) over the course of >3-month cultivation trials. We hypothesize that this is, in part, due to the unique capacity of our engineered *P. renovo* to sequester and grow on atmospheric CO_2. Per the reviewers' suggestion, TEAs will evaluate additional costs associated with TERA permitting in outdoor cultivation configurations. As indicated by reviewers, all milestones and deliverables are on track for Budget Period 3. We have made substantial progress to date, including achieving >40-g/m^2/day productivity in RAB systems on atmospheric CO_2 (exceeding go/no-go target metrics). Initial efforts in Budget Period 3 have already indicated that our CA-secreting variants of *P. renovo* display a growth enhancement on RAB systems on atmospheric CO_2 relative to wild-type cultivars, indicating that we are achieving effective CA enzyme concentrations. Efforts moving forward will assess model-informed, secretion-optimized CA variants; fabrication of thermoplastic composites derived from RAB biomass; and assessment of protein fraction suitability for plasticization. These wet lab efforts will be complemented by refined TEAs/LCAs defining key cost and sustainability drivers en route to commercialization.

MICROALGAE COMMODITIES PRODUCTION WITH A DIRECT AIR CAPTURE PROCESS

MicroBio Engineering Inc.

PROJECT DESCRIPTION

WBS:	1.3.4.006
Presenter(s):	John Benemann
Project Start Date:	10/01/2020
Planned Project End Date:	12/31/2023
Total Funding:	$2,528,795

Purpose: The technology to be advanced in this project is the utilization of CO_2 from air to cultivate microalgae and produce biomass for higher-value nutritional products in the near term, and commodities including feeds, biofertilizers, bioplastics, and fuels in the longer term.

Relevance and Impacts: The two approaches to accomplish this objective are:

1. DAC by a physical-chemical process provided by GT that delivers a near-100% concentrated CO_2 stream to the algal cultures. The GT-DAC process could become commercial at the Cyanotech facility in the near term.

2. The use of the algal cultures and cultivation systems themselves to provide CO_2 absorption from air at a rate supporting production targets.

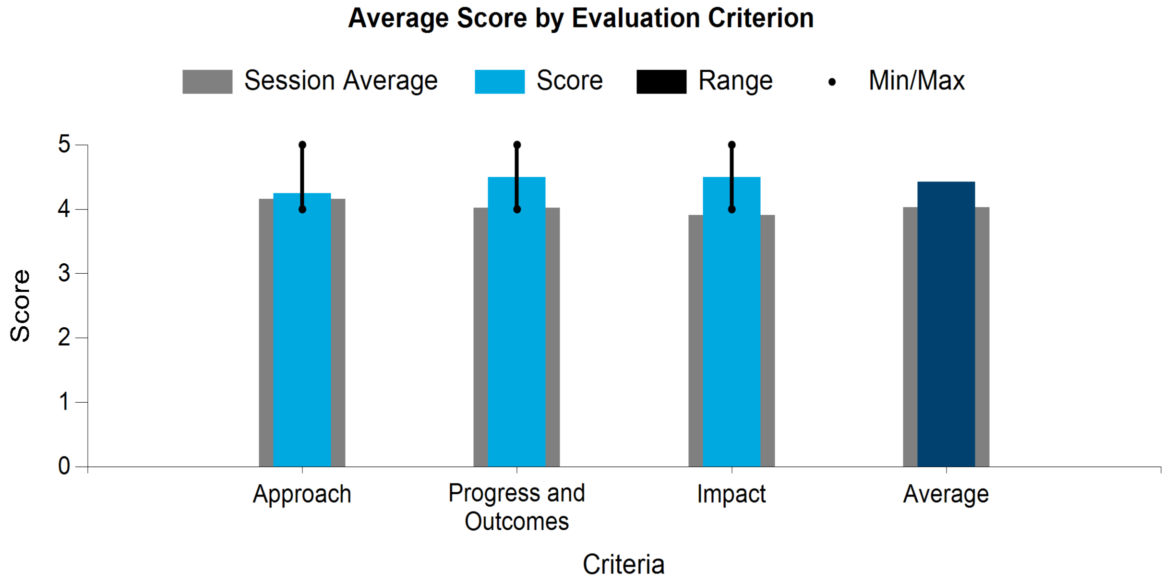
Challenges:

1. GT-DAC: Achieving similar productivities in raceway ponds with air CO_2, supplied by the GT-DAC process as with merchant CO_2, over several months of sustained cultivation.

2. For cultivation of algae directly on air CO_2: Achieving productivities in raceway ponds of >50% compared with use of enriched CO_2.

Outcomes and Technical Accomplishments:

- Completed design for GT-DAC pilot to provide 1–2 kg of air CO_2 per hour. Fabrication underway.
- Outdoor productivity met targets for commercial production of a high-value, whole-cell product.
- Validated an assay to identify presence/absence and relative levels of CA.
- TEA/LCA validated cost savings and reductions in GHG emissions by integrating DAC.



COMMENTS

- I love the graphics explanation of the approach demonstrating who is responsible for what portion of the work. Slide 9 showed a clear connection between the work and the department goals. The management Slide 17 with risks and Slide 18 with the schedule are particularly helpful for evaluation. Although pond depth will add storage capacity, what is the trade-off in productivity, as the lower levels of the pond won't be as well illuminated as the top layers?

- The progress is impressive; it will be interesting to see how it scales with Cyanotech. The impact is clearly identified and quantitative throughout. Graph legends would help to define the meanings of different colors, if these are different batches, different strains, or different conditions. Densitometry isn't a great way to do quantitation—an enzymatic activity assay would be much better. Optimization of pond depth for carbon sink function versus mixing and photosynthetically active algae will need to be done for the approach to be implemented.

- The project is early, awaiting equipment. Progress is being made consistent to the goals.

- Approach: The combined project team has well-established expertise and existing infrastructure in all the critical areas needed to conduct the research included in this project. Several approaches are being taken by the project team to enhance the prospects for using DAC for supply of CO_2 to algal mass cultures. The goals of the project are well aligned with the BETO goals of reducing cultivation costs in order to lower the cost of biofuel production. Pulling all the disparate parts of this project together in a cohesive and maximally informative manner will require significant communication, coordination of efforts, and appropriate timing of activities between the various teams.

- Progress and Outcomes: The carbon flux modeling provides good guidance on how to optimize carbon use efficiency under different cultivation conditions, which was used to shape parameters for supply of CO_2 via DAC.

- Cyanotech provided several eukaryotic algal strains (presumably that were isolated from their high-alkalinity ponds) to PNNL for alkalinity screening, medium development, and growth under various conditions, including outdoor pond evaluations. One of these strains (*Graesiella* CT3072, a member of the Chlorellaceae family) achieved the project's baseline productivity and had a carbon use efficiency >75%; this strain has been prioritized for further evaluation.

- The investigators also conducted research expanding earlier work on increasing CO_2 availability to algae by the addition of CA to cultures. Development of assays to measure the relative levels of exogenous CA in cultures and the CO_2 flux enhancement *in vitro* (without cells present) were reported, but data on the outcomes were not presented in any detail. Also, it was unclear which strain(s) will be looked at that may naturally secrete CA; see Slide 32. If it is the wall-less *Chlamydomonas* strain in the referenced paper, then the project team should bear in mind that this strain will likely have a difficult time surviving under outdoor cultivation conditions. Proof-of-concept lab studies with this strain may not translate well to outdoor conditions.

- A DAC skid is being manufactured by GT for delivery this summer to Cyanotech for testing with their ponds. The results from these studies will be interesting when the system becomes operable.

- Preliminary TEA modeling results suggest that in locations that are reliant on high-cost CO_2, the use of DAC can lead to a major reduction in biomass production costs. To put this in context, however, the project team needs to indicate what the existing baseline CO_2 cost used in the model was so that the results can be translated to locations where CO_2 is less expensive. It also doesn't look like capital costs (depreciation) or additional power for the GT-DAC system were added to the DAC model; this should be reconciled or explained.

- Impact: If the goals of this project are accomplished, it will provide useful data for determining the utility and practicality of the GT-DAC system. When combined with the additional topics covered (e.g., CA addition, use of high-alkalinity strains), the project results will provide relevant information about whether these combined strategies can reduce the cost of algal biofuel production by meaningful amounts.

- Approach: Project management was not discussed, but the project approach and methodology are good. Progress: The project is going well, as per the presentation; it looks like the carbon unit is not ready on time. Impact: The project will have an impact in expanding algae growth areas if successful; so far, results are not impactful, as they are not demonstrated at scale or with DAC technology.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: I love the graphics explanation of the approach demonstrating who is responsible for what portion of the work. Slide 9 showed the clear connection between the work and the department goals. The management Slide 17 with risks and Slide 18 with the schedule are particularly helpful for evaluation. Although pond depth will add storage capacity, what is the trade-off in productivity, as the lower levels of the pond won't be as well illuminated as the top layers? The progress is impressive; it will be interesting to see how it scales with Cyanotech. The impact is clearly identified and quantitative throughout. Graph legends would help to define the meanings of different colors, if these are different batches, different strains, or different conditions. Densitometry isn't a great way to do quantitation—an enzymatic activity assay would be much better. Optimization of pond depth for carbon sink function versus mixing and photosynthetically active algae will need to be done for the approach to be implemented. RESPONSE: We thank the reviewer for their helpful comments. Regarding the question, "what is the trade-off in productivity, as the lower levels of the pond won't be as well illuminated as the top layers," we point to McGowen et al. 2023 (https://doi.org/10.1016/j.algal.2023.102995), who found no statistical difference in average harvest yield productivity in ponds operated at 10-cm versus 20-cm depth over two cultivation campaigns with *M. minutum* 26BAM in 2019 and 2020. Surely there are other literature studies pointing to the opposite conclusion, and others in the literature that argue that depth primarily impacts biomass productivity via differences in diel pond water temperature (i.e., larger daily temperature extremes in the shallower pond). Productivity trade-offs at different depths is a complicated question, and one that our carbon utilization model does not yet account for. However, from a fundamental photosynthesis perspective, there would be no difference in productivity for different depths, as algae density per unit area is not affected. In regard to the CA densitometry assay, we agree that results here have so far been inconclusive but see value in confirmation of the presence or absence of CA that enzymatic activity assays alone may not provide. We feel that multiple analytical approaches will be needed to conclusively attribute any increase in air-CO_2 flux to CA. Given the inconclusive protonography results thus far, we are moving to a Western blots assay to verify CA presence and are validating a dansylamide fluorescence CA assay previously demonstrated on complex matrices (Mustaffa 2017; https://doi.org/10.1002%2Flom3.10182). We agree that there are many optimization variables, in particular alkalinity, and anticipate that the Cyanotech field trials, PNNL lab screening, and MicroBio Engineering TEA/LCA will make progress in identifying cost/productivity/carbon use efficiency/GHG trade-offs.

- Comments: The project is early, awaiting equipment. Progress is being made consistent to the goals. RESPONSE: We thank the reviewer for their assessment.

- Comments: Approach: The combined project team has well-established expertise and existing infrastructure in all the critical areas needed to conduct the research included in this project. Several approaches are being taken by the project team to enhance the prospects for using DAC for supply of CO_2 to algal mass cultures. The goals of the project are well aligned with BETO goals of reducing cultivation costs in order to lower the cost of biofuel production. Pulling all the disparate parts of this project together in a cohesive and maximally informative manner will require significant communication, coordination of efforts, and appropriate timing of activities between the various teams. Progress and Outcomes: The carbon flux modeling provides good guidance on how to optimize carbon use efficiency under different cultivation conditions, which was used to shape parameters for supply of CO_2 via DAC. Cyanotech provided several eukaryotic algal strains (presumably that were isolated from their high-alkalinity ponds) to PNNL for alkalinity screening, medium development, and growth under various conditions, including outdoor pond evaluations. One of these strains (*Graesiella* CT3072, a member of the Chlorellaceae family) achieved the project's baseline productivity and had a carbon use efficiency >75%; this strain has been prioritized for further evaluation. The investigators also conducted research expanding earlier work on increasing CO_2 availability to algae by the addition of CA to cultures. Development of assays to measure the relative levels of exogenous CA in cultures and the CO_2 flux enhancement *in vitro* (without cells present) were reported, but data on the outcomes were not presented in any detail. Also, it was unclear which strain(s) will be looked at that may naturally secrete CA; see Slide 32. If it is the wall-less *Chlamydomonas* strain in the referenced paper, then the project team should bear in mind that this strain will likely have a difficult time surviving under outdoor cultivation conditions. Proof-of-concept lab studies with this strain may not translate well to outdoor conditions. A DAC skid is being manufactured by GT for delivery this summer to Cyanotech for testing with their ponds. The results from these studies will be interesting when the system becomes operable. Preliminary TEA modeling results suggest that in locations that are reliant on high-cost CO_2, the use of DAC can lead to a major reduction in biomass production costs. To put this in context, however, the project team needs to indicate what the existing baseline CO_2 cost used in the model was so that the results can be translated to locations where CO_2 is less expensive. It also doesn't look like capital costs (depreciation) or additional power for the GT-DAC system were added to the DAC model; this should be reconciled or explained. Impact: If the goals of this project are accomplished, it will provide useful data for determining the utility and practicality of the GT-DAC system. When combined with the additional topics covered (e.g., CA addition, use of high-alkalinity strains), the project results will provide relevant information about whether these combined strategies can reduce the cost of algal biofuel production by meaningful amounts. RESPONSE: The project scope, involving CA produced and released into the culture media, is explorative in nature. The walled and cell-wall-deficient *Chlamydomonas* strains are our first targets, chosen as likely to be positive (wall-deficient strain, excreting periplasmic CA into the media; Kimpel et al. 1983 https://doi.org/10.1093/pcp/24.2.255; Coleman et al. 1984 https://doi.org/10.1104/pp.76.2.472; Ynalvez et al. 2008 https://doi.org/10.1111/j.1399-3054.2007.01043.x) and negative (walled strain, minimal CA released into the media) controls to demonstrate proof of concept and assay validity. The assay would then be applied to strains previously characterized by the MicroBio Engineering teams to perform well under the alkaline conditions required for air-CO_2 ingassing to take place, as well as more immediate commercial viability. These include strains identified in the present and previous (MicroBio Engineering, PNNL, and Qualitas Health) DOE-supported project, and include *Chlorella* (potential initially for a nutraceutical market), SSL1 (relatively productive at high pH), or *Porphyridium* (polysaccharides, pigments). The baseline cost for CO_2 at this site is quite high, severalfold higher than that on the mainland, and supply interruptions have taken place, further increasing the value of a DAC process at this site. Thus, this is a very promising site for deploying a DAC unit. However, it must be recognized that DAC technology is still at an early stage of development, and that actual capital and operating costs (and energy consumption) are not yet well established. This project will provide important information on these topics that will be incorporated in the final report. As stated by the reviewer, the in-pond DAC and GT-DAC technologies could reduce the cost of algae production and expand algal biomass resource potential.

- Comments: Approach: Project management was not discussed, but the project approach and methodology are good. Progress: The project is going well, as per the presentation; it looks like the carbon unit will not be ready on time. Impact: The project will have an impact in expanding algae growth areas if successful; so far, results are not impactful, as they have not been demonstrated at scale or with DAC technology. MBE RESPONSE: We agree that deployment and demonstration of the DAC unit will be impactful, particularly when integrated with the cultivation scale and experience at Cyanotech.

ACCESS CARBON – ALKALINE CARBON CAPTURE AND EXPRESSION-STREAMLINED SPIRULINA CULTIVATED IN AIR FOR RELIABLE BIOPRODUCTS, OIL, AND NUTRITION

Lumen Bioscience Inc.

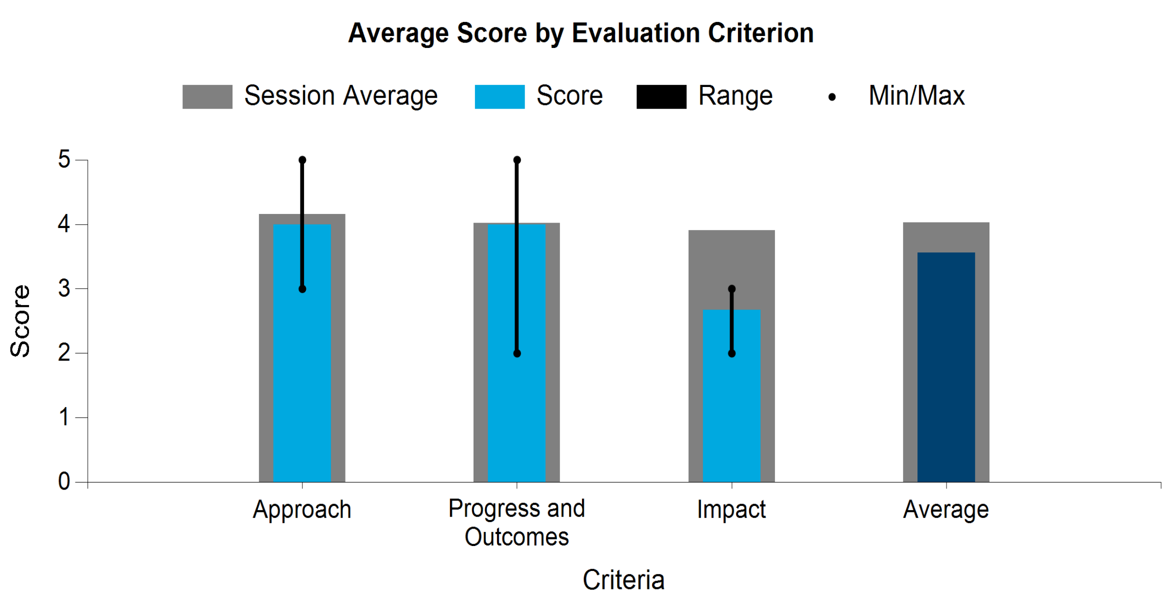
PROJECT DESCRIPTION

WBS:	1.3.4.008
Presenter(s):	Mark Heinnickel
Project Start Date:	10/01/2020
Planned Project End Date:	06/30/2023
Total Funding:	$2,500,000

Lumen Bioscience has developed a novel current good manufacturing practice (cGMP) biomanufacturing platform that enormously decreases the cost of developing and manufacturing new biologic drugs for certain illnesses. The platform builds on recently discovered methods that enable the bioengineering of the commercially important cyanobacterium *Arthrospira platensis*, also known as the common food algae spirulina.

We advanced the platform by developing strains to demonstrate the effectiveness of spirulina for mucosal delivery of protein biotherapeutics, including demonstrating intranasal administration of a spirulina-manufactured neutralizing antibody that can prevent disease by a respiratory virus SARS-CoV-2 in a hamster model. We describe production of this strain in photosynthetic culture using DAC of atmospheric carbon in alkaline pH. Optimal pH and alkalinity values were determined through machine learning. Conveniently, the modified media significantly increases (>100%) molecules convertible into biofuels (especially carbohydrates). Lumen also used a statistical design of experiments approach to increase therapeutic production (59%) with minimal replicates, significantly improving the economics of optimization.

LCAs were carried out with NREL to show that these adaptations lowered the carbon footprint of therapeutic production. In addition, computational flow dynamics are being employed to construct models that can lower this value in outdoor settings.



COMMENTS

- Making therapies from spirulina is a really interesting approach going for the maximum value type of products. This is a really compelling story because the value is so high. The missing part is fuel. The environmental drivers presented were a bit vague, quoting all U.S. health care, not the impact of the pharma industry. There are many reports detailing the impacts of the pharma industry. The data are available. I suspect the algae routes will be quite positive in an industry where the emissions are high. I think it will be a good story, it just needs to be told. The tie to DOE emissions and/or fuel goals is the only thing I found wanting. Really well presented, aligned with the project goals, and clearly showing progress.

- Approach: The project team is looking at ways to produce therapeutic proteins (monoclonal antibodies) in cyanobacteria (*Arthrospira*) at lower cost when compared to standard cell culture methods for monoclonal antibody production, and that have a lower GHG footprint relative to those current methods. Residual biomass would be available for conversion to biofuel products.

- Progress and Outcomes: The team reported that they had found conditions that resulted in a 59% increase in protein expression, but no information was provided on what those conditions were (Cultivation changes? Expression induction method? Changes to constructs?) or even what protein was being expressed. This makes it hard to assess the relevance of the outcome to BETO goals and the field in general.

- It would have been helpful to know what type of carbohydrate was elevated in the phosphate limitation experiments (e.g., glycogen versus small soluble carbohydrate versus cell wall carbohydrate); this can determine whether the increased carbohydrate content was relevant for fuel production from residual biomass.

- On Slide 14, the authors indicate that raising the pH of *Arthrospira* cultivation led to a large increase in CO_2 use efficiency. This is an expected result because of the higher capacity for carbon absorption into the higher-pH medium. *Arthrospira* is well known to be an alkaliphilic strain, so commercial production always occurs at high pH. Because no information was provided on the actual pH used, it is not clear whether the project team did anything different in their approach than what has been done in the spirulina industry for several decades.

- It is not appropriate to make side-by-side comparisons of carbon footprints for conventional monoclonal antibody production versus *Arthrospira*-produced monoclonal antibodies if boundary conditions for the analyses are not the same. The referenced paper for conventional monoclonal antibody production includes CO_2 emissions associated with the manufacture of steel fermenters and plastic bioreactors (and associated waste management, among other things), whereas this report appears to consider mainly CO_2 emissions associated with operating costs. In other words, to truly compare carbon footprints, the project team would also need to include CO_2 emissions associated with PBR manufacturing, all processing steps, etc. More clarity on the specific boundaries used in the reported LCA would be needed to make a true comparison possible.

- Impact: The amount of residual biomass from monoclonal antibody production would be very low relative to the biomass volumes necessary for meaningful fuel or commodity chemical production. As a consequence, although the research conducted in this project may very well have significant ramifications for the pharmaceutical industry, it’s not clear that the work will have a significant impact on technology development for large-scale algal-based fuel and/or commodity chemical manufacturing. Having said this, it is recognized that the successful commercial use of cyanobacteria to produce therapeutic proteins could boost interest in algae for other beneficial purposes, including fuels and related products.

- Approach: Good planning and good collaboration, clear management plan for the project, and risks and mitigations have been identified. Outcomes: The project is on target and on time, and the results exceed expectations/predictions/goals. Impact: It is not clear how this information will be shared and will drive the industry forward. Are publications planned? This is not a large enough industry for this research to have a large impact on carbon emissions or advance large-scale production of biomass for energy.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the time they took with our presentation and their feedback. Some of the comments focused on the broad applicability of the work presented. We view this work not only as a means to improve photosynthetic therapeutic production but also as a proof of concept that sets the stage for biomass, protein optimization, and increased carbon utilization efficiency, all of which extend beyond the Lumen algae systems and applications. These parameters are identified as critical components for the success of future algae biorefineries. While our volumes for COVID therapeutics would be small, the technology can be applied to protein products that apply to larger markets. If this occurs, it could have a more significant impact on the biofuel industry. Beyond publications (planned and in preparation), this project will have optimized toolkits whose applicability extends further than pharmaceutical production. These toolkits will be publicized in peer-reviewed publications and patents and could lead to further collaborations with commercial partners (e.g., the carbon utilization improvements can have impact across the value chain). The reviewers also highlighted the lack of experimental details underpinning some of the presented improvements. We are unfortunately constrained by disclosure limits in information that is deemed business-sensitive; we do plan to disseminate the methodologies applied in the public domain. The major accomplishments of this work revolve around the improved production of VHHs (Slide 4) and biofuel intermediates (carbohydrates) by *Arthrospira* in DAC conditions. The protein expression was increased by 59%; however, details of the conditions and protein identity are commercially sensitive and cannot be disclosed publicly. The carbohydrates (which also increased significantly) that were produced in this experiment were mainly glycogen, which can be fermented to ethanol. NREL confirmed that the glycogen content increased specifically by measuring the monosaccharide composition of the carbohydrate fraction as fucose, rhamnose, glucosamine, galactose, mannose, xylose, ribose, and glucose, and observed a significant increase in glucose content at the expense of a reduced contribution of the other monosaccharides. The DAC conditions were achieved by altering our standard media. Lumen's standard growth conditions are similar to those used in commercial spirulina production. As part of this work, Lumen raised the pH significantly above standard outdoor cultivation pH values. Details of the conditions are commercially sensitive and cannot be disclosed publicly. However, the methodology behind this optimization (machine learning and computational fluid dynamics) will be the subject of several forthcoming peer-reviewed publications. A last point was raised on the boundaries of the LCA of this project. This work was carried out at NREL and used standard emissions-burden approaches that have been well documented across BETO projects. The LCA showed that Lumen and NREL's technology could produce VHHs for a much smaller carbon cost in our facility. The inclusion of the facility footprint in the LCA, when amortized across decades of operating life, contributes minimally to the product GHG. This is particularly true for biorefineries like Lumen's that are similar to conventional chemical plants. For this reason, we believe the boundaries selected for this project are appropriate. While decades of DOE-funded research allow us to understand the emissions profile of our process quite clearly, as with many high-value specialty products, the LCA data on most pharmaceuticals are quite sparse. For this reason, a comparison of all of our projects to their companion products in the pharmaceutical industry remains challenging.

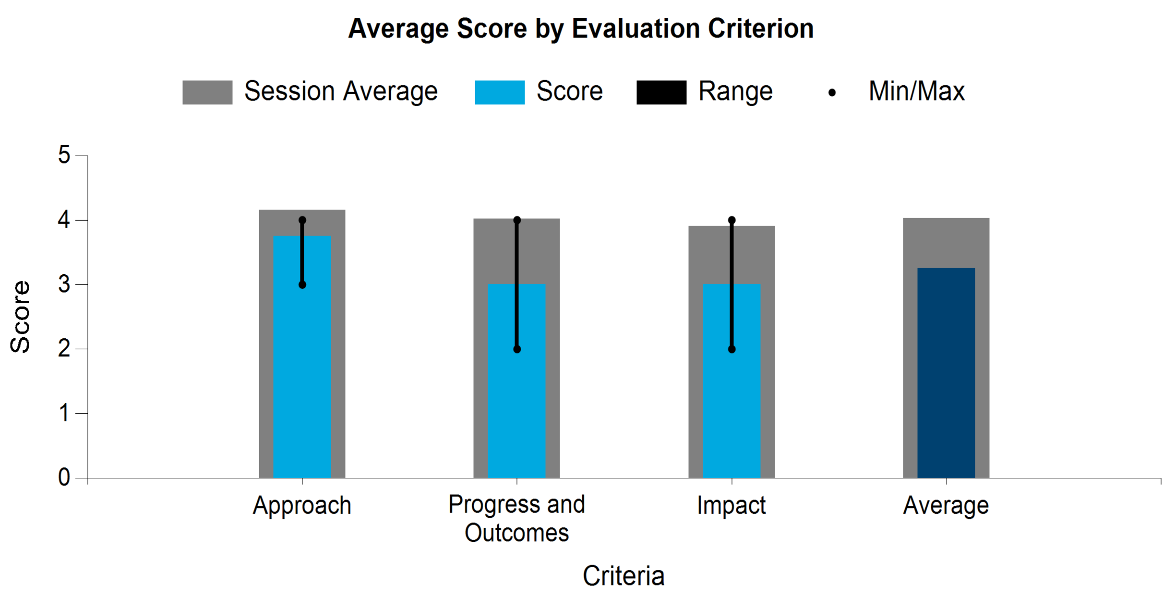
DEVELOPMENT OF HIGH-VALUE BIOPRODUCTS AND ENHANCEMENT OF DIRECT AIR CAPTURE EFFICIENCY WITH A MARINE ALGAE BIOFUEL PRODUCTION SYSTEM

Duke University

PROJECT DESCRIPTION

WBS:	1.3.4.010
Presenter(s):	Zackary Johnson
Project Start Date:	10/01/2020
Planned Project End Date:	12/31/2023
Total Funding:	$2,513,524

DOE FOA DE-FOA-0002203 Topic 3 has three major objectives: (1) increasing the revenue of the algae biomass while ensuring that the fuel specifications are met, (2) increasing productivity over baseline levels while using carbon supplied by DAC, and (3) increasing the percentage of carbon supplied by DAC while still reducing the costs associated with supplying CO_2. Our project's overarching goals are to (1) enhance the growth and productivity of marine microalgae through cultivation system design and operation improvements, (2) increase the market value of post-fuel algae biomass residuals by assessing alternative high-value products (i.e., collagen, whey protein substitute, and eicosapentaenoic acid/docosahexaenoic acid), and (3) demonstrate DAC as a source of CO_2 for algae cultivation. Although only approximately 1 year into the 3-year project, here we show substantial progress toward each of these goals, including development of a quantitative algae production model, screening of top biofuel candidate marine algae, and piloting of a novel DAC approach. Our project is on track with respect to its milestones, and our team continues to make substantial progress in marine microalgae commercialization.



COMMENTS

- An energy balance on the AHX module would have been helpful.

- Dewatering and further purification steps (HTL?) and other downstream operations are not included in the TEA/LCA, although they are not trivial in impact. The TEA should include throughput assumptions and wintertime mitigation strategies, particularly with respect to siting.
- There was no DEI approach included.
- The project appears to be doing interesting science largely unrelated to the goals. Reports on actual yields to high-value products, a centerpiece of the agreed efforts, appear completely lacking. The DAC component really has nothing to do with algae. Partners are developing a machine for air capture that will produce an enriched CO_2 stream, quoted to be at about 20% enrichment. The machine doesn't require algae, and integration, from what was presented, is nonexistent. It is a DAC machine capable of supplying any user of dilute CO_2, next to an algae facility capable of accepting any enriched CO_2.
- The description of why the DAC is advantaged failed to be convincing. The slides fail to paint a compelling case on where an advantage derives from and compared with what.
- Further, the discussion of bicarbonate was confusing, even when explicit questions were asked about it. The presentation certainly does not amplify the benefits of bicarbonate for storage.
- Product values appear exceptionally high, creating favorable TEA calculations. This is, of course, to be expected. Sensitivity to those product values is needed.
- Approach: The goals of this project—namely lowering the overall cost of biofuel production via a combination of increasing the coproduct value coupled to reducing CO_2 costs and availability through a DAC process—are fully aligned with the BETO goals related to algal biofuel production. The general approaches as stated are reasonable and similar to some other projects funded via this FOA. The management plan, including how the main collaborators interact, was not described. The role of the University of California, Santa Cruz, was not discussed.
- Progress and Outcomes: Fifteen strains, half of which were identified in the previous Marine Algae Industrialization Consortium (MAGIC) project and half of which were considered strains worthy of SOT status, were examined for high coproduct value potential. It was a bit confusing why collagen and whey (proteins) were included on this list, as collagen is known to be uniquely produced by animals and whey is a dairy (i.e., animal-produced) byproduct; these exact products simply cannot be expected to be made by naturally occurring algae. If the research team is looking for collagen or whey substitutes, they didn't indicate the desirable properties being screened for or how the screening is taking place. In any case, no substantive results were presented regarding coproduct development.
- The work presented on stocking density (inoculum level) and light field-related productivity was a large part of the presentation, but it was unclear what these somewhat narrowly focused studies had to do with the stated goals of the project involving coproducts, DIC control, or DAC-based CO_2 supply; this seems to be major disconnect. It was not disclosed what strains were analyzed and whether they produced high-value coproducts; if so, the impacts of growth mode on coproduct content were not mentioned. No results were presented on CO_2 use optimization or, in general, on CO_2 supply to cultures.
- Although behind schedule, information was presented on the MoleculeWorks AHX DAC module that will be tested outdoors at the Duke algal growth facility. If economical, this system has potential to provide CO_2 captured from the atmosphere to mass algal cultures, but since an operable system does not appear to be available yet, it is premature to assess the value of the system. The final TEA and LCA models will rely heavily on the costs and efficiency of the AHX-based system, and how the system integrates with algal cultivation.

- According to the quad chart, the project was scheduled for completion in December 2022, so a no-cost extension was apparently granted. It seems like there is still quite a bit of work to do to achieve the project objectives.
- Impact: If more progress is made on the various components of the project and they become better aligned and integrated, this project has potential to have a positive impact on the economics of algal biomass (and biofuel) production. It is not clear at this point whether the necessary progress will be made in the remaining time of the project, however.
- The publications listed in the supplemental slides don't seem to have much to do with this project.
- Approach: The overall approach is good, and risk mitigation is in place. The plan is reasonable. Feedback to other DOE portfolios is low, but there is collaboration within the group.
- Outcomes: It's very early on in the project, so strain screening is just initiating and outcomes are not completed yet. The work with DAC is very promising.
- Impact: Building on existing data increases the potential for higher impact, but it's too early to evaluate the impact of the overall project.

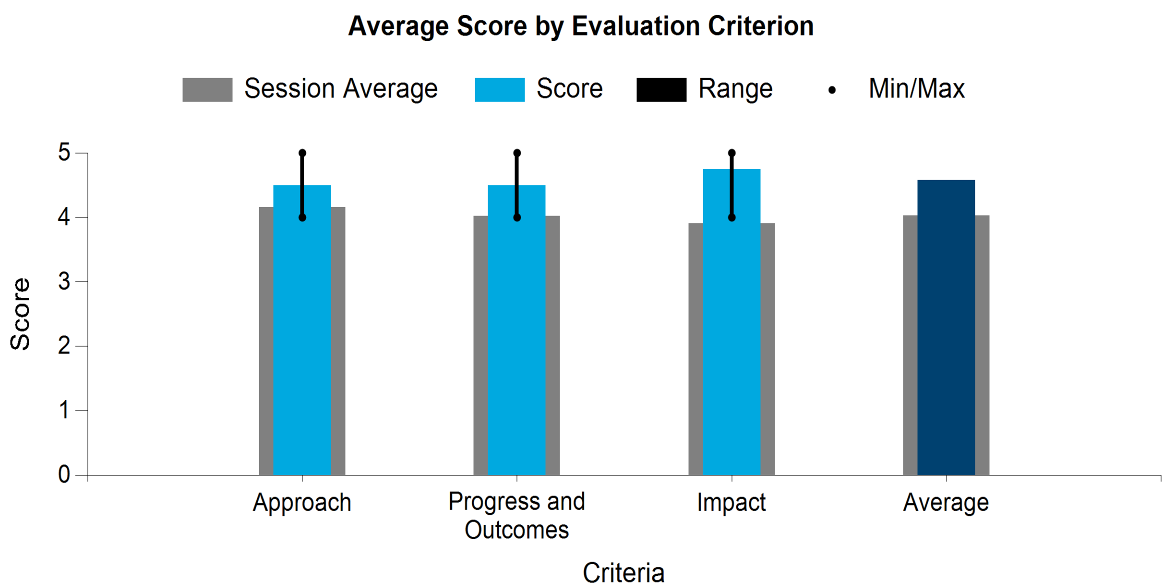
HTL DEVELOPMENT

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	1.3.4.102
Presenter(s):	Peter Valdez
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2022
Total Funding:	$1,575,000

The Hydrothermal Processing for Algal-Based Biofuels and Coproducts project is focused on developing advanced HTL methods to improve process efficiency and reduce capital and operating costs to produce carbon-negative biofuels and coproducts from algae. Cost-advantaged algal biomass is being investigated to enable cost-effective fuels and coproducts. Examples of cost-advantaged algae include residuals from algal-based products, algae used for remediation services such as wastewater treatment or pollution management, and harmful algal blooms collected and disposed in environmental services. Cost-advantaged sources, such as wastewater-grown algae, are available but underutilized (e.g., landfilled). New strategies are being developed to address high ash content, less energetic algal composition, and high-viscosity slurries. The project leverages experience with single-pass and sequential HTL to maximize the conversion of biomass. Coproducts such as extracted polysaccharides, fertilizer substitutes, and building materials are also being investigated. All data from these efforts directly support the algal HTL process model, economic and environmental impact models, and annual SOT reports. The SOT reports highlight key research and development targets to achieve DOE cost and production volume targets.



COMMENTS

- The collaboration slide and supplemental slides were very helpful to understand information sharing and project management. The DEI inclusion was also helpful. The success of the risk mitigation plan is great. Excellent job making the model and then iteratively validating it as more information came in. I also like the flexibility of using the available feedstocks and adjusting to seasonal changes, as this represents a more realistic scenario for different sites and weather patterns. This method is a critical unit operation for the feasibility of many biofuel projects and has broad applications. I would suggest looking into the anaerobic methods for material storage, as they are considerably less expensive than freezing; freezing will wreak havoc on your TEA. The Wendt lab in Idaho has done some work on this. Of course, the great interest of the moment is how to deal with sargassum nuisance blooms.

- This is that rare project trying to do something for everyone and with any feedstock. The analysis and work to date is impressive, showing more flexibility than I would have thought possible. That said, making a device capable of consuming anything and making products fit for established markets is an almost impossible task. The results obtained so far are commendable and in line with the description of the project goals.
- The DEI component is consistent with the established goals, but is more focused on outreach than aimed at increasing diversity. Reinforcing, they did what they said they would do.
- Approach: The project objectives and plans to achieve them are well described in the presentation. The project team members are well suited for the planned research, and the means that were established to communicate and collaborate are appropriate.
- An important objective that was not clearly stated would be to determine whether there really is a cost advantage to certain waste algal biomass sources relative to farmed algae. This would take into account the consistency of availability (impacting scale and uptime of processing facilities), feedstock stability, transportation costs, costs for making the biomass suitable for handling and HTL, etc. The assumption that waste biomass will be free (or at a negative cost), which is an important driver of the reduced costs, needs to be verified if the companies involved in water treatment, nuisance bloom harvesting, or other sources come to believe that there may be more value in the biomass than a straightforward savings on disposal fees. Different collection and transportation costs for a variety of scenarios should be examined in this regard.
- Developing methods to reduce ash content and improve the flowability of waste biomass is an important goal for this year. Identifying and verifying coproduct opportunities is also a worthwhile objective.
- Progress and Outcomes: Seven samples of low-cost algal biomass were acquired from collaborators; so far, one of these (algae from wastewater treatment) has been treated and processed via HTL with promising initial results. Even with the reduced yield, the TEA indicated a reduction in GGE cost to $2.61, which is near the BETO target. According to the related 2021 SOT, the costs associated with cultivation, harvesting, dewatering, and transportation of the wastewater-grown algae were not included when deriving this GGE cost, presumably because of counter savings by the treatment facilities for water treatment and sludge disposal. It will be important to determine the actual full total cost of the biomass when availability and processing requirements are better understood. Results from HTL of the other cost-advantaged biomass received will hopefully be conducted soon.
- Results of HTL using *Picochlorum* biomass (i.e., not a cost-advantaged algae as defined for this project) were reported, including a favorable comparison of the upgraded HTL oil properties with SAF requirements. Unless this information was included simply for future comparative purposes, it’s not clear why these studies were conducted (or at least reported) within this project. The HTL results will likely differ when processing waste algae biomass due to the differing chemical compositions and potentially variable heteroatom levels present prior to oil upgrading. It will be highly important to conduct such quality tests with actual biomass generated from wastewater treatment or other cost-advantaged biomass.
- Impact: The results of this project should shed light on whether algal biomass provided from waste sources (e.g., algae from wastewater treatment, harvested micro- and macroalgal blooms) can be collected, transported, and converted to fuels and coproducts in an economically viable manner.

- Information was not presented on the total volume of cost-advantaged algae feedstock that is expected to be available, which is important to know in order to assess the impact of the proposed technology. It is worth considering whether such low-cost algae could be coprocessed with farmed algae or stored and processed in farmed algae conversion processing plants during slow growth periods as opposed to making dedicated, distributed, lower-volume processing facilities.
- Approach: Safety considerations are industrially relevant and important; good work plan.
- Progress and Outcomes: On schedule with the project and good execution.
- Impact: Large impact from the work; it's good that it is agnostic to feed source.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful and constructive comments and questions. We will address key questions and areas that need further clarification. For storage topics, we have collaborated with Idaho National Laboratory to investigate the anaerobic storage of algae/wood blends prior to hydrothermal processing. Our published results (https://doi.org/10.1016/j.algal.2021.102622) of an algae/wood feedstock show that there is minimal impact to the quality of fuel products after 123 days of storage. Freezing algae samples is generally used to preserve experimental feedstocks for lab-scale processing. Current investigations in this project and other HTL projects at PNNL (3.4.2.301 and 2.2.2.302) are planned to assess the viability of any potential feedstock for HTL. When pilot- and commercial-scale operations commence, it will be the decision of the process operator to define a strategy for selecting a specific operating envelope for feedstocks and products. The objectives of the project are to produce experimental results to enable a broad selection for both feedstocks and products. We acknowledge that our estimates for feedstock costs and availability are still speculative. The current objectives of this project are to examine the technical feasibility and development of cost-advantaged algal feedstocks. We will work with the partners that provide the algal feedstocks and the project team leading the analysis work (1.3.5.202) to investigate current assumptions for cost and availability and determine the realistic potential of each feedstock. HTL of farmed monocultures of algal feedstocks to produce SAF was a previous objective examined during the project. It was included to demonstrate the national-scale potential for producing SAF from farm-cultivated microalgae and will be used in the future for comparative analyses against new results. The project team is focusing on outreach at K–12 programs as the first step in increasing diversity in STEM careers. The team will continue to think creatively to develop effective methods to improve DEI at PNNL and within STEM fields in general.

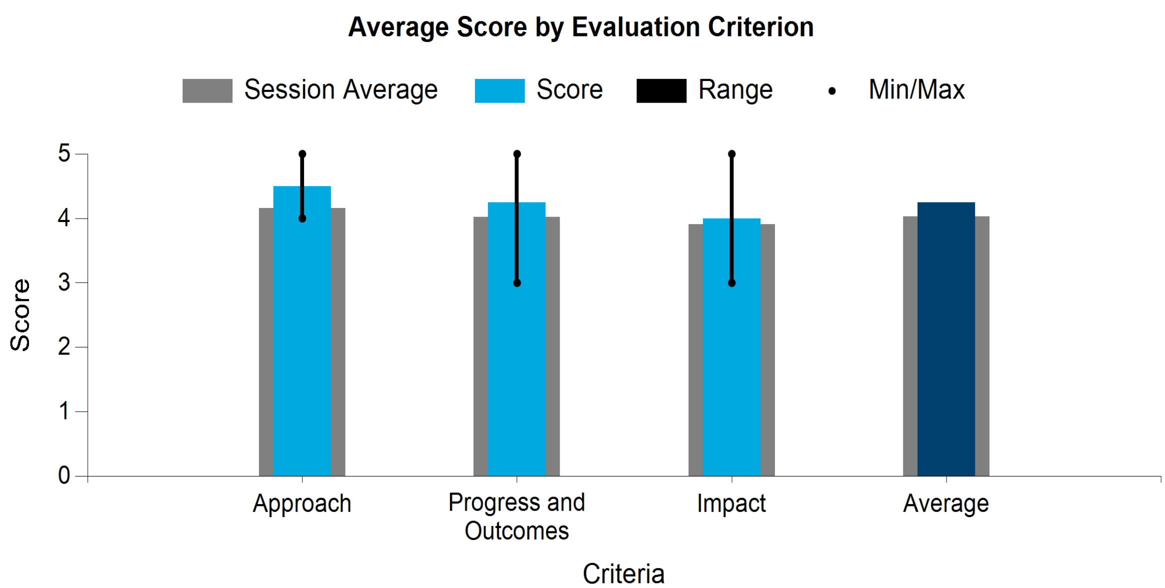
COMBINED ALGAL PROCESSING FOR THE SYNTHESIS OF LIQUID OLEOFUELS AND PRODUCTS (CAPSLOC)

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	1.3.4.204
Presenter(s):	Tao Dong
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,100,000

CAPSLOC aims to develop a biorefinery concept that is composition-agnostic and enables economically, environmentally, and socially viable biofuel production by maximizing the value from each fraction. To achieve this, we have employed an iterative approach between R&D and TEA/LCA to establish process targets and quantify improvements in the minimum fuel selling price, reduce carbon intensity, and support the SOT. We have surveyed various methods for biomass pretreatment and successfully demonstrated pre-pilot-scale pretreatment (100 kg) in batch mode. Using techniques such as lipid modification, fermentation, MOT, and carbonization, we have developed biofuel precursors and a range of value-added coproducts. Our project has demonstrated significant improvements in key aspects of algae processing, particularly in pretreatment technologies suitable for variable composition, coproducts available from lipid and extracted solid streams, conditioning and fermenting of high-protein hydrolysates, and recovery of nitrogen and phosphorus nutrients for recycling to cultivation ponds. We have demonstrated a pathway to generate drop-in algal biofuels at modeled cost of <$2.50/GGE and >50% GHG emissions reduction versus fossil incumbents. The success of this project will support the commercialization of a sustainable microalgal biorefinery industry.



COMMENTS

- Thank you for the slide explaining the management approach and communications strategy. The DEI approach is good, as it points to concrete actions taken. Downstream operations are critical to the success of commercialization, so there is clear impact and a strong connection to the economic case, especially of platform development as opposed to specialty chemicals. The use of machine learning to improve nitrogen availability is innovative. The connection to the Polaris licensing of non-isocyanate PU, Qualitas, Clearas, and GWT is excellent, but I would have liked to see a lipid fuels connection as well. There needs to be more understanding of the PU market in order to have more solid data for the TEA—how to get better market penetration. One hundred kilograms is a reasonable pilot scale for downstream operations. Ammonium sulfate can be quite expensive for the quantity needed; I would recommend looking at other options such as carbonic acid.

- This is one of the most wide-ranging projects reviewed; it has many moving parts and somewhat ambiguous goals. The umbrella goal is certainly good, and all projects are directed at that goal. There is a lot of quality exploration being done. Perhaps it was the short time allowed for the presentation, but there was a lack of coherence.
- Approach: Identifying and optimizing a downstream process that could be applied to multiple types of algal biomass feedstock to achieve a suite of products is a worthwhile goal that is in line with BETO's objectives. A good multidisciplinary team has been assembled for this project, and the communication and DEI plans are appropriate. Interim milestones and specific objectives were not provided in the presentation, however, so it's not really possible to know whether the approach being taken will meet the objectives in the project's time frame.
- Progress and Outcomes: Milestones and objectives for the subprojects were not specified, so measuring progress is not straightforward.
- Based on the presentation, MOT of acid-hydrolyzed algal biomass appears to be a good process for making such biomass a more viable feedstock for the fermentation step of the CAPSLOC process. An added benefit is the potential to recycle more nutrients back into algal cultures, which would be expected to reduce cultivation operating costs. However, although the MOT process was described in the 2019 and 2020 CAP SOT reports, it was dropped from the 2021 CAP SOT report, which would lead one to assume that it is no longer being considered a viable process option (perhaps due to the inability of the process to work at commercially relevant solids concentrations?). This disconnect should have been addressed in the presentation.
- A substantial amount of economic credit is being given in the TEA to the coproduct PU, but information on the assumed market size and sales price are not provided, again making it hard to understand whether the assumptions are reasonable or not. It is recommended that the research group obtain input from existing large-scale PU producers to validate the assumptions being made on product requirements, comparative manufacturing costs, potential market penetration, and bulk pricing of the algal-based isocyanate PU and non-isocyanate PU end products.
- Impact: A one-size-fits-all process to convert algal biomass from different sources to useful and profitable products would be quite valuable to the field. It would have been helpful for the researchers to report on the use of the CAPSLOC process for different types of algal biomass in order to know whether it is truly a universal process. It will also be important to know whether past issues with processing high-salinity strains have been overcome.
- More information in the presentation on the assumptions made in the TEA models as to which improvements are required in the existing CAPSLOC process to achieve the $2.50/GGE minimum fuel selling price target would have been useful. Without reading the current SOT in detail, which is beyond the scope of this review, it is hard to determine whether the TEA forecasts are reasonable, and thus the overall impact is difficult to assess.
- Approach: Good plan and working collaboratively with other BETO portfolio projects, adapting as needed to other project results to maximize output; risks and mitigation have been defined. Outcomes:

Met all project goals early and continuing to improve on targets. Impact: Large, as this is very practical due to wide variety of biomass streams; it may not work for all coproducts desired.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive and constructive comments. While the overall project goal is broad, we also have more specific goals delineated in quarterly milestones. We have achieved all seven of these milestones in the last 2 years, including comprehensively evaluating six pretreatment methods on nine different algal biomasses (Slide 9), scaling up pretreatment to the 100-kg scale (Slide 9), optimizing MOT regarding carbon and nitrogen yields to enhance lipid fermentation and nutrient recycling (Slides 11 and 12), demonstrating non-isocyanate PU production (Slide 13) and carbon products from posted extracted solids (Slide 14), and hosting one MEISPP intern (Slide 7). In the context of biomass conversion, we started at the pretreatment step and established that dilute acid is a universal approach to fractionate algal biomass with a broad range of composition. However, different algae give very different compositions of hydrolysate and solids, and establishing biomass-agnostic downstream conversion is an ongoing focus. MOT has been used as a tool to funnel carbons into biofuel precursors. Besides MOT of the post-extracted residuals, we will explore arrested anaerobic digestion for organic carbon funneling to produce volatile fatty acids as precursors for SAF production via sequential chemical and biological approaches. Though we have made significant progress, there's still a lot of work that needs to be explored and validated to establish a robust and universal algal biorefinery. While the TEA team did refer to MOT in prior SOT reports, it has never been a formal SOT pathway, and thus has not been the subject of focus in the SOTs to the same degree as the biochemical fermentation/lipid extraction pathways. We believe that MOT still exhibits potential for certain applications as a means of producing intermediates for subsequent upgrading while recovering nutrients, though challenges in conversion efficiency of insoluble solids have hindered its application as a stand-alone biomass conversion technology. After MOT, we extracted ammonium by ion-exchange resin, though regeneration of the resins has not been a focus of the research thus far. Regeneration with sulfuric acid to produce ammonium sulfate is a well-known baseline process, but we appreciate the reviewer's suggestion to use sustainable carbonic acid instead and will explore this option in our future work. In the last 2 years, we have been focusing on low-cost algal biomass (usually high in protein and low in lipid contents), but we do have a plan to recover lipid from the biomass and test its suitability for SAF production via the ASTM-approved hydroprocessed esters and fatty acids approach. This effort will be explored and benchmarked by the end of FY 2023. The PU foam market size is approximately 2.1 million tonnes/year (U.S.) or 14 million tonnes/year (global). These market sizes are significant and can support many algal biorefineries before reaching saturation. In addition, the price of PU has increased significantly to around $3.5/lb. This will be incorporated into future TEA models along with adjusting the prices of other raw materials and capital costs using price indices. We have realized the importance of working with existing large-scale PU producers to validate the assumptions being made on product requirements. The separate NREL algae TEA/LCA team has recently initiated a subcontract with an engineering contractor to assist in refining our understanding of non-isocyanate PU manufacturing costs in comparison to traditional PU production. Besides licensing this technology to Polaris Renewables, we have been working with several world-renowned companies, all delivering project cost share, as part of two consecutive DOE Technology Commercialization Fund-supported projects. These projects focus on developing non-isocyanate PU technology for market penetration and have yielded valuable insights that advanced commercialization. The CAPSLOC project works closely with NREL's TEA/LCA project (WBS.1.3.5.200) to better understand the improvements required to achieve minimum fuel selling price and decarbonization goals. To summarize recent SOT and design reports, further improving pretreatment efficacy to boost yields to fermentable intermediates, increasing catalyst performance (activity and stability) during upgrading of intermediates to finished fuels, and producing high-value, scalable coproducts from all non-fuel portions of algae feedstocks are areas with significant potential within the CAPSLOC scope.

MEDIUM OPTIMIZATION WITH RECYCLED ELEMENTS (MORE) FOR BETTER BIOMASS

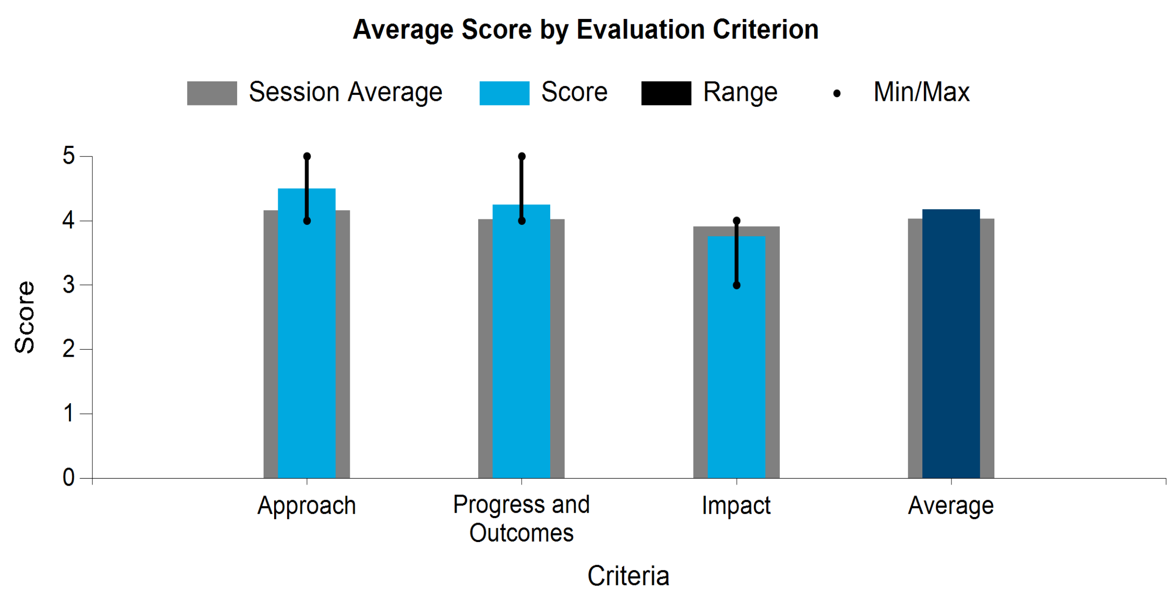
Los Alamos National Laboratory, National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	1.3.4.205
Presenter(s):	Claire Sanders
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,500,000

Microalgae offer great potential as a renewable source of biofuels and high-value bioproducts. However, the cost of algal biomass still remains a primary impediment to using algae for the production of biofuels and bioproducts. Past efforts to reduce biomass cost have included altering media components; however, the composition of primary nutrients has varied little from a standard starting nitrogen concentration [N] of 40–70 ppm and a nitrogen:phosphorus (N:P) ratio of 16:1 (Redfield's), with the aim of maintaining a nutrient-replete status during BETO SOT field trials. Nutrient inputs that are too low could adversely affect productivity, but conversely, the implications of overloaded nutrients are not understood.

In this project, we have leveraged multiple years of SOT data for *Picochlorum celeri* and *Tetraselmis striata* as inputs for machine learning to identify areas of improvement for N and P application and pond management. Machine learning has been combined with laboratory and outdoor testing using varying nutrient inputs, with which we have shown robust growth maintenance for both *P. celeri* and *T. striata*. TEA has been implemented to determine the MBSP cost savings of changing nutrient management strategies. Additionally, we are testing the use of recycled nutrients from biomass to support economically viable pond growth. Using these approaches, we have shown that data-directed nutrient input management will reduce the costs of biomass production.



COMMENTS

- The connections between all the different workflows are great. Very encouraging, especially the direct comparison of indoor PBRs to outdoor ponds. This has historically been a massive issue that is very challenging to address properly and is absolutely critical to resolve. Risk mitigation and connection of the approach to the impact is clear. I like that you are doing the model first and then validating against the data instead of leaving the model for last; it demonstrates that the authors know the value of *in silico* work and understand the point of the TEA. Thank you for the DEI slide; this is also helpful. I would have liked to see more of an industry connection. The Bayesian strategy for machine learning is solid, given the limited amount of data available to feed into the initial model and seasonal variability. I would like to know how the code versions are being tracked; versioning should be performed through GitHub or some similar validated method, which can also facilitate wider use of the code. The composition results and real-life media recycling data should be interesting when you have them.

- I will defer to the program about the approach, since this seems like very much a first step, almost a proof of concept. The presentation certainly did not leave the impression that the model is robust and useful across a range of conditions. It is curious that uptake rather than concentration is in the input and gives some pause. It would be best if the model relied only on controllable settings.

- It seems that progress has been made, but there is much left to be done. Good inclusion of DEI. Well considered and well presented.

- This project is trying something new, but it is still wanting. It is commonly said as a joke, but the adage "all models are wrong, but some are useful" is actually a statement carrying wisdom. It is insufficient to develop a model; it must be tested sufficiently to be proven useful. Perhaps those tests will come, but it is not clear they are being done or being planned based on what was presented.

- Approach: The project team members take advantage of existing data sets and use machine learning to gain insights into the impacts of nitrogen and phosphorus levels on algal growth (primarily *Picochlorum* and *Tetraselmis*). Additional lab testing is used to verify or refine the machine-learning results. Appropriate connections between team members at LANL, NREL, and AzCATI appear to have been made. The project goals are aligned with those of BETO, although it must be recognized that there will be limits on the applicability of the results to strains, cultivation conditions, and media that were not directly examined in this study.

- Progress and Outcomes: In the machine-learning correlation (Slide 11), NH_3 uptake is listed as the largest contributor to *P. celeri* productivity. This is most likely a result of high productivity rather than a cause. As shown on supplemental Slide 31, the actual NH_3 concentration in the medium didn't seem to have a large effect.

- It's important to recognize that, in addition to the impact that starting nutrient concentrations can have on productivity, the manner in which nutrients are added (e.g., once and done feeding, steady feeding over the duration of a cultivation, periodic feeding based on culture density) and the form of the nutrient (e.g., NH_3 versus NO_3 versus urea) can have large effects on productivity and nutrient utilization efficiencies.

- The analysis involving nutrient addition into environmental PBRs in which medium is recycled is interesting and shows the importance of balancing nutrient inputs with growth needs.

- Experiments indicating the possibility of utilizing MOT-extracted nutrients for growth are important because the premise has been that this process can reduce costs through nutrient recovery. Hopefully the inhibitory substances can be identified and easily removed.

- Impact: It would be more broadly impactful to the algae industry and research community if approaches similar to the ones described in this project could be used to understand nutrient use dynamics for a variety of available water types and for different types of algae, rather than a very limited scope (i.e., *P. celeri* or *T. striata* in f/2 medium). (Note that it is recognized that these were the most comprehensive data sets that were available for analysis.) Due to the effects of water chemistry on nutrient availability (especially metals and other micronutrients, which were beyond the scope of this study), as well as differing nutrient uptake systems associated with different types of algae, it will likely prove necessary to obtain empirical growth and nutrient use data for each unique cultivation system and strain. Therefore, a desirable outcome for this project would be the development of a general analysis tool and testing protocols that could be used by labs and companies for their particular situation.

- Approach: Data analysis is not necessarily novel, but the amount of data used is; good team interactions, good plan, and mention of equity and inclusion. What about media recycle? Is that being done? Not clear. Outcome: Good outcomes, with data analysis defining what is important and controllable with today's technologies. Impact: The impact is large if the industry listens to it. The take-home message is to feed your algae and control temperature if you can. Can salinity be considered as a variable, as it would most likely also be on the list of high-productivity impact metrics?

PI RESPONSE TO REVIEWER COMMENTS

- Thank you to the reviewers for committing their time to assessing the progress and outcomes of this project and for the insightful comments. We have integrated experimentation (both indoor and outdoor), machine learning, and TEA with investigators from LANL, NREL, and AzCATI to achieve the goals of this project, and we appreciate the reviewers recognizing our well-integrated team. We agree that there are many factors with nutrient inputs that need further study. Different macronutrient sources, micronutrients, types of media (e.g., fresh, marine), and timing of feeding have the potential to change the algae behavior, including biomass accumulation, and a valuable output of this work will be a framework that can be utilized in further studies. We are glad that it is recognized that the environmental PBR cultivation system is invaluable in predicting the behavior of outdoor cultures. Our ability to utilize this array has made the realistic study of a variety of media compositions possible. Recycled nutrients can be derived from two sources: media and biomass. In this project we are focused on the recovery of nutrients from extracted biomass; this has been little studied and is an important consideration as we work toward a reduction in waste from the production of algae. Media recycling is another important factor in waste reduction, and one that is currently out of the scope of this project but will be important in future research. Our work on macronutrient compositions in media and the resultant optimization will reduce loss of ammonia and phosphate (as N and P sources) during non-perfect media recycling, which improves MBSP, as shown by TEA. Development of a new machine-learning model takes considerable time and inputs. We have worked to ensure that the data inputs from multiyear outdoor growth trials are robust and have been screened for erroneous/missing data. The model was originally built to encompass all data, including deltas, directly available or directly calculatable, from the data sets. Now that the model is functioning and we have demonstrated its applicability on data sets from multiple species, we are working to identify parameters that are dependent and should not be considered in our analysis. Parameter input optimization will increase the robustness of the model and give further insight into pond performance. During development, software goes through many iterations, and we appreciate the reviewers recognizing the importance of version tracking. Currently, our machine-learning software is being tracked internally; when the software is ready for release, we will use a version control system, such as GitHub, where it will be publicly available. We do understand that dissemination of all our work to industry is imperative to realizing its significance in the field. We will continue to communicate our results at relevant conferences and publications, as well as by seeking opportunities for discussion. We appreciate the recognition of our progress in the first 18 months of this project and agree there is still much to do. We look forward to continuing our close collaborations and work to realize the impact of controllable factors, such as nutrient input, on biomass accumulation.

ALGAL BIOFUELS TECHNO-ECONOMIC ANALYSIS

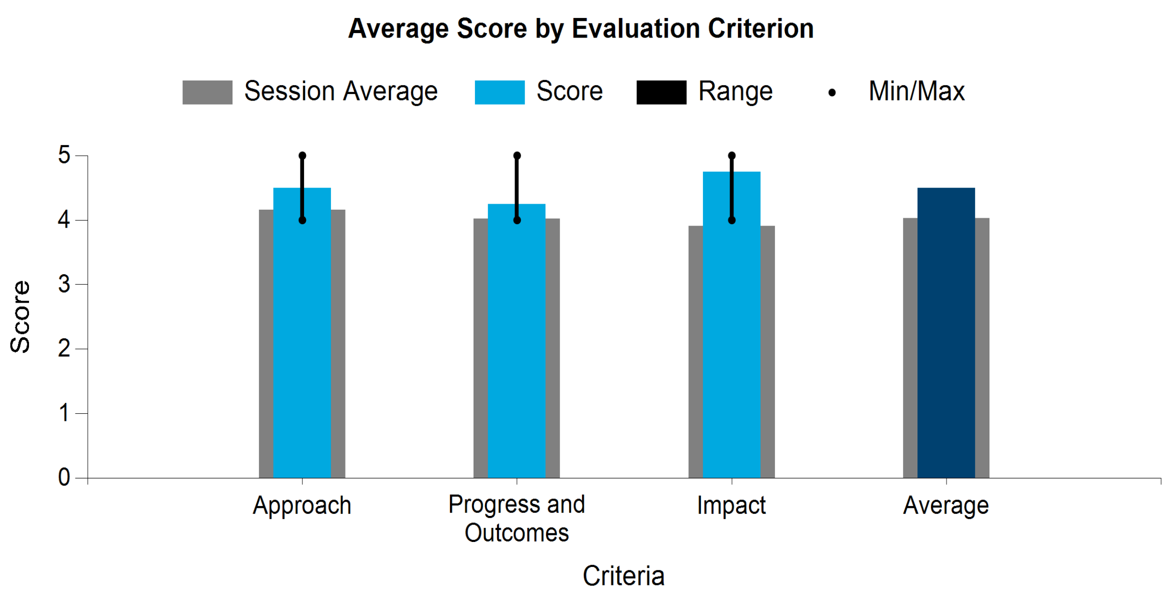
National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	1.3.5.200
Presenter(s):	Ryan Davis
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2024
Total Funding:	$1,050,000

The objective of NREL's Algal Biofuels TEA project is to provide process modeling and analysis to support algae program activities, utilizing TEA models to relate key process parameters with overall economics for cultivation, processing, and conversion of algal biomass to fuels and coproducts. By quantifying the economic implications of key process metrics, TEA models highlight the technical requirements to achieve future program goals for economic viability and sustainability, while identifying drivers and technology barriers that must be addressed through research prioritization.

This project provides high impact and relevance though the generation of critical cost data tied to funded research, with our analyses subsequently exercised by BETO to guide program goals and planning documents. This includes costs for both algal biomass production and downstream conversion, while working with lab partners to support LCA, ultimately to demonstrate paths to meeting the latest program goals for maximizing decarbonization potential at 70% or more GHG reduction while maintaining economic viability. This project has made numerous achievements since the 2021 Peer Review, including continued improvements to SOT cost benchmarks, publication of a high-visibility report documenting near-term opportunities for utilizing waste algae resources, and ongoing collaboration with other lab partners on an updated algae harmonization analysis.



COMMENTS

- The validation of the model with ongoing projects and industry experts is absolutely critical to the success of the model; this is great.
- It's also good to see multiple algae sources; this makes modeling more complex as the inputs shift, but it is also more practical.

- Good finding about the wastewater treatment and harmful bloom containment aspects.
- It's a very nice model, very detailed; I would like to see how it tech transfers to industrial organizations.
- The estimated time to build long term is 3 years, but that is with a fully developed facility that can be copy/pasted; realistically, after permitting, facility buildout, and modifications to optimize, you're looking at 7 years. The material storage assumptions are unclear. Is there a user interface in the future that would enable more sophisticated modeling than Excel can provide? I would also like to see a gap analysis between the current state and n^{th}-plant model to give a clearer idea of the path forward.
- TEA was certainly front and center of every talk. I am heartened to see that TEA is as important as it is in the program. I certainly hope there is some harmonization of assumptions used in those TEAs. Based on a line of questioning, tracking the database of assumptions used in any particular TEA would seem to be useful. What is disconcerting is that project-to-project comparison requires understanding what the assumptions are, or at least whether they are based on the same assumptions.
- Concerns are directed at the program. For the program, it would be useful for some indication of whether projects are using the same assumptions. Assumptions will be the main drivers. Some version of being able to track assumptions to allow for updating and harmonizing results from different times would be useful.
- Approach: The general approach for collecting input and conducting TEAs for algal biomass production and conversion is robust and has been formulated and shaped over years of interactions with multiple research groups and industrial partners. The feedback from knowledgeable consultants and stakeholders is an important element of this effort in order to enhance the accuracy of modeling outcomes. The harmonization efforts with other groups in this field are very important in order to enable meaningful comparison of results and enhance the reliability of the ensuing research guidance.
- Progress and Outcomes: The new effort to examine waste sources of algae from wastewater treatment, algal bloom collection, extracted biomass associated with nutraceutical manufacturing, etc. is interesting in that it can provide information on smaller-scale, distributed conversion processes. This could help with gaining operational knowledge for potential larger-scale, purpose-grown algae facilities. Regarding the collection of bloom algae, the investigators need to ensure that collection and dewatering costs and energy requirements for such dilute algal biomass streams are fully accounted for, especially considering the rather large water remediation credit needed for a positive outcome.
- Impact: The results of this ongoing project help to provide economics-driven research guidance in order to focus on the most impactful areas, as well as to provide credibility (or not) to new ideas on cultivation, processing, and commercialization of algal-based technologies.
- The fact that there are many downloads of publications and reports from this analysis/modeling group attests to the breadth of impact for the project.
- If not already doing so, the primary investigators should make sure that input on coproduct market prices and costs for certain services (e.g., wastewater treatment costs to municipalities, including biomass disposal, bulk prices for PUs and precursors, and fusel alcohols) are vetted by companies that are actually producing these products or providing services with conventional processes (i.e., don't rely strictly on prices/costs provided by small aspirational companies).
- Approach: Nothing novel here, but good to keep this updated each year and available for updating. Progress and Outcomes: It's critical to keep updating the model with new information. It would be

interesting to see if the models work if systems are not scaled in size as much—but are scaled in modules. Impact: Impactful to the community due to open access to the work and Excel sheet.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive comments and recognition of the importance of this project. We agree with the second reviewer's comments regarding the importance of understanding and harmonizing assumptions made between different projects who use our (and others') TEA models to make economic projections, though recognizing that comment is directed more toward the BETO algae program than to this project specifically (although we are happy to assist in that capacity as we can). Regarding the comments pertaining to specific inputs/assumptions made in the models—e.g., facility scale, construction time, storage assumptions—the parameters attributed to our "base case" scenarios (as documented in the pertinent report links shown in the slides) are reflective of n^{th}-plant conditions with sufficient economic and technical maturity to enable 5,000-acre algae farms modularized for construction to be completed in a 3-year period. Variances to those base case assumptions can be readily investigated, and in many cases are already reflected in sensitivity analyses published in the accompanying reports. Interested users can also vary such parameters directly using our public TEA algae farm model tool (https://www.nrel.gov/extranet/biorefinery/aspen-models/). While our TEA modeling efforts to date have historically focused on such an n^{th}-plant framework per BETO work scope authorization, there has been more interest recently in better understanding n^{th}-plant versus pioneer plant comparisons, and we will investigate options for expanding into such a comparison (in this project or elsewhere) moving forward. We also agree with the comments regarding the need to use well-validated inputs for both processing costs (e.g., for harmful algal bloom/wastewater treatment biomass collection and processing) and coproduct credits/market values. To this end, we have worked closely with industry collaborators such as AECOM on the harmful algal bloom study and Gross-Wen Technologies on the wastewater treatment study to understand key processing details for collection and dewatering of such biomass sources, and resultant water treatment remediation credits. Market values for algal-derived chemical coproducts are typically sourced from industry databases reflecting macro-industry pricing. The TEA sensitivities to both of those considerations are documented in the pertinent reports as sensitivity analyses; time constraints did not allow for presenting such sensitivities in the slides.

ALGAE TECHNOLOGY EDUCATIONAL CONSORTIUM

National Renewable Energy Laboratory

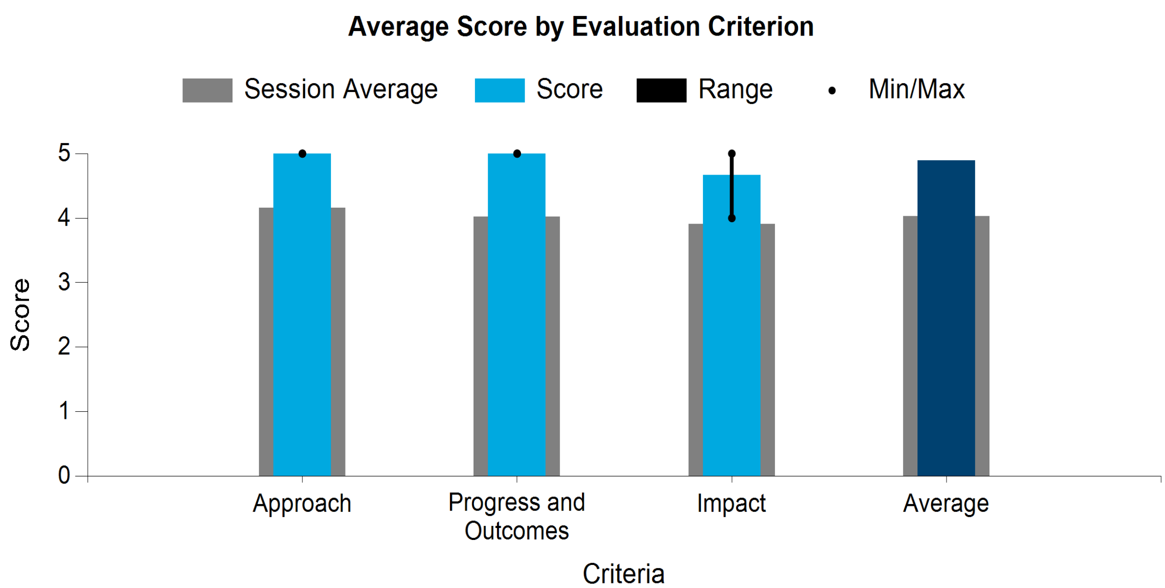
PROJECT DESCRIPTION

WBS:	1.3.5.201
Presenter(s):	Cindy Gerk
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2025
Total Funding:	$1,650,000

The ATEC project is a collaboration of academics, national laboratory researchers, and commercial algal experts to develop state-of-the-art workforce development, education, and training programs serving ages 5–80, in all 50 U.S. states and 100 countries. ATEC has a 7-year history of developing two separate collegiate curricula in algal cultivation and algal biotechnology. Additional efforts include three algal MOOCs, Algae Academy (a K–12 STEM education program), Algae Cultivation Extension Short-courses (ACES), and a digital badging program, supporting the development of the next generation of algal professionals. Future efforts include formalizing relationships with minority-serving institutions, including historically Black colleges and universities and Hispanic-, Native American-, and Native Hawaiian-serving institutions.

ATEC initiated the DOE-supported AlgaePrize 2022–2023, a national student-based 18-month research competition enhancing the algal-based bioeconomy. The culmination of the inaugural AlgaePrize is scheduled for April 14–16, 2023, at NREL in Golden, Colorado.

ATEC entered into a formal collaboration with Prairie View A&M University focused on the development of the Algae Center of Excellence for Climate Resilient Food-Energy-Water Systems, intended to be the nation's ultimate algae-based research, workforce development, education, and training center.



COMMENTS

- The risk mitigation slide is helpful, especially the COVID disruption. The collaborations are impressive, especially the industrial advisory board. As DEI is absolutely critical to this particular project, it's wonderful to see so much outreach. The impact on student learning and careers is wonderful; the quantitation and clear success of the program are fantastic.

- The curriculum is frequently updated based on feedback from industry and networking events to ensure the relevance of the material. Many students choose entrepreneurship and work in related fields rather than directly in algae cultivation, as the jobs anticipated have not materialized; however, the transferrable skills are strong and readily used. For example, Austin Community College is part of the program, yet there is no algae cultivation ongoing in Texas. The program specifically provides more in-depth experience than many kit-based labs can provide, as there is more hands-on work, and a richer understanding of the course materials is required in order to perform the work.

- Most impressive was the way in which the course was able to transition to online education with materials shipped from various facilities. The program leadership was able to anticipate a potential shutdown with an earlier experience of a bird flu epidemic and had already preadapted their programming by leveraging online education connections at Santa Fe Community College and some other collaborators who were already online.

- This was a very enthusiastic presentation and had a clear commitment to education about algae. In general, very positive with two very minor concerns: goal alignment and metrics. The move to heterotrophic growth is one example. I find it hard to relate this to the stated program goals. It may well benefit the students but seems unaligned with BETO goals. The second is about metrics for success. I've been involved with education programs in the past. The data on student surveys as a measure of success are certainly wanting. If the intent of the program is a prepared workforce, some more meaningful metric such as post-training employment would be a more reasonable metric. For secondary education, a post-class survey is not compelling as a measure of success for classroom learning but may be a bit more acceptable, as more rigorous data collection is likely difficult. Lots of excitement and engagement; my only question is about the measure of impact relative to programs attempting to provide certifications for employment.

- Approach: The approach taken by ATEC is comprehensive and addresses some key general BETO goals regarding education and workforce development in the bioenergy field, as well as specific program goals related to algal systems for energy production.

- ATEC has developed and rolled out training curricula at levels everywhere from elementary school through colleges and universities. Multiple disciplines are covered, including algal biotechnology and cultivation science. Both microalgae and macroalgae are covered, which adds to the depth of the training offerings.

- Progress and Outcomes: The number of students who have participated in training modules developed through ATEC over the years is really quite impressive. This has certainly had a positive impact on getting the word out about the potential for algae in the bioeconomy, both in the United States and abroad.

- The addition of new modules to the MOOC series and the expansion of schools that participate in ATEC offerings will continue to further the reach of ATEC and ensure that the curricula are kept fresh, comprehensive, and up to date.

- Impact: The various ATEC programs continue to be impactful for generating interest in algae for students of all ages and for providing skills and knowledge that should enhance the job prospects for college-level program participants who choose to pursue jobs in algal-based businesses and research labs. This impact is confirmed by the large and growing number of students who have participated in ATEC programs and products, including MOOCs, the Algae Academy, community college courses (including earned certifications), AlgaePrize applicants, etc.

- As the algae industry expands in the future, there will be numerous qualified job applicants for open positions that will already have many of the skills required for successful integration into the industry.

PI RESPONSE TO REVIEWER COMMENTS

- The ATEC team is very grateful to the BETO reviewers for their recognition of accomplishments and to BETO for continued support of bioeconomy workforce development, algal education, and training. The ATEC curriculum and the Algae Academy have reached all 50 states and more than 100 countries. We continue to expand the ATEC partnering collegiate network through our collaborations with historically Black colleges and universities, InnovATEBIO, and Future Farmers of America. It is deeply gratifying to receive such a strong positive review. It sends us a clear message that we are on the right track and encourages us to continue to focus our energies on expanding the program to bring algae awareness to more and more students. We acknowledge the reviewer's comments concerning analytical metrics measuring impact and have scheduled this as a major area of effort over the next 2-year period. Regarding the comment about aligning with BETO goals, the example given was the development and inclusion of heterotrophic cultivation of algae within our cultivation curricula. Currently, the United States' microalgae market is split between the phototrophic and heterotrophic, with the corporate giants DSM and Corbian relying on heterotrophic cultivation for omega-3 fatty acids (eicosapentaenoic acid and docosahexaenoic acid), along with the development of Thrive, an algal-based cooking oil. With the inclusion of bioplastics, biofeeds, and biofoods along with algal-based fuels, heterotrophic cultivation techniques are a valuable arrow in the quiver of current cultivation expertise. Our industry relevance is reflected in NREL including ATEC experience as a preferred qualification for job applicants and Corbian lowering the degree requirements from a 4-year degree to a 2-year degree for graduates with an ATEC algal cultivation certificate.

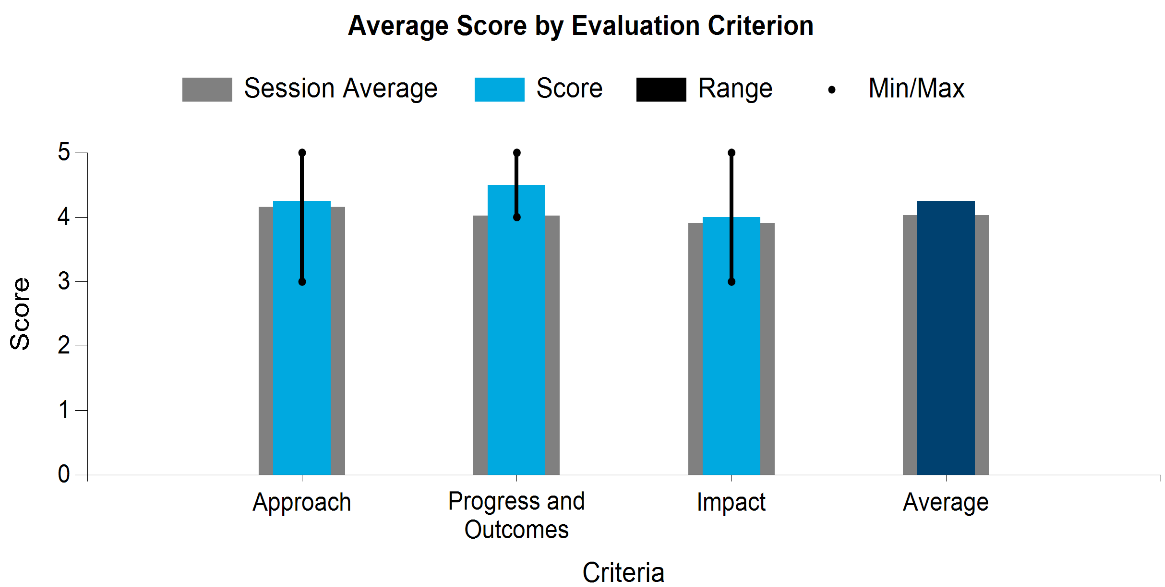
HTL MODEL DEVELOPMENT

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	1.3.5.202
Presenter(s):	Peter Valdez
Project Start Date:	10/01/2017
Planned Project End Date:	09/30/2023
Total Funding:	$600,000

The HTL Model Development project provides TEA and sustainability inventory for algae conversion via HTL and upgrading to fuels and coproducts. A conceptual biorefinery model was first developed in 2014, and since then, SOT assessments have been reported annually. The purpose of the SOT assessment is to identify barriers, cost reduction strategies, and sustainability impacts to track research progress toward BETO's 2030 cost target of producing fuels at $2.50/GGE. The annual SOT report documents the modeled costs and the associated research incorporated into the modeling. Synergistic work between the analyst and experimentalist teams directs research toward high-impact results, driving conversion costs toward the cost target. In the 2022 SOT report, the cost of HTL conversion of *Picochlorum celeri* was $0.35/GGE, compared to $0.88/GGE reported in 2019. The reduction is achieved through the value of recycled nutrient credits. The conversion cost is nominally affected by the inclusion of a denitrogenation step to produce high-quality distillates for SAF. However, the cost of the farm-cultivated feedstock results in a minimum fuel selling price of $5.42/GGE. A no-cost algal feedstock, as reported in the 2021 SOT report, resulted in increased conversion costs but achieved the lowest reported minimum fuel selling price of $2.61/GGE.



COMMENTS

- The slides are telling me that you are communicating and that you have some industry collaborations, but how are you communicating? Is it with meetings, online, Slack, or what? Who in the industry are you collaborating with specifically? On which aspects of the project? Slide 11 reads like a decrease in production after optimization; is this correct? Slide 14 states that 23% of the biocrude is within range of jet fuel, but this doesn't seem to be what the graph is showing. The mixed materials with wood waste blend will be helpful. I would have liked to see a gap analysis of how long it will take to get to the *n*th-plant scenario.

- There is still considerable ambiguity. Within that ambiguity, the project has done a great job of attempting to get to actionable conclusions. I am particularly impressed with the ability to accept changing feedstocks, including even non-algae feedstocks like wood. My only negative comment is that the results still show that considerable improvement is needed to be viable.
- Approach: The project team includes different groups that are able to provide good input for the various analysis parameters. The team helps to identify processing pathways that increase the economic value of the overall HTL process.
- There appears to be quite a bit of overlap between this project and the other HTL project reported by the same presenter (Hydrothermal Processing for Algal-Based Biofuels and Coproducts). Comments for this presentation should be considered in tandem with the comments made for that presentation.
- Progress and Outcomes: Modeling results have been completed in the past 2 years for HTL of purpose-grown algae, indicating a minimum fuel selling price of $5.42. These results, including a higher credit for nutrient recycle, were provided as input for the 2022 SOT report. Information from this study was also used for the upcoming version of the algae harmonization report.
- Emphasis was placed on protein coproduction in order to lower the achievable fuel selling price and to reduce GHG emissions from farmed algae (*Picochlorum*). Because of the significant modeled cost reduction, it will be important to validate that the protein quality is suitable for use as a feed or food product, as well as to ensure that the GHG displacement credits are accurately calculated.
- Considering the large credit being given to struvite as a coproduct of HTL of algal biomass from wastewater treatment, it will be important to actually test the struvite coproduct for use as a fertilizer for crop plants (and possibly algae) to make sure that there are no growth-inhibiting substances present to validate the assigned economic value.
- It is important to understand whether the products from the HTL process have characteristics that are acceptable for their intended purposes, and thus whether the assigned values are appropriate. The small-scale testing of the HTL oil products from *Picochlorum* suggests that it would be suitable for use as a jet fuel; this is a good outcome. Similar studies will need to be conducted for HTL products form other algal biomass sources.
- Impact: The team has published SOTs and other reports the last couple of years that provide research guidance for further areas for HTL process improvement. In combination with SOTs for alternative downstream conversion processes, funding decisions on the most promising paths forward can be made.
- Approach: Good; good collaboration on the project. Outcomes: Meeting goals, advancing the SOT. Impact: High due to lots of publications and patents.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful and constructive comments and questions. We will address key questions and areas that need further clarification. With respect to our collaborative activities, we interact via emails and meetings (in person and virtual) with providers of the algal feedstock, equipment vendors, and others implementing HTL technology. We typically engage with our industrial collaborators to learn about current trends that impact the development of algae HTL, such as feedstock availability and costs, market potential for HTL products, and equipment capabilities. An abbreviated list of collaborators is included in the presentation for project 1.3.4.101. In the presentation materials, the draft results for the optimized scenario show that there is a reduced production volume of fuel. In the optimized scenario, the production volume of protein concentrate is unconstrained, resulting in a higher production of protein products, which are favored over fuel products because of their higher value. However, please refer to the final, published version of the harmonization report for full details of the analysis and results. In upcoming work, to produce the design case study report, we will investigate scenarios related to the first-of-a-kind plant and the predicted costs and anticipated design challenges. We will continue investigations in the experimental project (1.3.4.101), working with collaborators and relevant product experts to validate the process assumptions that are used in the analyses for this project. Additional analysis work in this project and with support from Argonne National Laboratory (4.1.1.10) will ensure the accuracy of our process and environmental model calculations to assess the project's economic and environmental impact.

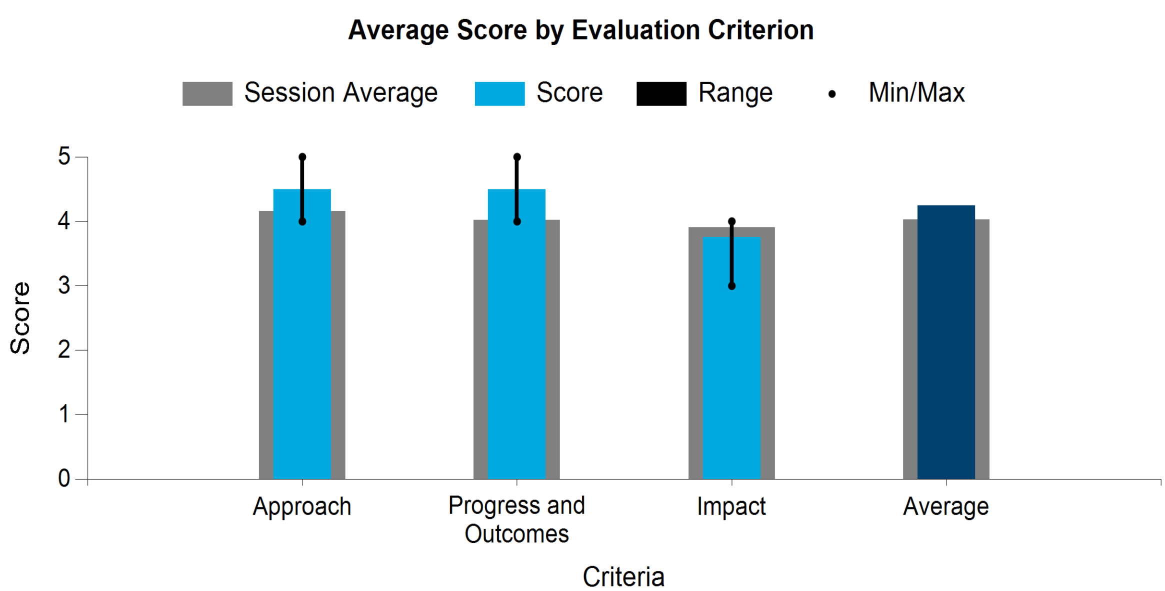
MICROALGAE ANALYSIS

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	1.3.5.203
Presenter(s):	Andre Coleman
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,725,000

The Biomass Assessment Tool (BAT) provides a core capability in the BETO program, enabling a linked geospatial, biophysics, and partial techno-economics model and analysis tool for linking key BETO and industry research activities to achieve high-impact objectives. To date, project technology transfer has been successfully achieved through 31 peer-reviewed publications, the technical assistance program, workshops and conferences, direct collaboration with academia and industry, and integration with the Bioenergy Knowledge Discovery Framework. Outcomes from the past annual operating plan (AOP) cycles have continually addressed priority issues for the emerging algal biofuels industry. Under the current AOP, the project objectives are to (1) continue participation in the BETO SOT for experimental design and scale-up of field studies in time and space; (2) parameterize and model two high-performing saline strains from DISCOVR; (3) provide resource assessment and limited techno-economics for the multi-lab Microalgae Model Harmonization effort that includes water and nutrient collocation opportunities; (4) perform resource assessment and techno-economics for offshore macroalgae cultivation; (5) develop microalgae and macroalgae chapters for Oak Ridge National Laboratory's Billion-Ton report; (6) complete the development, validation, and documentation of the enhanced high-rate algae pond model; and (7) develop, mature, and demonstrate the microalgae biomass forecasting system.



COMMENTS

- This project focuses on modeling the sustainable supply of cultivated biomass by employing open-pond PBRs, saline water, wastewater, and CO_2 collocation. Their approach includes development, enhancement, and application of available tools and resources to understand opportunities and trade-offs and realize new pathways.

- The team appears to be well managed with well-defined task structure and leveraging team expertise and previous experiences. The team highlighted some challenges with the various approaches and identified mitigation strategies.
- The team has made significant progress in using a microalgae biomass forecast system to demonstrate improvement in biomass productivity by over 40%. They have identified collocation opportunities and offshore macroalgae biomass potential. The team should consider the impact of water quality from the different location on biomass productivity for the selected strains. The algae industry will benefit from the work done here and may provide inputs and new technologies that are currently missing from this analysis.
- The goal of this project was to provide an algal biomass assessment tool to BETO and industries as a harmonized model for building a systematic assessment of site-scale capability considering all environmental factors related to land, water resources, and other such parameters. Several partners have contributed to this project, improving and updating the model. It now involves parameterized assessment for both macro- and microalgae, salinity, drought, and other such variables. The project has been well coordinated between the partners and employed in several experimental operations. It would be helpful to know how many industries have adopted this BAT model to their benefit. The project has resulted in several publications in peer-reviewed journals.
- This project has very clear management and communication, and they appear to have exceeded their goals/milestones. The project goal is to deliver a national assessment tool that can answer where, who, and how for algae cultivation. The team appears motivated to get the tool into the hands of industry but has had little success so far. It is concerning that no industry link has been made to date, as this was a topic of discussion during the 2021 review. It is unclear if this is due to the lack of companies that could utilize the model or a shortfall of the project. Once it is in the hands of industry, the model should become a highly valuable tool, particularly informing technology trade-offs for various geographies. One of the project's biggest limitations is the quality and quantity of data inputs, but it is understandable that these data are either IP protected or just do not exist. It was refreshing to see a project in the BETO portfolio taking a national view on the algae industry's potential and not just for the limited locations where most algae work has been done. Hopefully the data will catch up with the model capabilities. The recent inclusion of macroalgae is also good foresight.
- This project approach focuses on a national assessment of where algae production can occur, how much nutrients are required, land and water resources required, how much biomass/energy is produced, and what interactions/trade-offs exist between technologies. The development of this BAT is an important part of the BETO algae cultivation program. The project is on schedule, and the project team has accomplished most project tasks. It is not clear what would be displaced (houses, farmland, etc.) in the sites identified in California, Texas, Louisiana, and Florida.

PI RESPONSE TO REVIEWER COMMENTS

- Reviewer #1 Response: We are grateful to the reviewer for providing an accurate summary of the research topics and including constructive comments. The work elements included in this project provide insights on BETO research priorities while being informed on needs, gaps, and questions in the community (BETO SOT, DISCOVR's industry advisory board, Advanced Research Projects Agency – Energy [ARPA-E] Macroalgae Research Inspiring Novel Energy Resources [MARINER] industry partners). Our focus has been to provide high-resolution, site-scale, national analysis that can help inform industry on a range of location and configuration trade-offs for use in their own strategic operations. The same analysis is also informative for helping to set future production and sustainability targets that can ultimately provide input into policy. The reviewer noted the consideration of water quality into the BAT analysis. In some aspects, water quality has been considered, specifically with respect to avoiding potential algal cultivation sites that would use groundwater with constituents (e.g., arsenic) that exceed standards established by the Environmental Protection Agency, and establishing waste resource budget models to utilize wastewater and associated nutrients from municipal wastewater treatment plants where algae cultivation sites can be potentially collocated. For our open-pond microalgae model, we have generally assumed this to be a closed-loop system for freshwater, where harvested or centrifuged water is recycled back into production ponds. The new BAT-enhanced pond model will also track pH and nutrient balance, and a future expansion of the model could include water quality measures if we assume water is being routed elsewhere after harvest. On another point, for the saline water open-pond model, blowdown volumes are processed through a forward osmosis system, where the freshwater fraction (~85% of the processed blowdown) is recycled to the pond for salinity management, and the remaining hypersaline fraction (~15%) is disposed of via deep-well injection. Alternative forms of hypersaline water disposal have also been investigated, including evaporation ponds. Our team will further consider how water quality can be better incorporated and represented.

- Reviewer #2 Response: We thank the reviewer for their favorable comments. A key pillar in the BAT modeling work is to link the resource assessment (i.e., what is required and consumed and how much biomass is produced under varying locations and operational configurations) with the expertise and capabilities of our lab partners. This has been exercised under three separate BETO model harmonization efforts and provides a unique coupling of resource assessment, techno-economic modeling (NREL), LCA (Argonne), and modeled biomass-to-energy conversion pathways. In addition, the BAT team has contributed to the BETO SOT efforts with the microalgae biomass forecast system; informed on DISCOVR experiments; and brought microalgae, and now macroalgae, into the Billion-Ton studies. Our recent addition of macroalgae modeling is possible through partnerships with the ARPA-E MARINER program (and industry partners) and the University of California, Irvine. The BAT team has long participated in and contributed to various consortia efforts, directly supporting and informing industry partners and contributing analysis data to support research at other national labs outside of the BETO model harmonization effort, as well as to numerous individual universities. With respect to the reviewer's comment about industry adoption, we've had strong industry collaboration in the past, directly providing analysis for informed decision-making. We also recently submitted a new project proposal with an industry partner focused on scaling up SAF and renewable diesel production. Unfortunately, our team has not kept a tally of users, but the primary use of BAT is through its data products, which have been published as open-source data sets through Oak Ridge National Laboratory's Knowledge Discovery Framework, and the methods and analysis results have been documented in 25 peer-reviewed publications and several reports. We regularly field requests for data and analysis products and are happy to provide these to the community.
- Reviewer #3 Response: We thank the reviewer for the positive comments, but also for sharing concerns. As noted to Reviewer #2, the BAT team is a regular collaborator and partner on many fronts, including the BETO SOT efforts, the Algae DISCOVR experiments, and multi-lab efforts such as the BETO model harmonization study and the Billion-Ton studies. Our recent addition of macroalgae modeling is possible through partnerships with the ARPA-E MARINER program, the program's industry partners, and the University of California, Irvine. Additionally, the BAT team has long participated and contributed to various consortia efforts that included private industry, as well as directly supporting and informing industry partners and numerous individual universities. Our methods and data analysis products have been regularly peer-reviewed and improved upon by those in industry. We would like to clarify some points, as these likely weren't made clear in the Q&A session of the presentation. First, some of our team's closest industry partnerships are fragmented due to the volatility of a still nascent industry. Having said that, there is more our team can do to continue outreach and build relationships so industry can benefit from tailoring BAT's data and analysis capabilities. In addition, with the recent publications of the microalgae forecast system model, we feel this will be of interest to industry, and near-term efforts will focus on establishing industry collaborations. Second, our team has continued to publish our

methods, analysis, and data to make them publicly accessible or accessible by request. In fact, our team regularly fields data requests from various entities, including academia, industry, government organizations, and national laboratory partners, though admittedly, it is hard to quantify what the specific impact has been for industry. Third, the BAT is a complex collection of big data, numerical models, interaction mediums, high-performance computing components, and Linux OS implementations that currently does not lend itself well to a downloadable and easy-to-use model for industry. Admittedly, if there were industry interest, a future project effort could be established to move the modeling platform to a higher technology readiness level and make this a deliverable product. As a note, a version of BAT was instituted in a web-based interactive platform, though it was later taken down due to emerging security vulnerability risks in the underlying web technology used. Additionally, there hasn't been significant sponsor interest to revive or establish a goal toward a transferable or web-interactive model. As a final response, the reviewer noted that "one of the project's biggest limitations is the quality and quantity of data inputs." The BAT team continually strives to use the highest-quality, most resolute, and latest publicly available data to inform the various models. We believe that the reviewer's comment here was specifically referring to open-pond observation data that we use for model validation; this ties to a question posed and a time-limited answer provided in the Q&A session. In our experience, the open-pond observation data have not been abundantly available, not appropriate (i.e., 100-L raised ponds), and/or not ready for release, but what we have received through industry and academic partners reveals very good open-pond modeling performance. We will continue to work with collaborators to acquire data so we can assess the modeling performance of the open-pond model, PBR model, biomass growth model, and nutrient and pH models.

- Reviewer #4 Response: We thank the reviewer for their comments and recognition of BAT as "an important part of the BETO algae cultivation program." Regarding the reviewer's comment on displacement by potential algal cultivation sites, it is worth briefly explaining BAT's multicriteria land suitability model. The land suitability model provides the fundamental basis for all other models in BAT, specifically identifying potential cultivation locations that meet a user-specified minimum area requirement (i.e., 1,000 acres). A key building block in the land suitability model lies at the currency and quality of spatial data used to inform the scenarios, and thus efforts are taken to process and use the latest high-resolution (10–30-m) national (contiguous and outside contiguous United States) data available. The model first identifies areas with slopes <2%, and then from these areas proceeds to eliminate open water bodies; wetland and riparian areas; forested lands; productive agricultural and pasture lands; urban area boundaries; various density developed areas; roadways and airport runways; military lands; protected lands, including local, state, and national parks, wilderness areas, fish and wildlife lands, and environmentally sensitive lands; and lands with significant levels of net primary productivity (high carbon storage). Brownfield sites, 25% of U.S. Department of Agriculture-defined marginal croplands, and defined croplands that have been idle for >5 years are added back into the screening pool. Finally, from the remaining screened lands, all contiguous areas less than the user-specified area threshold value are eliminated. Further site screening is implemented in additional models with regard to sustainable freshwater or saline water availability, minimum annual average biomass productivity of 25 $g/m^2/day$, access to existing infrastructure, access to collocated waste resources, and so on. This rigorous screening process is intended to provide the locations that have the greatest potential for success, while minimizing displacement impacts. Because this screening is occurring nationally, it is still necessary to understand site-level conditions and nuances that cannot be captured with available mapping data.

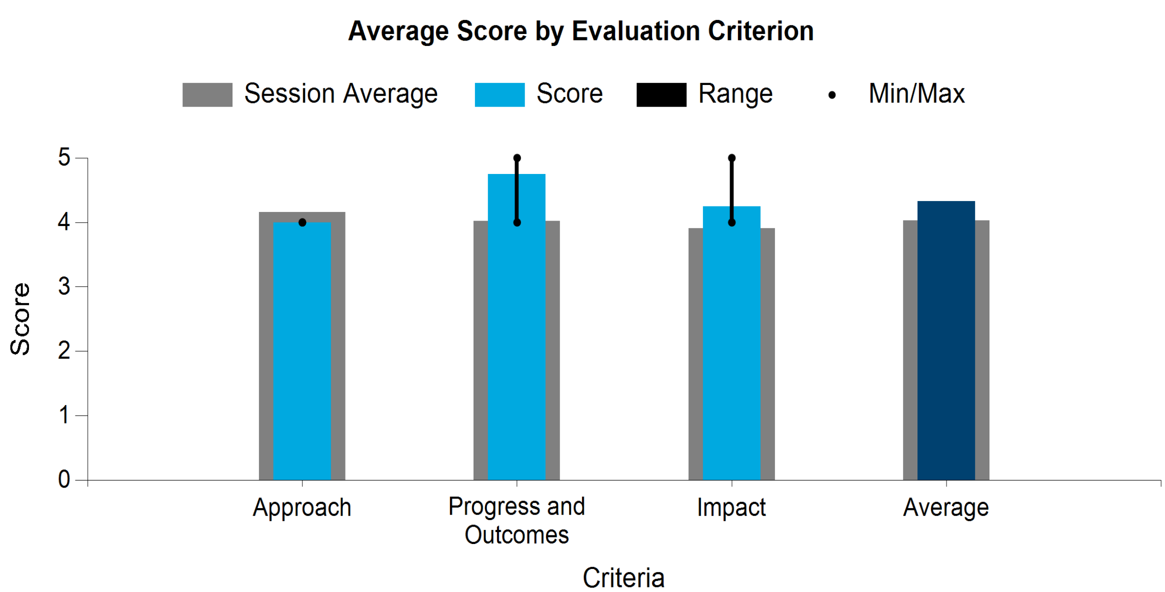
LIFE CYCLE ANALYSIS

Argonne National Laboratory

PROJECT DESCRIPTION

WBS:	1.3.5.204
Presenter(s):	Troy Hawkins
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$500,000

This project provides energy and environmental LCA of advanced algal systems to support BETO R&D decisions and to provide reliable benchmarks for algae production and fuel/product pathways and estimates of their life cycle energy and environmental metrics for BETO stakeholders. It is a continuation of a task that has been active at Argonne for 10 years. In the first year of this new project cycle, the project team is analyzing the life cycle energy and environmental benefits and trade-offs of alternative carbon dioxide sources for algae production, considering CO_2 from DAC, electricity generation, industrial sources, and high-purity sources. We are collaborating with the National Energy Technology Laboratory (T. Skone) for this effort and will leverage LCA data sets for DAC and capture from fossil energy sources. During the first year, the team is also analyzing algae production in saline water, continuing a collaborative effort with PNNL that began in FY 2020 focusing on understanding the energy and environmental implications of salinity maintenance and brine management. In the second and third years of the project, we will expand the focus to LCA, examining production of higher-value products from algae and integration of algae production with wastewater/manure management systems.



COMMENTS

- The goal of the project is LCA for algal systems that include CO_2 sources, saline algae, algal bioproduct, and integration with wastewater. This has clear relevance to BETO's goals of increasing the supply of sustainable algae and reducing the resource intensity, as well as system integration and resource recycling.

- The team appears to be well managed with well-defined task structures and leveraging team expertise and previous experiences. They identified risk and outlined mitigation strategies. The project performers are constantly refining and harmonizing data across models to make them more relevant to the field and have good collaboration with research partners. The team has delivered several milestones and is well on its way to achieving the goals outlined for this project.

- The project analysis demonstrated that fossil fuel CO_2 will result in the highest GHG emissions when compared to biogenic or atmospheric CO_2. It is unclear if this analysis includes the use of CAs and other improved CO_2 capture methods like operating at high pH and the iteration process for integrating data and technologies into the model. The project performers should consider integrating industry feedback into the model, as most of the inputs are based on national lab data. Overall, the team has made significant progress in delivering on goals.

- The project, focusing on LCA of advanced algal systems, runs out in September of this year but is in a situation where it can extend to another 3-year period by filing another application. The team talks about its success on being able to align their tasks with BETO's goals as projected on five areas by (1) providing LCA data for algae production, salinity management, and pond operations; (2) evaluating and comparing carbon dioxide sources affecting algae production; (3) integrating algae cultivation with wastewater and manure management; and (4) harmonizing TEA and LCA within BETO's AAS Program. It is a little difficult in certain parts to understand how the harmonization analysis data flow was achieved across the models between the other national labs and Argonne's Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model. It would be very affirmative if the team could share some success stories that users are benefiting by implementing these models (like an example from the GREET users), which is BETO's mission. There is not much mention about the task on algae cultivation with wastewater and with manure management, which currently falls under the last 5 months of the grant's lifetime. The team has disseminated their findings to the community and stakeholders by publications in peer-reviewed journals, conference presentations, and reports.

- Team management and communication are well outlined, and this appears to be a well-organized project. The goal of this project is to deliver LCA for key production/conversion pathways. They have had a few key findings, including identifying PU from algae as a highly valuable and influential coproduct. The concern with this project is that it is only sourcing data from the national labs, which may be a bit insular and limit the applicability of the findings as the industry grows, although it is unclear if the scope of data required to input is available from other sources. The team does appear to be working with two industry partners directly involved in algae. The focus areas of this project are well aligned with BETO goals. The timeline on the last slide was very helpful. Hopefully the topic areas of focus remain live after each stage such that they can continue to be updated and remain current as the industry emerges.

- The approach of analyzing algal systems using a life cycle approach is important and crucial for BETO to meet its targets. The project team has made good progress in analyzing LCAs for saline algae production, cultivation with CO_2 from DAC, comparisons of CO_2 sources for CO_2 production, and algae bioproduct pathways. The project is on schedule, and the project team is on track to complete its last task involving LCA integration of algae cultivation with wastewater and manure treatment systems. The impact of the project is clear and should provide the value proposition for algal biofuel and bioproduct technologies.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' feedback on the project and support for this analysis to guide the development and scale-up of algal systems capable of delivering on BETO's strategic goals related to decarbonization of transportation, industry, and agriculture. We are dedicated to focusing on the key issues and driving consensus among stakeholders regarding the promising opportunities. The reviewers' comment regarding integration of industry data and perspectives in the project resonates with our plans. We have established relationships and data-sharing agreements with industry partners related to analysis of their technologies and will continue to expand these interactions. We have also leveraged the capabilities developed through this project in work on projects with the Office of Fossil Energy and Carbon Management and ARPA-E, as well as other BETO FOA projects involving engagement with industry partners. We regularly attend the Algae Biomass Organization Conference to present our progress and meet with industry stakeholders. We will continue to seek out opportunities for interaction with industry as we move forward in analyzing options for maximizing the economic and GHG benefits of algal systems through different product strategies and options for improving wastewater resource recovery through integration of algal systems. The reviewer's point about keeping the topic areas "live" as we move forward to explore new questions is well taken. We revisit the algae models in GREET with each annual release to consider updates to reflect the current state of the industry and our understanding. Moving forward, we hope to have the opportunity to renew this project so we can continue to update the GREET algae models, support the SOT assessments for algal biofuel systems, continue building deeper connections with industry stakeholders, and address new issues such as those suggested by the reviewers related to approaches for improved CO_2 utilization to enrich BETO and the community's understanding of the promising opportunities for algal systems. This is a rapidly evolving field with a strong need for analysis to guide research, development, and deployment efforts, and we are honored to have the opportunity to provide actionable results.

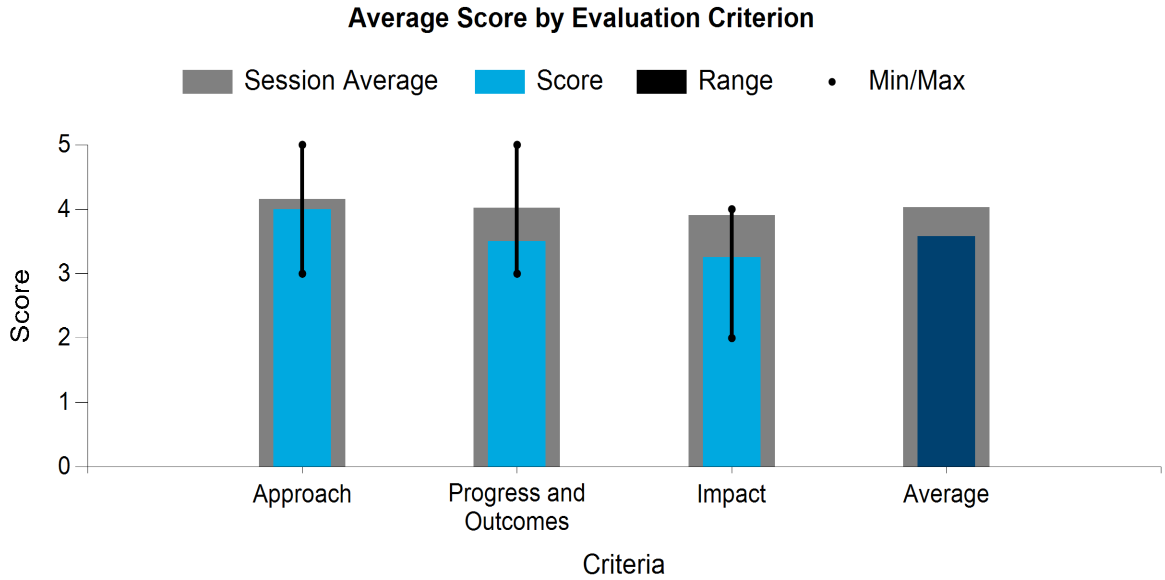
OPTIMIZING SELECTION PRESSURES AND PEST MANAGEMENT TO MAXIMIZE ALGAL BIOMASS YIELD

New Mexico Consortium

PROJECT DESCRIPTION

WBS:	1.3.5.280
Presenter(s):	Alina Corcoran
Project Start Date:	10/01/2019
Planned Project End Date:	02/01/2024
Total Funding:	$6,289,829

The Optimizing Selection Pressures and Pest Management to Maximize Algal Biomass Yield (OSPREY) project responds to a critical industry need to improve annualized productivity, stability, and quality of algal production strains for biofuels and bioproducts. We aim to generate process innovations rooted in outdoor cultivation for strain selection, maintenance, cultivation, improvement, and pest management that will result in a 50% improvement in harvest yield and robustness and a 20% improvement in conversion yield. Our project's components are built on a single foundation: the year-round cultivation of a field-adapted algal biofuel strain in outdoor systems at Qualitas Health (Imperial, Texas), Cyanotech Corporation (Kona, Hawaii), the California Center for Algae Biotechnology (San Diego, California), and the Fabian Garcia Science Center (Las Cruces, New Mexico). We envisioned that the unique environmental selection pressures of each outdoor system would allow us to naturally develop robust cultivars with different environmental tolerances. Project components include tracking trait drift and evolution in the field and lab, using metagenomic tools to identify and track pests/pathogens, using non-genetically modified approaches to improve the baseline field-adapted strain, implementing process improvements, and assessing the effects of improvements through sustainability modeling based on open-raceway pond growth architectures. To date, our technical accomplishments include (1) the cultivation of industrial field-adapted strains at three additional locations since summer/fall 2020, (2) phenotypic and genotypic trait tracking every 6 months, (3) metagenome characterization across sites, (4) detection of novel pests, (5) development of a fieldable qPCR tool, (6) application of selection and mutagenesis/selection to drive cold and hot tolerance, (7) hindcasting of productivities across sites, and (8) exploring the effects of shifts in biomass composition on the minimum fuel selling price. Selection pressures were not strong enough and/or the time was not long enough to capture cultivars in the field. This project responds directly to DE-FOA-00029 with an indoor/outdoor experimental framework and the development of tools to monitor cultivation health.



COMMENTS

- The risk mitigation, decision-making, and project management are all clearly laid out and easy to follow. It seems like the risk mitigation initial estimate wasn't as accurate as it could have been due to field selection pressures not being thoroughly understood; Qualitas and Cyanotech should be tracking the generations of field cultures and periodically sampling and should have shared these data to give you an initial working idea of how many generations are required to realize trait evolution. I love the overview of progress on Slide 16; this is perfect. There are no y-axis markings on the left side of Slide 17. It would be helpful to know if the field PCR analysis would be run in a time window sufficient to mitigate the infection/predation. Adding the data regarding ultraviolet kill of pests and its effect on the algae would have been helpful, as well as the data for clonal isolation from the mutagenized volumes that underwent clonal selection. The cryopreserved reference strain is a good benchmarking practice; it would also be good to select either single nucleotide polymorphisms (SNPs) or some critical gene to monitor for mutation as well.

- The project scope change complicates reviewing the goals against the objectives. It appears that the changes remained true to the goals of BETO, were made with the blessing of BETO staff, and were executed well. It shows the involvement of BETO staff in shaping and maintaining projects. Great example of active project management.

- The approach is thorough and sound. The team composition is complementary. qPCR in the field was promised and delivered. The outside mutagenesis and cryopreservation data being out in the open literature is a plus. In a program funded by public money, there is certainly a desire to have project learnings shared with the entire community. This is, of course, counter to the desires of a company seeking to develop and maintain a proprietary competitive advantage. This project is sharing some data, which is a good thing. I'm happy to see the team is thinking about how to strike a balance.

- Approach: This project is a collaboration between several well-qualified companies, universities, and government labs, each of which brings established strengths to the project. The general approach being taken is directly relevant to BETO and AAS goals, although the results may be applicable to a relatively small subset of strains (*Nannochloropsis*, in particular, if in fact that was the strain being evaluated throughout these studies, which was not entirely clear). However, the presentation did not reveal a well-integrated strategy; rather, it seemed that several fairly disparate research activities were undertaken that didn't have an obvious connection (e.g., strain preservation methods, qPCR for pest evaluation, in-field mutagenesis, SNP analysis to check on genetic drift).

- Progress and Outcomes: The mutagenesis experiments to develop a cold-tolerant strain were interesting, but more work would need to be done to see if this represents an industrially relevant advance (i.e., is the improvement great enough to actually enable profitable growth in cold seasons?). Due to the multigenic nature of cold adaptation, this reviewer feels that mutagenesis for enhanced growth under cold conditions is unlikely to yield strains that are significantly and stably improved such that the overall production economics are significantly improved. Efforts to find native strains that are naturally adapted to colder temperatures may be more successful, although even then the thermodynamic constraints of physiological and biochemical processes at low temperatures will likely limit potential enhancements.

- Fieldable qPCR is interesting from an R&D perspective, but it may not enable mitigation of pest strain contamination events unless the particular contaminant strains being tested for are amenable to specific or broadly applicable pest control efforts that can be initiated in a rapid and meaningful time frame.

- Higher levels of SNPs in strains that have gone through many generations is not altogether surprising, considering that many (or most) of these may represent silent or neutral mutations. It wasn't clear, at least to this reviewer, whether the SNPs were found in DNA isolated from the bulk population or from single cells that had been isolated from the cultures and grown up for DNA extraction as clonal cultures. This would help to understand if there are multiple SNPs occurring in single strains or across a whole population. Estimating the numbers of cell divisions (generations) for the different cultures being compared would be useful information.

- Impact: Determining the composition of contaminant populations and making correlations of particular species with periods of poor (and possibly good) productivity will help to build a database that informs culture maintenance strategies. For maximal value, this type of analysis should be conducted across multiple sites with several algal species and cultivation protocols in order to identify possible commonalities.

- It is well established in industrial microbiology (e.g., fermentation companies) that cryopreservation of strains and periodic reestablishment of inoculum seed trains with cryostocks is an important and necessary means to preserve strain integrity and maintain consistent production results. Although this work confirms this well-established principle for algae, it may not be worth continuing such studies beyond getting a better understanding of how long a semi-batch or continuous culture can be run, although even then, empirical productivity measurements will best define strain stability.

- Approach: Had to be changed in regard to trait drift and evolution. Unable to show trait drift in the field, which could relate to the amount of time permitted for drift. Progress and Outcomes: Had to change approach due to lack of progress; data output is here. Not clear that the data were particularly impactful. Better presentation of the data is needed to show the improvements claimed. Impact: The qPCR tool could have some impact; the data do not have a lot of impact other than to prove to industry that their strains should be stable in production. However, proving a lack of strain drift in the field is important, as consideration of trait drift in productivity decreases can prevent producers from finding the real root cause of production issues. The qPCR equipment work approach is good. This information is impactful.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for evaluating our project and welcome the opportunity to address key comments. We will start with the project approach. One reviewer noted that our project had a lot of components that were not strategically integrated. Our project's components—(1) balancing indoor and outdoor selection pressures, (2) optimizing pest management, and (3) improving field strain performance, resiliency, and composition, all to enhance biomass production and stability—are built on a single foundation: the long-term cultivation of *Nannochloropsis* at different field sites. We aimed to start with a field-adapted strain and use lab-field iterations to overcome some of the challenges associated with the lab-to-field pipeline commonly followed in R&D. We also want to clarify that the aim of the first component was not to confirm reestablishment of inoculum seed trains with cryostocks as a key practice. Rather, we planned to establish local cultivars that would show phenotypic advantages over the cryopreserved strain. As this result was not obtained, we shared the results we did have. With respect to qPCR, the analysis can be run in a few hours, such that if pond samples are taken in the morning, ponds can be treated in the afternoon. This approach has previously been used on specific pests at industrial scales. Regarding strain improvement, mutations were found in DNA isolated from the bulk populations. Generation number varied across sites, with the most at the University of California, San Diego, the least at New Mexico State University, and Cyanotech being intermediate. Additional work will focus on mutations that are linked to cell function. For our cold adaptation work, we agree that strains might not be improved enough to affect overall production economics. However, if successful, we will validate a pipeline that can be used in other seasons.

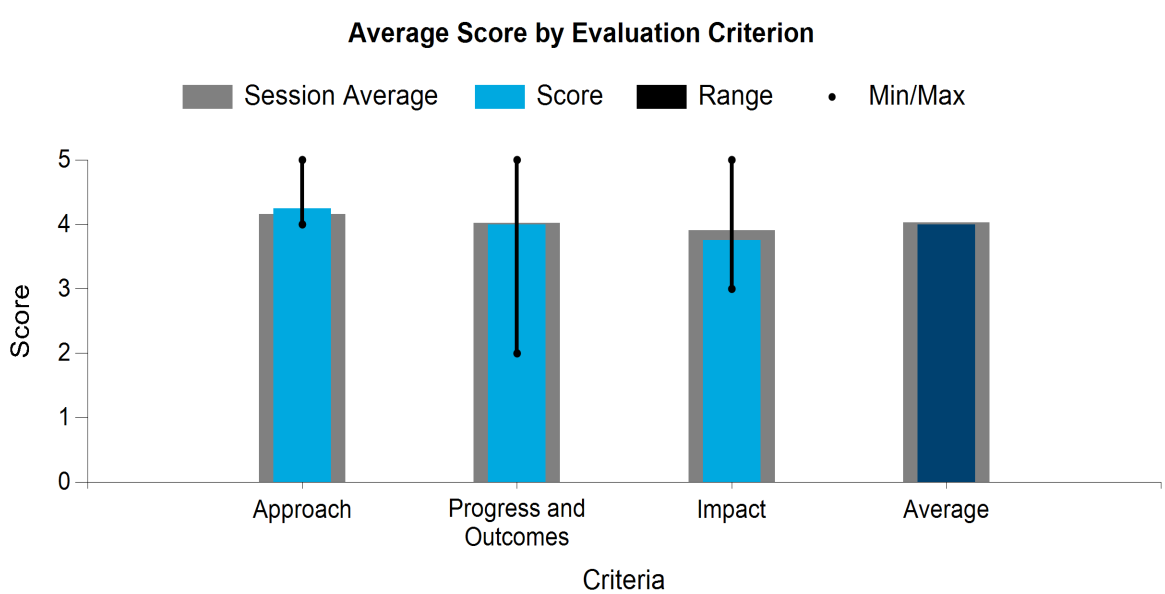
ALGAL PRODUCTIVITY ENHANCEMENTS BY RAPID SCREENING AND SELECTION OF IMPROVED BIOMASS AND LIPID PRODUCING PHOTOTROPHS (APEX)

Colorado School of Mines

PROJECT DESCRIPTION

WBS:	1.3.5.282
Presenter(s):	Matthew Posewitz
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2024
Total Funding:	$4,920,378

We are using random mutagenesis techniques (e.g., atmospheric and room temperature plasma mutagenesis) to generate genetic diversity in two oleaginous strains of algae (*Nitzschia inconspicua* and *Nannochloropsis granulata*). Mutant pools are grown in solar-simulating bioreactors to enrich for robust growth, and then high-lipid strains are sorted using fluorescence-activated cell sorting to isolate higher-oil-accumulating strains. After multiple rounds of enrichment and rapid growth campaigns, single cells are sorted from the highest-lipid cultivars during fluorescence-activated cell sorting. To date, we have downselected to four strains of *Nitzschia inconspicua* of interest. One strain (GAI-370) is able to attain diel yields of ~40 g/m^2/d in solar-simulating bioreactors and attained lipid yields of 60% in lipid phase growth. Initial outdoor growth campaigns yielded sustained productivities of ~22 g/m^2/d through lipid phase, with lipid yields >31% during lipid phase. Strain stability is being validated through sustained growth campaigns and after freeze/revive cycles. Diatom breeding is also being explored as a potentially powerful approach to generate biomass diversity for the screening and isolation of more oleaginous strains with phenotypes of interest. Initial libraries of *Nannochloropsis granulata* have been isolated and are being screened for high-growth/high-lipid isolates.



COMMENTS

- The risk mitigation, metrics, and decision points are clear. Fluorescence-activated cell sorting selection is good; it's a very proven method. The clone screening is excellent; thank you for picking enough clones. The screening criteria are clearly defined and relevant. It would be helpful to see how strain/clone 370 compared to other GAI strains. Other than GAI, it would have been good to see more industry engagement.

- Phenotypic screening and freeze/thaw behavior of the culture is not sufficient to ensure cell line stability: Genetic monitoring should also be used, particularly since another distribution of cells is observed after bioreactor cultivation and the observation of smaller cells present in the culture. The environmental enrichment for photobleaching events and oxygen tolerance is a good strategy.

- This project is well presented and well aligned with goals. Easily all aspects of the goals are comprehensively addressed. There are significant strengths.

- This is an example of a company being funded where information will remain proprietary. In a perfect world, information would be "free" once obtained on the public dime. This is, of course, directly opposed to company goals of protecting IP as a competitive advantage. I am impressed that the speaker indicated that attempts were being made to share widely, where appropriate. This is a very reasonable approach, and I commend it.

- Approach: The project personnel are attempting to use classical strain development strategies (e.g., mutagenesis and breeding, coupled with screening based on fluorescence-activated cell sorting) to increase at the same time both the lipid content and overall biomass productivity for *Nitzschia* and *Nannochloropsis*, and in a manner that is manifest in outdoor cultivation trials. This is clearly in line with AAS goals to lower the cost of algal biofuel production.

- The project team is well qualified to conduct the research, both with respect to strain development and testing in the lab and outdoors.

- Progress and Outcomes: Strains of *Nitzschia* were chosen after several screening rounds that demonstrated faster lipid accumulation upon induction; this is certainly a favorable outcome that can have a positive impact on the economic bottom line.

- Data were not provided as to whether the isolates selected using fluorescence-activated cell sorting with high BODIPY staining maintained that phenotype after numerous generations. Such data would help to assess whether the strains were truly stable mutants or whether the higher BODIPY staining was based more on the physiological state of particular individual cells or transient morphotypes (e.g., different stages of cell division).

- Without parallel, contemporaneous data for the control strain (GAI-337), it is hard to assess whether improvements seen for GAI-370 at lab scale translate into similar improvements in outdoor field trials. Retesting outdoors for GAI-370 alongside control ponds with GAI-337 will be critically important to answer this question.

- In the 2021 Peer Review, it was stated that strain collection/discovery efforts were underway, with one goal being to identify *Nitzschia* strains that could serve as mating partners for improving the existing *Nitzschia inconspicua* strain via sexual breeding. No updates were provided on this topic, including information on gamete formation of the existing strain or any new isolates. In addition, no information was provided regarding *Nannochloropsis granulata*, other than a statement that mutant libraries were being screened. Considering that the project has been up and running for 2.5 years, the overall progress seems somewhat behind; however, a timeline chart was not shown, so it's not possible to track actual progress in the different project elements against expected progress.

- Impact: The demonstration that improved *Nitzschia* strains were able to achieve high lipid levels faster than the parental strain would likely have positive financial implications because more commercial batch cultures could potentially be completed in a given amount of time. It will be important to demonstrate that there is a statistically significant improvement of the new strains versus the control (parental) strain in outdoor cultivations.

- Progress and Outcomes: The project is on track with goals, perhaps slightly behind with the *Nannochloropsis* work, with just 1 year left to run the project. *Nannochloropsis* will not make it outdoors for much time at all, if at all. However, progress with *Nitzschia* is significant in terms of accomplishing established productivity goals. Impact: The impact and outcomes from publications and patents are good; the ability for industry at large to access these adapted strains does not seem to be possible. If the concept is that every company would have to go through this process to improve their own strain, then the impact is limited in scope.

PI RESPONSE TO REVIEWER COMMENTS

- Strain 370 is actively being compared to other GAI strains in use at the GAI farm site. To date, 370 has been among the best performers, but it is important to compare under more extensive and diverse conditions. We are in the process of filing initial IP claims on the strains selected, at which point it is expected that the strains can be utilized by other researchers. We agree that freeze/thaw is not sufficient for assessing strain stability. We are in the process of genome resequencing of the top-performing strains, determining whether genetic loci can be mapped, and then using DNA sequencing to verify strain maintenance and phenotype correlations. We thank the reviewer regarding their support for publishing our data. This is actively ongoing, and we agree that data sharing is important for the community. We are certainly monitoring phenotypes through generational grow-out campaigns. The reviewer is correct in identifying this critical issue, and experiments are underway to monitor growth/phenotype over a 1-year period. In the summers of 2023/2024, growth campaigns monitoring 370 relative to controls at the farm are planned to demonstrate comparative differences. To date, we have not identified any mating partners to *Nitzschia inconspicua*. These experiments are ongoing. The *Nannochloropsis* library has been generated. Screening efforts are planned for summer 2023. We agree that statistical significance of the improved strains is important to demonstrate at the pond, and efforts are underway to attain these data. It is hoped that *Nannochloropsis* will be run outdoors in summer 2024. The project still has ~1.5 years to run, and there should be time for outdoor *Nannochloropsis* work. It is our hope to make strains available to other interested parties as we publish our results.

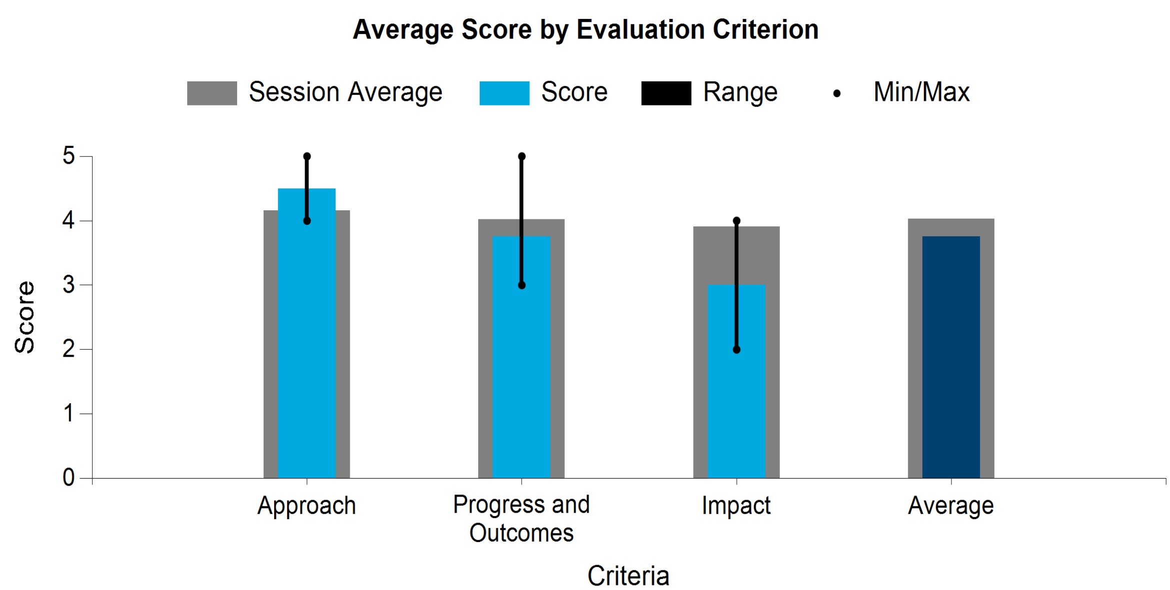
INNOVATIONS IN ALGAE CULTIVATIONS

Global Algae Innovations

PROJECT DESCRIPTION

WBS:	1.3.5.284
Presenter(s):	David Hazlebeck
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2024
Total Funding:	$5,625,000

GAI has developed low-cost algae production technologies aimed at achieving commercially viable production of biofuel and high-protein meal. Radical advances have been designed and implemented throughout the entire process, resulting in many industry breakthroughs for large-scale algae cultivation, harvesting, and processing. The goals of this project are to overcome the challenge in translating results between laboratory and mass cultures and to increase algal productivity by 50%, cultivation robustness by 50%, and lipids by 20% while achieving cost and LCA targets. A series of seven innovations in cultivation methods and three innovations in cultivation monitoring tools were developed, and a chain of test systems from laboratory-scale microplates through outdoor raceways producing kilograms of algae biomass was developed and tested to accelerate the indoor/outdoor cycle rate and improve the translation of laboratory results to mass culture. Through these advances, the lipid content at harvest was increased by 50% of the ash-free dry weight, which is a 90% improvement, and the productivity was increased by 15%–50% depending on the season, with greater improvement in the winter. During the next budget period, the lipid formation approach will be investigated in greater detail to provide greater understanding of the impact of abiotic and biotic conditions and to routinely achieve greater than 50% oil content in open outdoor cultivation. Additionally, a rapid compositional measurement tool was developed using near-infrared that accurately predicts the lipid and protein content of the algae. During the next budget period, the measurement tool will be optimized, used to support greater understanding of lipid formation, and moved toward a potential commercial product to make it widely available.



COMMENTS

- The goals are clear and quantitative. It wasn't clear how kLa and other scale factors are being compared across the methods, especially because mass transfer and mixing challenges are difficult to replicate at very small scales and the intermediate-scale systems leaked. It's great that the author is tightening up sample handling and processing, as this is the first step to process analytics with real-time controls, something that will be critical to some of the DAC implementations. The biotic versus abiotic information is really interesting; it would be nice if there was more explanation, even though many of the interventions are proprietary, particularly when it comes to impact and what the relative costs of those methods are. For the analytics, it would help to understand from an implementation perspective if this is something that could be done with an original equipment manufacturer Ocean Insight system or if it requires a custom build and peak validation.

- Several times it was mentioned that the project ran out of time during the budget period. Reasons were not given in detail. This is certainly a negative when asked whether the project is delivering appropriately against goals.

- The number of process patent applications was held up as a sign of progress. It does not come across as a compelling example of progress. One positive outcome of a patent is that it eventually becomes public information. Concerning is that these advances cannot be talked about for fear of wrecking a patent, making it impossible for us to review the novelty or impact. There are negatives. The biggest one is that process patents are difficult to police and frequently easy to circumvent. The patents were described as being in oil purification. This is a well-populated area due to the history of seed oil purification. It seems unlikely that there is an area of huge novelty remaining, and nothing said provided clear evidence that these were powerful aids to eventual success.

- In a program funded by public money, there is certainly a desire to have project learnings shared with the entire community. This is, of course, counter to the desires of a company seeking to develop and maintain a proprietary competitive advantage. It's good that equipment designs are being shared, great that tools are being used at multiple institutions, and great that there is a public toolkit for a new strain evolution method.

- Approach: This project is focused largely on the development of new tools, primarily small-scale growth systems along with equipment for determining the lipid, protein, and carbohydrate composition of algae. The tools are being used to assess new cultivation procedures to enhance the lipid content and productivity. Hamilton Robotics is listed as a project partner for certain aspects of the project, although their specific role was not defined in the presentation.

- Progress and Outcomes: Some of the tool development work reported in this project represents basically the same research topics that have been carried out and described by numerous groups (e.g., microplate and flask testing of strains, lab PBRs, automated monitoring for nutrient levels [and coupled feed systems], pH, DO, temperature). It wasn't clear in many cases what was actually novel, other than perhaps the small-scale sloped raceways.

- It appears that good progress is being made on biomass and/or lipid productivity, although details on results, methods, or procedures were not provided due to the desire to protect IP. Hopefully more clarity will be provided soon on the proprietary biotic and abiotic methods used to increase productivity. It would have been informative to know more details about how these experiments were conducted, including scale, whether the controls were run concomitantly or at different times, etc. More information on the lipid formation method (induction) and respiration control would also have been helpful to assess the progress and novel aspects of the project.

- Perhaps this is by design, but there seems to be overlap between the Colorado School of Mines project (1.3.5.282) and this one with respect to the results on improving the lipid production rate.
- Results were presented indicating that a spectroscopic tool had been developed that enabled measurement of lipid, protein, and carbohydrate levels in at least one strain. This would be a good outcome if it provides advantages over standard infrared measurement systems for these algal components and can be applied to multiple, disparate species.
- Impact: Assuming that the increases in lipid content and productivity that were reported are validated and that the methods that result in the enhancement are ultimately published or patented in a manner accessible to others, then the project results should be beneficial to the algae industry as a whole, especially if the methods are applicable to multiple strain types.
- It will be interesting to follow the commercialization and implementation of the spectroscopic compositional analysis equipment and procedures that were developed in this project. The specifics of the system and sample preparation methods weren't disclosed, which makes it difficult to assess the novelty and utility of the system, but hopefully it becomes a useful and widely applicable tool for the algae research community.
- Approach: It isn't clear why new cultivation testing tools were being developed (lab PBRs are not new). Why were on-the-market PBRs not viable as testing vessels? It is clear that this company has unique pond engineering and that mini-pond research specific to their ponds would require some modifications to most mini-ponds on the market. The spec methods for composition are a very nice new tool. There is only one collaborator for spectrophotometric work but no other lab, academic, or industry participants. The project seems to be managed well, but not much information on project management was presented. There was not enough forethought into difficulties with commissioning new systems, no mitigation plan in place for risk, and not enough resources to overcome issues during the project. Outcomes: Not all the areas that were planned to test to improve cultivation were done (nutrient addition and timing). Outcomes were not presented, as they were reported to be confidential. This makes determining outcomes and impact very difficult. The project greatly underestimated the effort to set up new systems, which limited outcomes significantly. Impact: Hard to evaluate—patents and confidential outputs, so impact is extremely limited as a result. Spectrophotometer methods are impactful.

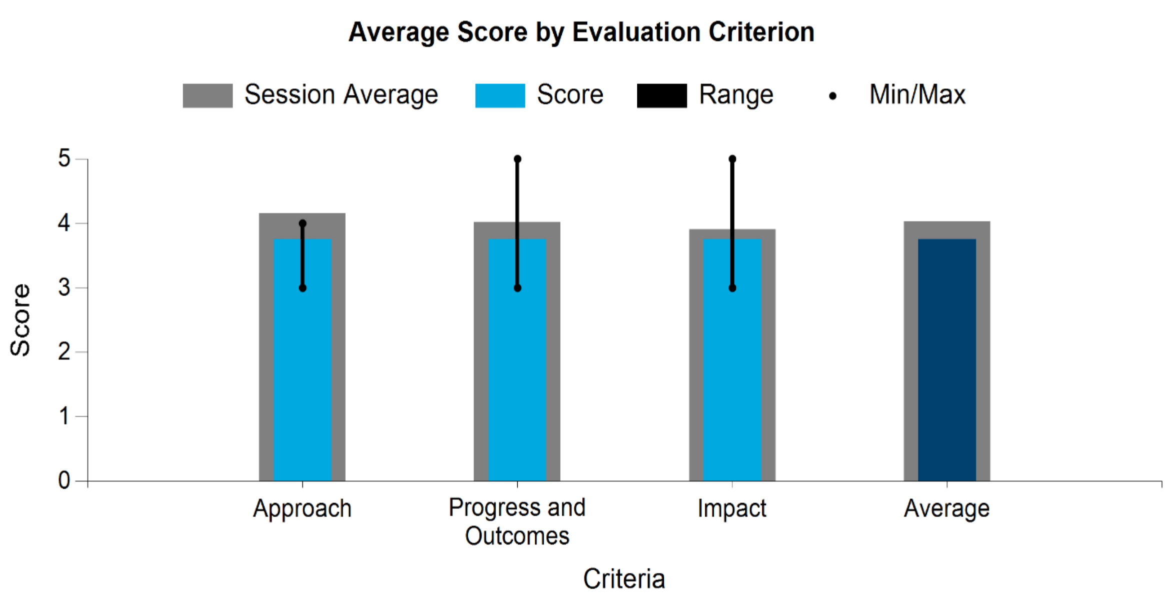
IMPROVING THE PRODUCTIVITY AND PERFORMANCE OF LARGE-SCALE INTEGRATED ALGAL SYSTEMS FOR WASTEWATER TREATMENT AND BIOFUEL PRODUCTION

University of Illinois at Urbana-Champaign

PROJECT DESCRIPTION

WBS:	1.3.5.286
Presenter(s):	Lance Schideman
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2024
Total Funding:	$3,764,553

Producing biofuels from algal biomass is currently one of the most promising approaches for meeting society's need for sustainable energy, because algae grows faster than other biofuel feedstocks while using marginal land and low-quality water resources that compete less with food production. However, high biomass production costs remain a significant challenge that limits the practical use of algal biofuels. Thus, the overarching goal of this project is to develop and demonstrate an integrated system for algal biofuel production and wastewater treatment that can reduce biofuel costs below DOE's minimum fuel selling price target ($2.50/GGE). This approach is compelling because of the significant coproduct value of treated wastewater and dual-use infrastructure, and because wastewater provides a low-cost source of major algae cultivation inputs (e.g., water, nutrients). In this project, we are developing novel biological and engineering approaches to enhance the biomass productivity of a commercially available algal wastewater treatment system, called Algaewheel, and conversion of the resulting mixed algal biomass to biofuels via HTL. The methods being studied to improve algae cultivation and biofuel conversion include bioaugmentation with bacteria that provide algal growth promoters, stress-induced endoreduplication to increase cell size, integration of adsorbents, dynamic control models, and nanofiltration of HTL aqueous products for improved carbon efficiency. The integration of these techniques at pilot scale has been shown to increase biomass productivity by more than 50% (>30 g/m^2/day) and has increased the efficiency of biofuel production by more than 20%. In the current budget period, these improvements will be validated in demonstration-scale testing at an operating Algaewheel plant used for domestic wastewater treatment.



COMMENTS

- The project timeline slide is good, though you have a lot of milestones all occurring at the same time, which could make risk management more challenging. The progress and outcomes look great, exceeding productivity goals, especially in the nanofiltration unit operation. More explanation of what happened to Lake 2 would be helpful. There is not much industry engagement in the impact section. The selection of two weather conditions (cold and warm) is good, as this has been problematic in past field work. Wild-type bacteria isolated from the environment would have been a more useful test than ATCC strains, which tend to be less robust and have a history of being problematic in the past (cross contamination, incorrectly identified, etc.). You will likely have to shift to a tangential flow filtration method of nanofiltration (whether hollow fiber or flat sheet), and this may add significant economic challenges.

- The definition of "pilot" was a bit ambiguous. Pilot is a word used with inadequate definition. This is a criticism that falls both on this project team and the algae program. I prefer defining a pilot as the smallest scale that can be operated to gain understanding sufficient to move to the next stage of scale-up. Ideally, a pilot allows the move to full production. For this particular technology, I don't know exactly what will define pilot. I believe this requires both the wheel and pond to be of sufficient size to be able to move with confidence to the next scale. If the thought has already been expended, it was not articulated. It appears the wheel is pilot scale. This may be OK, but it was not clearly stated. It is not clear how this is building to the future.

- The trends observed are all positive, whether productivity or ash content. The project appears consistent with the goals outlined for the project.

- Approach: The project has the primary goal to increase the productivity of the Algaewheel system for wastewater treatment, coupled to fuel production via HTL processes. A variety of treatments were applied to cultures to enhance productivity, and a process step was added to increase the yield of HTL-produced bio-oil. Field demonstrations at two sites in the United States are planned for the coming year. The approach and stated objectives are aligned with BETO and AAS goals to improve algal productivity and develop cost-effective biofuels and related coproducts.

- Progress and Outcomes: Data were presented indicating substantial increases in productivity and HTL-based bio-oil yield for Algaewheel-grown mixed algal/bacterial cultures.

- The premise that the formation of polyploid cells will improve productivity was not well explained or documented; in fact, the data indicating that genome duplication has occurred are not at all conclusive in this reviewer's perspective. It is not clear whether saline-induced polyploidy, if true, is a stable change or whether the increase in salinity simply transiently halted physical cell division. No data were presented indicating whether the larger cells reported to be polyploid cells actually led to enhanced productivity. Without corroborating data, it is not clear that continuing down this endoreduplication path is a worthwhile venture.

- It is also not clear from the data that the addition of *Azospirillum* cells made much of a difference in productivity, especially considering that there appeared to be a large (albeit delayed) increase in growth for both the control and treatment tanks upon increased carbon substrate addition (glycerol or tryptophan malate). The claimed 20% increase over the control was attributed to IAA production by the added *Azospirillum* cells, but the lack of error bars makes it hard to assess whether the increase was statistically significant or not. The presenter indicated during the Q&A session that experiments had been conducted that showed similarly large increases in productivity upon the direct addition of IAA, but the actual data weren't presented.

- The presenter showed a 73% improvement in HTL yields upon recycling the nanofiltration retentate, which is quite remarkable. In order to determine the fuel potential of the HTL oil produced in this manner, it would be helpful to know more about the organic composition of the retentate and the molecular weight range of HTL-derived oil products with and without recycling the retentate.
- It was not indicated in the presentation how harvesting would be accomplished with the Algaewheel system in a commercial-scale system, or how those costs were included in the interim TEA.
- Impact: If field trials scheduled for the coming year validate the data obtained to date, and if the assumptions in the TEA are verified by others in the field (e.g., NREL and PNNL analysis teams), then this research would align well with the BETO/AAS initiative to investigate low-cost algae with coproduct (i.e., wastewater treatment) potential for biofuel production.
- Approach: No input on the management plan was presented. Outcomes: Great work with presenting data and outcomes; I can see the progress from the project. Impact: Good impact with this work—if implemented by industry, it looks to be a game changer to a few issues. The next year will determine the amount of impact, depending how it goes in full deployment.

PI RESPONSE TO REVIEWER COMMENTS

- The timing of milestones, with many occurring simultaneously at the end of Budget Period 2, was designed to give the technologies that included bench-scale work more time to refine desirable operating conditions prior to upscaling to greenhouse pilot work with the Algaewheel rotating algal contactors. This did make the pilot testing for those technologies a bottleneck that contributed to the need for a no-cost extension, but ultimately, we were able to demonstrate a 50% increase in productivity and meet the Budget Period 2 go/no-go criteria. The HTL biomass conversion data for Lakes 1 and 2 show a range of results for different algal biomass sources when using nanofiltration to concentrate the HTL aqueous product. Both lake biomass samples were natural microalgal blooms collected by dissolved air flotation and further dewatered using a screw press. The recycling of the nanofiltered HTL aqueous product from Lake 1 did not improve oil yield, which we believe is primarily due to having a significantly lower biomass concentration and concentration of organics in the HTL aqueous product than the other samples. To achieve a higher oil yield when recycled, the Lake 1 HTL aqueous phase would likely require a more concentrated nanofiltration retentate. The recycling of the nanofiltered HTL aqueous product from Lake 2 did improve oil yield for some operating conditions (membrane type, chemical pretreatment, etc.), but other operating conditions did not increase oil yield. Overall, these supplementary data highlight that the nanofiltration process needs to be optimized for each source of biomass and HTL aqueous product. Since we wanted to test a variety of nanofiltration conditions, we decided to perform our experiments in a dead-end filtration system, which requires less volume of feed to be operated than other filtration systems. Tangential flow filtration systems offer enhanced scalability and will be a good option for the future scale-up of this process. Additional pretreatments to decrease fouling and flux decline, along with optimization of operational conditions, will help overcome the said economic challenges. It is worth mentioning that nanofiltration would still be less costly and uses less energy than the current state-of-the-art technology for aqueous-phase treatment (hydrothermal gasification), which can cost as much as HTL itself. Our commercial partner on this project is OneWater Inc., who is the commercial supplier of the Algaewheel system. They have more than 10 operating wastewater plants in the United States, which will provide a direct link for delivering the results of this project into the wastewater market. However, we agree with the need to do more general industry outreach in the future. Because the next phase of the project will incorporate the demonstrated productivity enhancements into two of the operating wastewater treatment plants, we feel that the resulting data from this upcoming effort will be more compelling for the wastewater industry. Some bench-scale testing was started with ATCC cultures so as to provide a more consistent starting point for our experiments that could potentially be replicated by others and compared with other literature data using these strains. Once in our lab, we struck out these strains to confirm purity and used matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) to confirm identification. Routine microbiological techniques such as single-colony plate streaking and MALDI-TOF were then used to prevent contamination and monitor culture purity over time. Ultimately, our work with pure cultures is a simplified experimental precursor to using the same productivity-enhancing techniques with the complex, mixed-species, algal bacterial cultures that are used in the Algaewheel system. Thus, the techniques must eventually have broad applicability beyond the single cultures used in our lab experiments. Each pilot-scale tank that we used is a six-wheel, 180-gallon system with an average flow of 60 gallons per day. We used the smallest of the commercially available Algaewheels that are currently used in most of their full-scale installations. Due to space and other location constraints, we opted for using a longer hydraulic retention time with a more concentrated simulated wastewater feed, but the daily loading of key wastewater contaminants (COD, NH_3) at the pilot scale was set to be within the range of long-term historical conditions for full-scale Algaewheel systems. Due to time constraints, we only briefly touched on our upcoming (Budget Period 3) full-scale demonstrations, as this experimental period has just recently begun. All the successful pilot treatments will be upscaled for use in an operating full-scale Algaewheel treatment plant. The first demonstration with full-scale Algaewheel tanks will have 50 wheels (same size as our pilot) and a volume of approximately 1,300 gallons and will receive an influent wastewater flow rate of 6,333 gallons per day. There are 12 Algaewheel tanks of this size at the first full-scale demonstration testing location in Gardner, Illinois, which recently began testing. The second full-scale testing location will be in Florida, which is being planned now and is expected to start demonstration testing in fall 2023. Due to time constraints, we did not provide as much information on the premise and potential for increased biomass production via endoreduplication. We provided some more information on these topics in the 2021 Peer Review and focused on other more recent pilot work in 2023. One of our collaborators has worked extensively on endoreduplication in terrestrial plants (https://doi.org/10.1007/s00442-019-04458-1) and has shown the potential for increasing biomass. More recent work has shown that endoreduplication can also be induced in algae to produce an increase in desirable biomass products (https://doi.org/10.1016/j.biortech.2019.121332). We subjected our productivity with and without the addition of *Azospirillum* cells to a pairwise Student T-test and found that it was statistically significant ($p < 0.05$). The average relative standard deviation of these data was 4.8% of the productivity value, which provides a general understanding of the size of the error bars. Experiments with the direct addition of IAA were conducted at bench scale with cultures of individual algae (e.g., *Chlorella vulgaris*) and showed biomass production that was 50% higher than controls. We did not conduct pilot tests with direct addition of IAA prior to the 2023 Peer Review meeting, but they are now being conducted. Our goal for the HTL experiments we presented was to identify the conditions that resulted in the highest oil yield increase. In our current and future experiments, we will perform gas chromatography–mass spectrometry for analysis of key chemical groups with thermogravimetric analysis to have a better understanding of the effects of recycling the aqueous phase on biocrude oil quality and fuel potential. Harvesting of biomass in our pilot system and in current full-scale Algaewheel systems occurs by natural sloughing and subsequent sedimentation in a clarifier. We have shown that increasing the aeration rate and spin rate of the algae wheels can enhance the rate of sloughing and amount of biomass harvested, while also reducing the ash content of the sloughed biomass. We believe the latter benefit is due to reduced time for predation on the surface of the wheels.

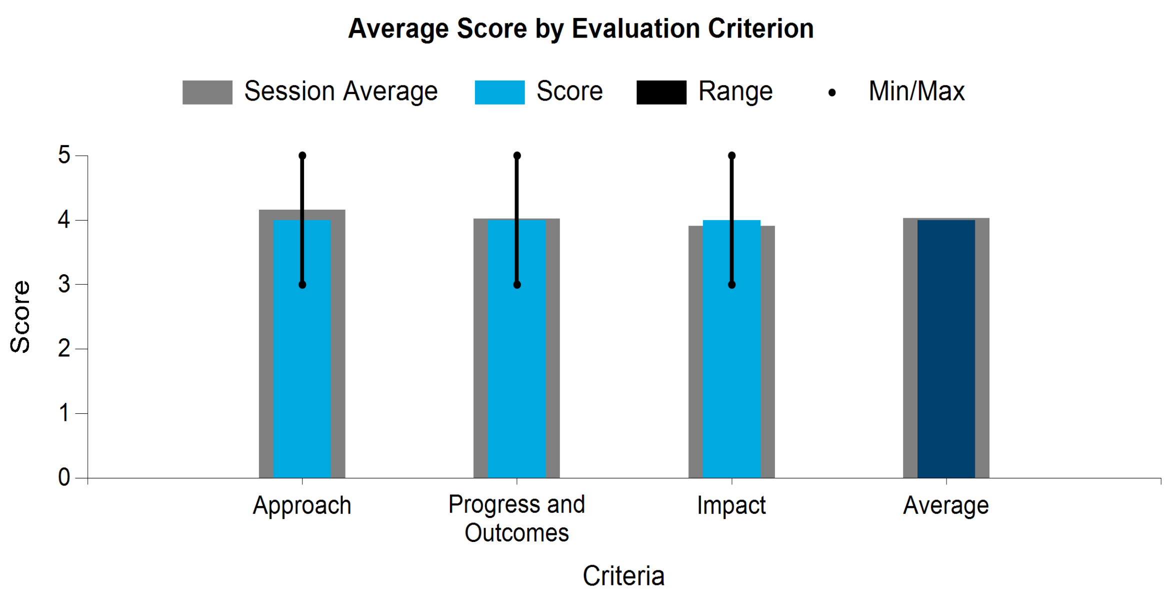
DECISION-MODEL-SUPPORTED ALGAL CULTIVATION PROCESS ENHANCEMENT

Arizona State University

PROJECT DESCRIPTION

WBS:	1.3.5.287
Presenter(s):	John McGowen
Project Start Date:	10/01/2019
Planned Project End Date:	06/30/2023
Total Funding:	$4,375,000

Current decision support models (TEA, LCA, and growth/productivity) for large-scale algae cultivation systems lack critically important quantitative, culture-failure risk data. At very large scales, semicontinuous versus full-batch cultivation strategies present very different risk profiles with respect to the consequences of culture failures from pathogens, grazers, and competitors. These uncertainties constitute a critical knowledge gap that must be closed to guide major investments in commercial algal biofuel systems and enable systems for crop insurance. We will quantify the economic and technical risks associated with different cultivation strategies through an integrated program of indoor lab studies, cultivation simulation and optimization, and multiscale "omics," including robust outdoor cultivation campaigns informed by more than 6 years of outdoor cultivation data generated at AzCATI. Through the development and deployment of a suite of novel real-time sensors for nutrient and water quality monitoring, we will gain better process control though novel insights, plus the ability to optimize productivity, robustness, and biomass quality of our selected high-performance strains. System optimization will include concurrent economic and life cycle modeling coupled with production process variability modeling. This work will directly integrate with experimental systems to understand the impact of the advancements and provide data feedback for focused investigations.



COMMENTS

- The explanation of communications and information management is helpful.
- Unfortunately, bacterial and fungal predation are very common and tough to address with lab-grown algae strains. Even if antibiotics and antifungals were cheap and plentiful, the costs and containment

especially are really difficult, and you can't use a good fraction of your products as they are too contaminated by the antibiotics and antifungals to be useful for fermentation media or fine chemicals starting materials. It also eliminates the possibility of using any of your products for human or animal consumption in any form, even as fertilizer for fields. You'll see a drop in culture health a day or two before you can detect the contaminant.

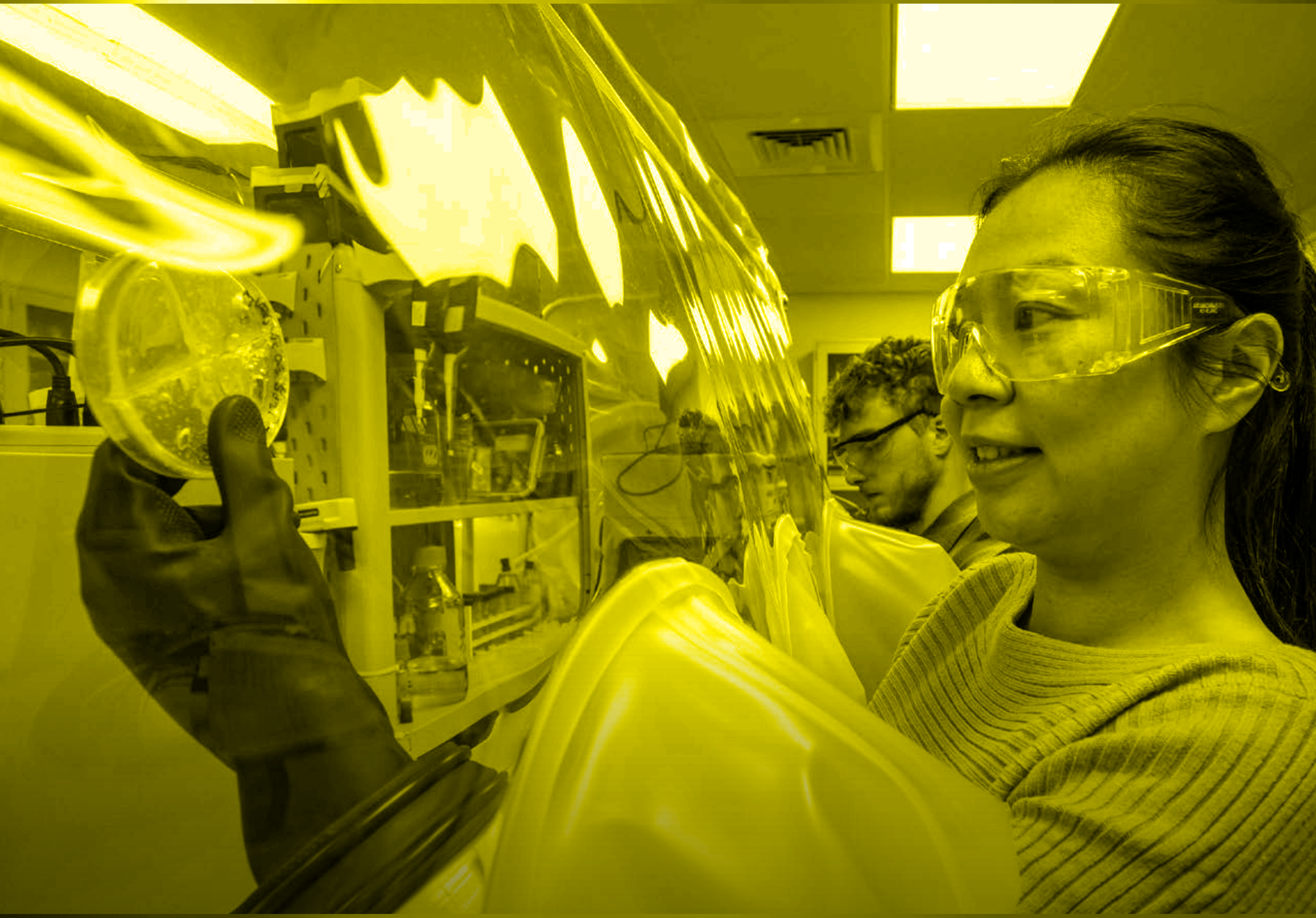
- The AzCATI site is a good robustness test due to the harsh environment. It appears that they actually went backwards in productivity based on the data in Slides 12, 15, and 17; is this correct? The fungicide used is slated to be banned based on its breakdown products. Although the fungicide itself isn't detected, its breakdown products are known to be problematic. Additionally, resistance tends to develop very quickly.
- Nice checking calculations with experiment.
- I'm not sure how to internalize the novel parasite impact on the project. Certainly, it looks like they failed to reach goals while taking very reasonable steps. The contamination issue is certainly daunting, yet it is hard to see that the project met the goals as defined.
- It's a little troubling that they are using a per- and polyfluoroalkyl substances (PFAS) fungicide. It seems like that should be on the sustainability slide.
- I believe staff decisions to alter scope and goals were good. The parasite issues, while preventing the attainment of the initial goals, warrant further exploration. Good example of active project management.
- Approach: The goal of this project was to identify and quantify factors that limit productivity and the length of time between culture crashes in outdoor ponds, and to develop mitigation strategies to overcome those negative factors. This is an ambitious project, but AzCATI and other project team members are well positioned to collect and analyze relevant data from outdoor cultivations. The goals of the project are well aligned with BETO objectives.
- Progress and Outcomes: Progress in increasing the mean time to failure of outdoor cultures was being made, based in part on the development of fungicidal treatment protocols to mitigate fungal parasitoid infection. Tolerance that developed to the fungicide used, along with new invasions by predatory bacteria, caused the mean time to failure to drop down again in 2022.
- The observations that contaminating fungi developed resistance to fungicides, along with the identification of new pests (i.e., predatory bacteria), are not surprising when considering the multitude of potential contaminants in nature and the diversity of ecological niches that they occupy. Although frustrating, this points out the realities of open mass cultivation systems that are generally not amenable to sterilization procedures.
- The identification of contaminating pests via genome analysis, followed by the development of qPCR assays, will be helpful for determining the prevalence of these (and some closely related) microbes at AzCATI and other outdoor sites.
- The TEA and LCA work done in this project is helpful for assessing the pros and cons of batch versus semicontinuous cultivation systems.
- Impact: Although undoubtedly frustrating for the research team, the reality is that they are subject to real-world challenges of outdoor mass cultivation of microalgae, especially the unpredictable problems related to contamination with destructive microbial pests. As such, AzCATI and collaborators are well positioned to try to find and report on solutions to these problems. It is anticipated that different locations

and different species of farmed algae will be impacted by different pests, so the value of this project is probably more in developing a framework for how to evaluate and establish robust culturing procedures and general contamination control strategies that other sites could leverage, as opposed to trying to identify mitigation procedures that might be specific to AzCATI's common contaminants but not universally applicable to all sites and algal types.

- Despite being academically interesting and based on solid science, the use of qPCR to identify a very limited number of known contaminants, and the use of elaborate real-time nutrient measurement systems, may be challenging to perform in an economically viable manner. Likewise, it's not clear if such data would be timely enough and specific enough to prevent culture failures in a commercial-scale production field. An indication of how these systems would be implemented in multi-acre facilities and the impacts on the capital and operating costs would be helpful to determine the value of continuing to pursue these particular lines of research.
- Approach: This project has a good plan, meeting goals, a good communication system, and good collaboration across the project. Outcomes: Good outcomes with probes; even a decrease in productivity over time (also could be looked at as site variability over time) is a good outcome, as it is a real-world variable that can teach industry what they need to be prepared for as their sites mature over time. Flow cytometry for higher throughput is good, and this reviewer disagrees that it is not cost-effective. However, this could become true as more cost-effective tools come to market. It's unfortunate not to be able to detect contaminants, etc., earlier with flow cytometry; however, perhaps current detection timelines are early enough. Could a look at the data from this perspective provide additional value? For example, we can detect pests with flow cytometry and pond monitoring by day *X* of them being present in the system, and this has proven to be early enough for mitigation tactics to be used successfully. In industrial settings, it is not just detection that needs to be fast; the trick is getting operators to act fast enough, so mitigation techniques need to be rapidly deployable. Impact: Far-reaching, as all data are open access. Development of tools and protocols for industry saves thousands. Protocols should also be open access and ready for deployment into a GMP document control program, as this is key development work for commercialization.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the time and effort put into the review process by the reviewers and the constructive and insightful comments. In response to the overall challenge of identifying and implementing effective integrated pest management for algae cultivation, we think while the overall results—in particular decreased time to failure and decreased productivity observed in the project primarily due to the novel predatory bacterial contaminants, which as of yet have not been reported in the literature—give a clear example of the iterative cycle of integrated pest management. In other words, one pest identified, mitigated, and managed, only to have a new pest appear, is valuable information to put out into the public domain. AzCATI remains relatively unique within the BETO portfolio, as we have years of seasonal cultivation data with the same strains, and thus we are able to observe trends and associated challenges, actually building a knowledge base for algal agronomy. We have pest models that have been developed and are in a good position to bring additional solutions to the table as part of the overall cycle of integrated pest management; in fact, we will be doing so as we wrap up this specific project in 2023. We clearly demonstrated the ability to mitigate contamination and keep productivity higher through operational shifts (e.g., batch versus semicontinuous) and clearly identified the trade-offs with respect to TEA and LCA based on those approaches, something that had not been delineated well in the literature and backed up by actual cultivation data. With respect to concerns about the fungicide used, this fungicide is in fact used in food production now and remains one of the few that, as of yet, is not banned in the United States. However, we acknowledge it's likely to be banned, and while technically *not* a PFAS compound, it is fluorinated and thus of concern. Resistance as well is of course always a possibility and an issue to be concerned with for any treatment methodology. Understanding and characterizing that while looking for ways to prevent it are key aspects in developing any effective integrated pest management program. The challenges faced in this project with respect to developing approaches to manage pests are the same ones any site will face in bringing algal cultivation forward. As described in the presentation, and to extend the impact of this BETO-funded work, our data are being made publicly available and also include any protocols as well as pest models we have or will develop. We have already transferred pests to collaborators at the national labs and other academic institutions.



AGILE BIOFOUNDRY CONSORTIUM

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Agile BioFoundry (ABF) Technology Area is one of 11 technology areas reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 31 presentations were reviewed in the ABF session by six external experts from industry, academia, and other government agencies. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer the corresponding Program and Technology Area Overview presentation slide decks, which can be accessed here: https://www.energy.gov/sites/default/files/2023-04/beto-00-project-peer-review-abf-apr-2023-bentley.pdf.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $86,928,379.00, which represents approximately 12% of the BETO portfolio reviewed during the 2023 Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Gayle Bentley as the ABF Technology Area review lead, with contractor support from Frank Fields (Boston Government Services LLC). In this capacity, Gayle Bentley was responsible for all aspects of review planning and implementation.

AGILE BIOFOUNDRY REVIEW PANEL

Name	Affiliation
Karen Draths*	Michigan State University
Brentan Alexander	Synonym
Doug Friedman	BioMADE
Hanny Rivera	Ginkgo Bioworks
Gale Wichmann	Amyris
Fuzhong Zhang	Washington University in St. Louis

* Lead Reviewer

AGILE BIOFOUNDRY REVIEW PANEL SUMMARY REPORT

Prepared by the Agile BioFoundry Review Panel

INTRODUCTION

The Agile BioFoundry was established by BETO in 2016 and currently exists as a distributed consortium of seven national laboratories: Lawrence Berkeley National Laboratory (LBNL), Argonne National Laboratory (ANL), Sandia National Laboratories (SNL), Pacific Northwest National Laboratory (PNNL), Los Alamos National Laboratory (LANL), Oak Ridge National Laboratory (ORNL), and the National Renewable Energy Laboratory (NREL). A ***biofoundry*** provides an integrated infrastructure that combines biological, chemical, and engineering disciplines and tools that enable automation, high-throughput measurement, integrated data acquisition/analysis, artificial intelligence, and machine learning (ML) to enable rapid design, construction, and testing of genetically reprogrammed organisms for biotechnology applications. The ABF exists to support BETO's decarbonization mission of the energy-intensive chemicals industry and transportation sector by accelerating development of optimized routes to direct replacement chemicals, performance-advantaged bioproducts, and CO_2 utilization for chemicals and by leveraging design-build-test-learn (DBTL) infrastructure to meet opportunities and challenges related to sustainable aviation fuels (SAFs).

Thus, the ABF is a public infrastructure investment that is intended to expedite advancement of the bioeconomy by accelerating innovation and encouraging adoption of new biomanufacturing methods. The specific objective of the ABF is to develop and deploy state-of-the-art tools and technologies that enable commercially relevant biomanufacturing of products. ABF partnerships with industry and academia enable adoption and utilization of advanced tools, infrastructure, and expertise to facilitate growth of the bioeconomy. The ABF's stated goal is to reduce bioprocess scale-up time for its partners by 50% from a current average of 10 years.

In this review, the ABF presented progress reports for the following activities: (1) DBTL infrastructure, demonstration products, and beachheads; (2) host onboarding and development; (3) process integration and scale-up; (4) techno-economic analysis (TEA) and life cycle analysis (LCA); and (5) industry engagement, outreach, and management. Internal ABF activities within these areas are funded via annual operating plan (AOP) funds provided by BETO. Outward-facing, partnership-related research is funded via funding opportunity announcements (FOAs) or directed funding opportunities (DFOs). Five FOA projects and 10 DFO projects were reviewed.

The ABF recently presented a plan for the 2023–2025 funding cycle, and subsequent reviews indicated that although the ABF has completed significant and meaningful work, quantifying reductions in development time and costs remains challenging. This analysis echoes the 2021 Peer Review, which cautioned that the current ABF approach might not be well suited to achieve its high-level goals. For reference, the ABF has received more than $124 million in BETO funds since its inception. As a result, BETO program management directed the ABF to suspend research activities for two quarters and to dedicate all efforts to devising a new strategic plan with defined implementation tasks. The new strategic plan and corresponding budget allocation were described by ABF leadership and extensively discussed with the review panel.

STRATEGY

During the recent strategic planning process, the ABF defined its mission as follows: Develop biomanufacturing tools, processes, and partnerships that enable sustainable industrial production of renewable fuels and chemicals for the nation. To advance its mission, the ABF is now organizing itself in goal-oriented units in place of the previous task-oriented units (e.g., DBTL, host onboarding). The new strategic plan calls for advancing pathways, strains, and processes for production of two types of SAF (thermophilic ethanol and microbial alkanes) and two biochemicals (muconate and 3-hydroxypropionic acid [3-HP]). Tools development will continue within the framework of advancing strains for sustainable fuels and chemical production, and an invigorated emphasis on partnerships will target funds-in relationships with industry in addition to the standard FOA and DFO partnership mechanisms. The review panel agrees that the revised mission and goals align better with BETO's mission. There is concern that the ABF vision of "sustainable biomanufacturing of affordable fuels and chemicals" overstates ABF's bioeconomy role beyond infrastructure to include production. The panel advises caution regarding writing performance metrics specifically tied to bioproduction. Furthermore, CO_2 reduction metrics were not contextualized (e.g., actual versus theoretical CO_2 reduction), which may introduce new challenges when ascertaining whether ABF has achieved its goals. Although the panel agrees in principle that internal research should focus on a small number of specific targets, no rationale was provided for selection of muconate and 3-HP over other bioproducts ABF has previously targeted. SAF is admittedly well aligned with the BETO mission; however, its economic viability remains uncertain. The panel recommends ABF revise their newly stated goals. For example, details surrounding tool benchmarking to "equivalent industry-accessible, state-of-the-art baselines" are not well defined, which makes categorizing tools for further development or sunsetting particularly challenging. Panel members would have appreciated more details describing the mapping of specific capabilities, tools, and personnel onto the strategic goals to ensure efficient expenditure of resources.

To fulfill its role as a biofoundry and achieve its high-level goals, the panel agrees that the ABF must interact extensively with both industrial and academic partners. Both the FOA and DFO funding mechanisms were deemed appropriate. Overall, the panel was impressed by the quantity, quality, and research progress for the reviewed ABF partnerships. One goal of the new strategic plan is to direct greater than 50% of ABF funding to partnership-related research. This is viewed favorably by the panel and is expected to strengthen ABF skill sets and provide companies, regardless of size or resources, access to cutting-edge technologies. The ABF acknowledges that oversubscription to ABF funding opportunities is critical to maintaining a competitive process, which the panel agrees will provide the best opportunity to develop impactful research programs. Echoing sentiments of the 2021 Peer Review, current panel members are concerned that ABF efforts to disseminate information regarding technological advances fall short of expectations. Panel members perceived an emphasis on journal publications as a measure of accomplishment and productivity, although this was not explicitly stated by ABF leadership. Because journals are not universally available to potential industrial partners, publications may not be the most effective means to reach the appropriate audiences. The panel recommends more extensive description of advances via other means, including the ABF website (e.g., text, videos, presentation slides) and newsletters. The Advanced Biofuels and Bioproducts Process Development Unit (ABPDU), which is fully under the ABF umbrella but maintains its own website, provides an effective model for information dissemination. Among the strongest concerns raised by the panel was the lack of a consistent, coordinated strategy for the ABF to engage industry stakeholders, despite various outreach and engagement activities. The absence of engagement with the industry advisory board (IAB) during the recent strategic planning process provides evidence that this is the case. The panel recognizes that industry stakeholders and their corresponding needs vary widely, which likely results in conflicting messages. The panel encourages the ABF to develop a consistent strategy to gather and catalog stakeholder feedback and then determine methods to provide maximum benefit to the industry.

Reviewer attention tightly focused on the new strategic plan, leaving less time to thoroughly evaluate the inward-facing ABF technological portfolio. Review of the task-oriented units of (1) DBTL infrastructure, demonstration products, and beachheads; (2) host onboarding and development; (3) process integration and scale-up; and (4) TEA and LCA indicates that ABF research is generally of high quality, and that unique synthetic biology (synbio) and bioprocessing capabilities are being developed. The ABF team has developed many core technologies, including pathways, products, strains, sensors, multi-omics tools, computational tools, and modeling tools. Multiple challenges remain before biomanufacturing processes will be economically competitive, particularly at commodity scale, which is required for SAF and biochemicals. The ABF plan to advance a small number of targets in these spaces may highlight the technological gaps, which can then be addressed. Panel members have concerns related to reducing resources to enable host onboarding and genetic tool expansion for nonstandard organisms, which falls squarely within the ABF mission. Reviewers recommend judicious, continued investment in host onboarding/genetic tool expansion. Conversion of the lauded Host Onboarding Tool (HObT) web portal to an outward-facing, publicly accessible tool in a timely fashion is imperative.

As stated above, panelists are pleased that the new strategic plan includes a strong emphasis on partnerships and a commitment to invest at least half of BETO funds on partner-related research. Funding partnerships with the National Science Foundation (NSF) and BioMADE and a funding opportunity specific for minority-serving institutions broaden access to ABF tools and capabilities, which is viewed positively. Current and future partners are encouraged to clearly highlight how the partnership benefits the company/academic effort, the bioeconomy, and the ABF. The 2021 Peer Review recommended exploration of a fee-for-service mechanism for ABF engagement. Reviewers support the new effort to initiate strategic partnership projects, which are expected to increase engagement with industrial stakeholders. Details relating to recruitment of industrial partners, execution of partnership agreements, and intellectual property (IP) management were lacking, however. Reviewers encourage the ABF to work closely with their national lab partners to streamline and standardize these processes.

STRATEGY IMPLEMENTATION AND PROGRESS

The ABF continues research on a range of projects closely aligned to its mission. This includes internal projects focusing on tool development, capabilities, and demonstration projects, as well as outward-facing partner-related research. The ABF is in active partnerships with organizations ranging from small biotechnology startups to large, mature corporations. The ABF also has multiple academic partners. All task-related units are involved in a mix of internal and outward-facing research projects. Host onboarding/genetic tool development is engaged by many partner organizations, while TEA/LCA has performed a large body of work focused on internal projects related to beachheads and demonstration projects. This TEA/LCA work provides a foundation of research that enables prediction of the strongest drivers of both economic and environmental impacts. Reviewers note that the strength of the portfolio would be positively impacted by increased competition for research funds within the FOA and DFO selection processes. More widespread and thorough dissemination of ABF tools, capabilities, and advances through all possible means must be a focus for ABF management going forward. Similarly, a consistent approach for interacting with industrial stakeholders is an important need.

Reviewers characterized many of the partner-related projects as on the leading edge of the field. For several projects, even if characterized as on the leading edge, the combination of research status and product requirements make it difficult to envision a path to economic viability over the next decade. Across the board, reported progress indicated that assigned researchers are working diligently. Outward-facing projects to be discussed at future reviews should include a single slide aligning project status with all proposed milestones, tasks, and timelines. Reviewing projects before completion of five quarters of funded research is not recommended. Communication, technology transfer, and data sharing between the ABF and partner organizations appears to be adequate.

Past accomplishments for technology-related, task-oriented activities justify an optimistic attitude regarding achievement of near-term and midterm goals described under the previous strategic plan. For example, several beachhead molecules were produced in multiple host strains with impressive titer, rate, and yield (TRY) metrics. This progress was enabled by contributions across the ABF infrastructure, including DBTL, biosensors, host onboarding/genetic tools development, multi-omics analysis, and process integration/scale-up. Under the new strategic plan, the ABF is well positioned to make significant progress on SAF and biochemicals. The panel notes that deliverables for fiscal year (FY) 2025 were provided, but in many cases, these lacked context or specific details. Midterm ABF goals were not included.

Panelists agree that the ABF management team provides an appropriate level of project management to ensure beneficial outcomes for both partners and the government.

RECOMMENDATIONS

Modify ABF Management Structure

The panel unanimously recommends the ABF adopt a management structure whereby one individual oversees all ABF activities, including allocation of research funding. The new ABF director should be in alignment with BETO's vision for the ABF and should devote their full professional effort to ABF management. The panel recommends the following changes to the ABF organizational chart proposed in the new strategic plan. The director would report to the BETO technology manager. Direct reports to the director would include (1) engagement and outreach, (2) business development and partnering agreements, and (3) strategic implementation. The director would seek advice and counsel from the executive committee and the IAB. At least one reviewer advocated for selection of the director from candidates outside the current ABF management structure. The committee arrives at this recommendation following observations of protracted high-level decision-making and failure to address review recommendations adequately and in a timely fashion.

Standardize Research Agreement Templates

Protracted timelines for negotiation and finalization of research agreements are a powerful disincentive to work with a national laboratory consortium such as the ABF. The panel unanimously recommends that the ABF prioritize development of standard cooperative research and development agreement (CRADA) templates that outline IP management plans, licensing, and royalty rates. Templates from other national laboratory consortia such as Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment (BOTTLE™) may provide a starting point. The review panel believes the quality and quantity of ABF partnerships with industry will determine whether ABF is successful in its mission to expedite advancement of the bioeconomy. Reducing barriers to establishing strong partnerships must be a top priority.

Allocate BETO Funding to Partner-Driven Projects

The panel unanimously recommends that the ABF set a more ambitious goal of allocating 75% of BETO funds to partner-driven research projects. Following 6 years of allocating much of its funding to internal research projects, ABF has developed an impressive list of tools, capabilities, and infrastructure. The panel suggests the ABF is now in a strong position to assume its originally envisioned role as a service provider. The panel reminds ABF management that more effective dissemination of ABF capabilities and consistent engagement with industrial stakeholders are recommended to increase competition for ABF funding and services. Ultimately, the level of interest to form productive research partnerships and the extent of industry use of ABF capabilities will provide ABF with validation and proof of impact.

Map Partner-Driven Projects Onto Specific ABF Tools, Capabilities, and Infrastructure

The panel unanimously recommends that ABF management map all partnerships (past, current, and future) onto the specific tools, capabilities, and infrastructure being utilized, and at the conclusion of a project, clearly indicate for each all meaningful contributions to research progress. This exercise will highlight the extent of interest/utilization for each tool, capability, or infrastructure component and is expected to be useful to ABF management, BETO, and future panel reviewers.

AGILE BIOFOUNDRY PROGRAMMATIC RESPONSE

INTRODUCTION

BETO would like to thank the reviewers for the thoughtful and careful review of the ABF research portfolio, particularly in light of ABF's ongoing implementation of its revised mission and goals. This feedback is extremely helpful as BETO seeks to ensure the ABF is successful in achieving their newly defined objectives. Many of these comments provide clear direction that BETO will use to inform directives to ABF moving forward. This program response will address several of these comments directly, but BETO appreciates and will consider all of the provided comments in the ABF's management moving forward.

The reviewers note that the new vision to support "sustainable biomanufacturing of affordable fuels and chemicals" may potentially overstate the ABF's bioeconomy role. While this comment is well taken, BETO believes that the ABF can indeed meet this new mission by clearly understanding and overcoming barriers to production of the strategically chosen bioproducts and biofuels. While ABF may not develop the entire bioprocess and lead the full-scale demonstration, ABF can contribute to overcoming critical barriers to scale-up and thereby enable biomanufacturing at large.

The program agrees that additional, clearer metrics around the goal to reach CO_2 reduction targets and other critical objectives are needed. These comments will be taken into consideration specifically regarding the noted benchmarking task and other critical milestones.

The program agrees that improved dissemination of the ABF's tools, capabilities, and advances will improve awareness of ABF's value to the community. External communications are also related to the reviewers' comments regarding industry engagement. The program appreciates this feedback and agrees that the ABF's industry relationships can be strengthened and partnership agreements can be streamlined along with improved IP management.

Recommendation 1: Modify Management Structure

The unanimous recommendation for a dedicated ABF director is appreciated. BETO recognizes the need for more efficient decision-making processes. Implementing a streamlined management structure will enable the ABF to progress their research objectives and improve timeliness. The program also acknowledges that this consortium is led by researchers at national laboratories, where the structure of those laboratories often prevents investigators from being able to focus on a single project.

Recommendation 2: Standardize Research Agreement Templates

The program appreciates the reviewers' assessment of the research agreement process. The program fully supports the improvement of the research agreement process in order to facilitate collaborative projects and interactions with industry.

Recommendation 3: Allocate BETO Funding to Partner-Driven Projects

The program notes the recommendation to set a more ambitious goal to dedicate 75% of BETO funds to partner-driven research projects. This suggested goal and the currently proposed target of 50% partnership projects both reflect a commitment to intensified industry collaborations. While BETO may not recommend that the ABF reach the 75% budget target, the program is committed to ensuring that the spirit of the partnership metric is met as the ABF proceeds. The reviewers noted that the ABF's originally envisioned role was as a service provider. While the ABF can indeed provide valuable services to the bioeconomy, BETO still sees great value in investing in the catalytic infrastructure that develops the scientific tools and capabilities that will ideally enable transformative improvements in microbial strain engineering and bioprocess design. As the ABF matures, it will be important to ensure that the scientific engine driving the ABF's value to the community is running strong, in addition to working hand in hand to solve specific technical challenges.

Recommendation 4: Map Partner-Driven Projects Onto Specific ABF Tools, Capabilities, and Infrastructure

Furthermore, the recommendation to map all partnerships onto specific tools, capabilities, and infrastructure is appreciated. The program agrees that it is important to provide clear indications of meaningful contributions to research progress.

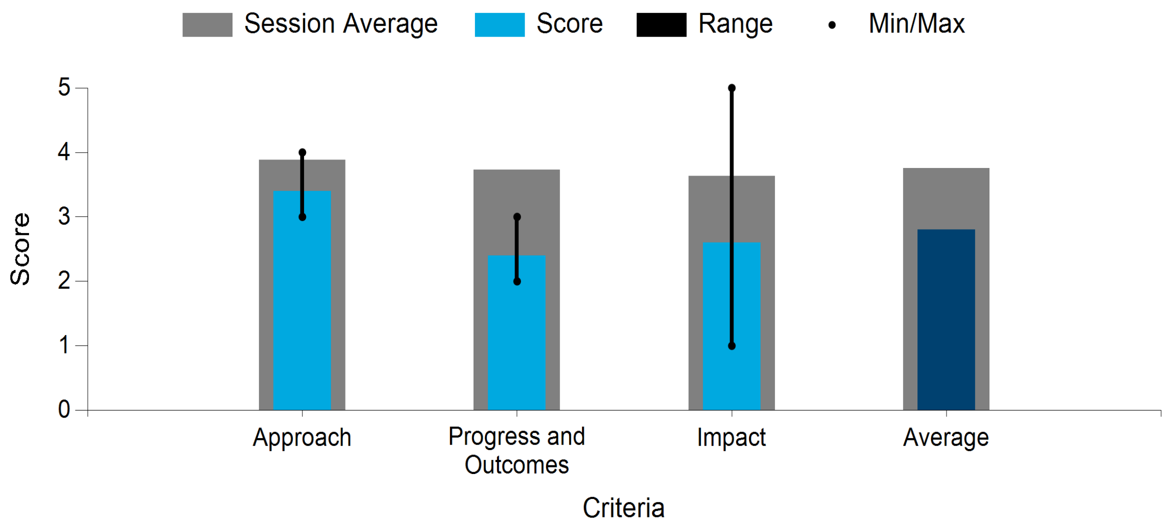
In conclusion, the review panel has provided valuable guidance for the ABF as they embark on a new strategic direction. BETO is committed to addressing the recommendations provided, and seeks to reflect on these recommendations in the management of the ABF moving forward. The program would like to again thank the reviewers for their time and expertise.

ACCELERATING ENGINEERED MICROBE OPTIMIZATION THROUGH MACHINE LEARNING AND MULTI-OMICS DATASETS

Lygos Inc.

WBS:	2.3.2.209
Presenter(s):	Bryce Dille; Nick Ohler; Rebecca Lennen
Project Start Date:	10/01/2018
Planned Project End Date:	09/30/2022
Total Funding:	$2,857,142.00

Average Score by Evaluation Criterion



COMMENTS

- This project began with some ambitious goals to generate significant quantities of data to use to drive an ML tool to rapidly accelerate performance of the target strain using multiple DBTL cycles. The experimental design appears to be aimed at capturing as much data at as many points as possible in order to train the ML model. This approach is a strong one in both demonstrating ML capabilities and validating the ability of ML models to find useful insights in the noise that drive strain development.

- Unfortunately, both pandemic and partner financial issues appear to have taken a major toll on the progress of this award. Only one DBTL cycle was completed, and as such, the learnings from that cycle were not returned to the ML model for further cycles. The success of the first cycle is muted: Although improvements were seen in a number of strains, the improvement did not reach targets (although such success was not expected after a single cycle). Salvaging some learnings from this study would be important. Passing data back to the ML model to see how its predictions change based on the first cycle could provide interesting insights into what has been learned thus far and what new pathways may yet emerge. Review of the weights in the ML model may give guidance to which data (from the 80,000 points collected) were most useful and impactful, providing guidance and direction on where to focus limited data-gathering resources in future activities. Without this closing work, the impact of this study is muted.

- Strength: This project benefits from the ABF's multi-omics capabilities, which helped Lygos generate a large proteomic data set.
- Weaknesses/areas for improvement:
    - The team proposed to complete six DBTL cycles, which is not a lot considering a total budget of $2 million. Even more concerning, only one cycle was completed, representing a major failure of the project.
    - Although the team generated a large number of omics data sets, the data set was not used to inform engineering targets, as a continued round of engineering was not performed. The data set also failed to provide any useful knowledge. So, it seems nothing can be learned from the large data set obtained. It is not clear what useful output this project has produced.
    - The impact of the project is quite limited. No improvement on TRY was mentioned. Although new strains were created and were claimed to be Lygos's highest producers, it is not clear how much improvement was obtained and to what degree these strains helped the commercialization process.
- I'm not sure what happened between 2021 and 2023 for this project. Back in 2021, they were nearly done, or significantly done, with the first DBTL cycle, and here 2 years later it's just finishing with the data. As the presenters stated, it was overly ambitious from the start and didn't need so many samples for the first DBTL cycle. Still, the project clearly advanced learning for both the ABF and the company. The first DBTL cycle was ultimately successful in generating useful data and improvements, but it seems it came too late, and it's not clear these learnings will be incorporated. The work merits more cycles if the partner is still developing this strain, although I recommend fewer samples and getting through it more quickly.
- This project really needed a table of all metrics and tasks and percent completion toward them. This project fits well with the mission of both the ABF and BETO. The value proposition and impact to the U.S. bioeconomy is clear.
- It's not clear how many key performance indicators were in the process/milestones.
- Given the really low ability to actually build the recommended interventions, I would like to better understand why that was the case—whether that was a big deficiency of the ML model or the ability of Lygos or the ABF to synthesize constructs.
- The project focused on malonic acid production using the acid-tolerant, nontraditional host *P. kudriavzevii*. Project goals include leveraging multi-omic data sets to populate ML networks, making predictions for strain modifications to increase product formation, and iterating the DBTL cycle a total of six times. As described, the project was a good selection for the solicitation. Management plans were sparsely addressed, and ABF partners were not specified. Although complex, interdependent workflows were a recognized risk; communication plans were not provided. An initial set of 24 strains were cultured in fermenters, and omics data were obtained; however, the project was discontinued early. The overall impact is minimal due to failure to complete the project. Project strengths are as follows. Selection of malonic acid as the targeted product was well justified. Focus on Key Performance Indicator 2 over Key Performance Indicator 1 was appropriate and justified. The initial strains analyzed indicated the possibility of good advancement in strain development if it had been completed as described. Project weaknesses are as follows. No improvements in ML algorithms were realized. A description of the

>80,000 data points per cycle was not included (e.g., number of strains, time points examined, multi-omic methods). Strain engineering was a skill assigned to Lygos but appeared to be not as expected given that only a single gene deletion was completed. Whether reliable workflows and data collection schemes were developed remains unclear.

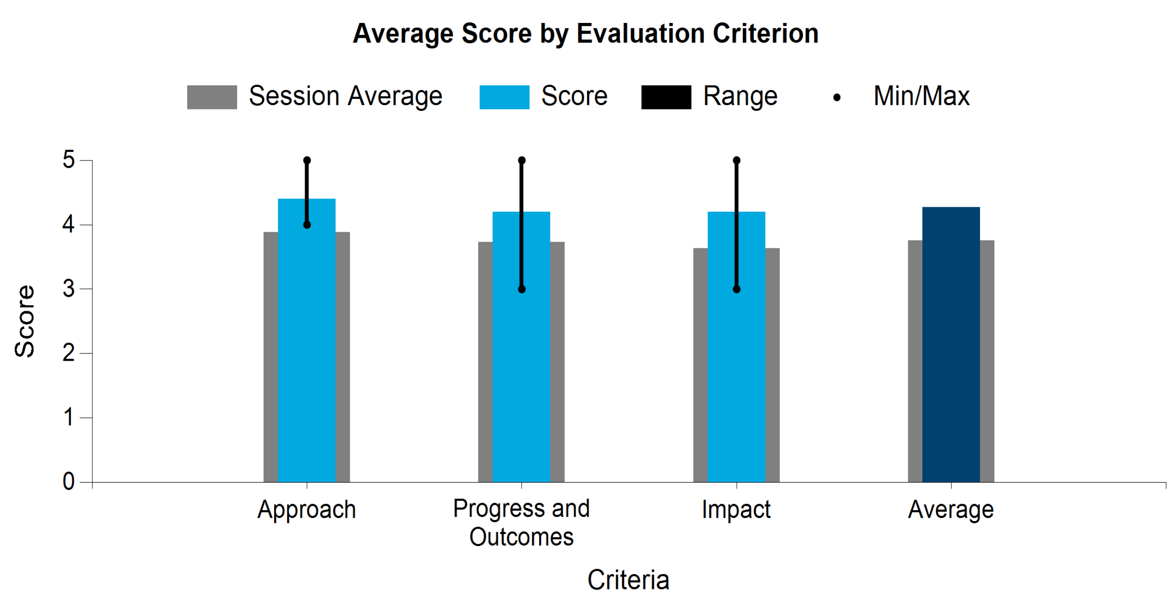
DEVELOPMENT OF *BACILLUS* AS AN INDUSTRIAL HOST FOR THE MICROBIAL PRODUCTION OF BIOPOLYMERS

ZymoChem

PROJECT DESCRIPTION

WBS:	2.3.2.213
Presenter(s):	Harshal Chokhawala; Thomas Mand
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2023
Total Funding:	$1,666,908.00

Biotechnologies that target high-value products hold immense long-term promise, yet efforts to bring these technologies to market are often hampered by low titers, high cost of feedstock, and organisms that are difficult to engineer. Thus, it would be beneficial to develop microbes, bio-based processes, and related process technologies that are tailored for utilizing sugar-rich feedstocks derived from low-cost lignocellulosic biomass. Biopolymers are an example of high-value bioproducts due to their ability to replace petroleum-based polymers used in many industries. *Bacillus* strains are currently used as industrial producers of some biopolymers. However, these fermentations generally require feedstocks supplemented with expensive components, which limits economic viability. To address this challenge, ZymoChem partnered with the ABF to develop genetic tools in a non-model strain of *Bacillus*, utilize the tools to construct a carbon-conserving strain of *Bacillus*, optimize biopolymer production in minimal media containing C5 or C6 sugars, and demonstrate biopolymer production at the 300-L scale. We demonstrated success in each of these endeavors and surpassed the final milestone titer by 3.6-fold through a combination of strain engineering and process development. With this successful partnership with the ABF, we were able to significantly decrease the overall risk to our commercialization efforts by lowering the cost of biopolymer production.



COMMENTS

- The carbon-conserving C5 pathway developed by ZymoChem represents an interesting production pathway that would improve the carbon efficiency of molecule production. The research work was designed to implement this pathway in a new organism while increasing overall strain performance. The result of this work is a bit of a mixed bag: A host with the C5 carbon pathway was created, but its performance was poor, and the strain does not appear to be near commercial viability at current TRY levels. Further process optimization work and piloting appear to have been done on C6 sugars, and so do not use the carbon-conserving pathway. The benchmark used in the study also appears to be essentially a starved wild-type strain, so it is unclear why this serves as a useful benchmark instead of the wild-type alone, which is much closer to the performance levels of the engineered strain. The overall impact is therefore a bit muted; however, the toolkit developed within the *Bacillus* host may find use in further studies with ZymoChem or other users.

- Strengths:
  - The ZymoChem team has clearly benefited from strains and tools (promoter library) developed by the ABF.
  - The ABPDU helped to scale up the production and purification.
  - Clear improvement on titer and rate metrics, exceeding the project milestone. High titer (75 g/L) and high rate (2 g/L/h) were achieved. These values are impressive, although details on how it worked were not provided.
  - A majority of the proposed tasks were completed.
- Weakness/area for improvement: Elimination of sporulation was identified to improve product titers. It is not clear why removing sporulation would help. The final strain that produced high titer and rate seems to be from another mechanism. It is difficult to evaluate its scientific impacts.
- Thank you presenters for Slides 6 and 7 stating progress on all milestones and tasks! This is needed in all slide decks. There were also clear impact slides and value proposition to BETO and the U.S. economy. Overall for the ABF this is a great project. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. The work in this proposal clearly advances the capabilities of the ABF, and at the same time, the partner gains knowledge and access to capabilities it does not have in-house.
- This has been a highly successful project in which all the milestones and goals were reached. The overall project timeline seems a bit long to me for the improvements achieved, though it is not entirely clear what drove the timeline or if there were delays in contract negotiation, etc. The presentation of the data here was rather confusing—for instance, the scale of "titer" changes in each of the slides, at first being 10 g/L in the engineered strain (Slide 8), but then 45 g/L in the wild-type (Slide 14). It was not clear exactly which conditions the final improvement was under and whether that was the end result/goal that ZymoChem originally desired.
- An unidentified strain of *Bacillus* was engineered for production of an unidentified biopolymer. Project goals included implementation of ZymoChem's carbon conservation technology in a non-model organism, which required genetic engineering tool development. Fermentation and process development was also included. The project was a good selection for the BioEnergy Engineering for Products Synthesis FOA, whose areas of interest include development of non-model organisms and production of data sets to enable ABF learn methodologies and the metric of demonstrated titers exceeding 20 g/L. The project achieved good overall progress and has future commercialization potential. Project strengths are as follows. Project milestones and tasks were articulated for all participants. Strong progress was made in the development of genetic engineering tools for the non-model organism, which enabled forward progress on strain development. Transcriptomic data, which will have utility for future stain development strategies, enabled elimination of sporulation without a negative impact on biopolymer production.

Fermentation and process development for strains growing on glucose enabled significant improvement in product formation by the wild-type organism (45 g/L), while combined strain and process development afforded products (72 g/L) at 300-L scale. Project weaknesses are as follows. It is unclear whether the *Bacillus* strain is fully onboarded by the ABF for use by the community at large. The strain is not listed on the ABF website of onboarded organisms. Implementation of carbon conservation technology was not described beyond initial demonstration, which is disappointing given the 4-year project timeline. Strain development will be necessary before carbon conservation technology bears fruit: The carbon-conservation-enabled strain grew approximately twofold slower and produced fourfold less product relative to the wild-type. I'm curious about the long-term strategy for the carbon conservation pathway given the need for C5 feedstock streams. Ultimately it will be necessary to engineer the strain to co-utilize C5 and C6 feedstocks.

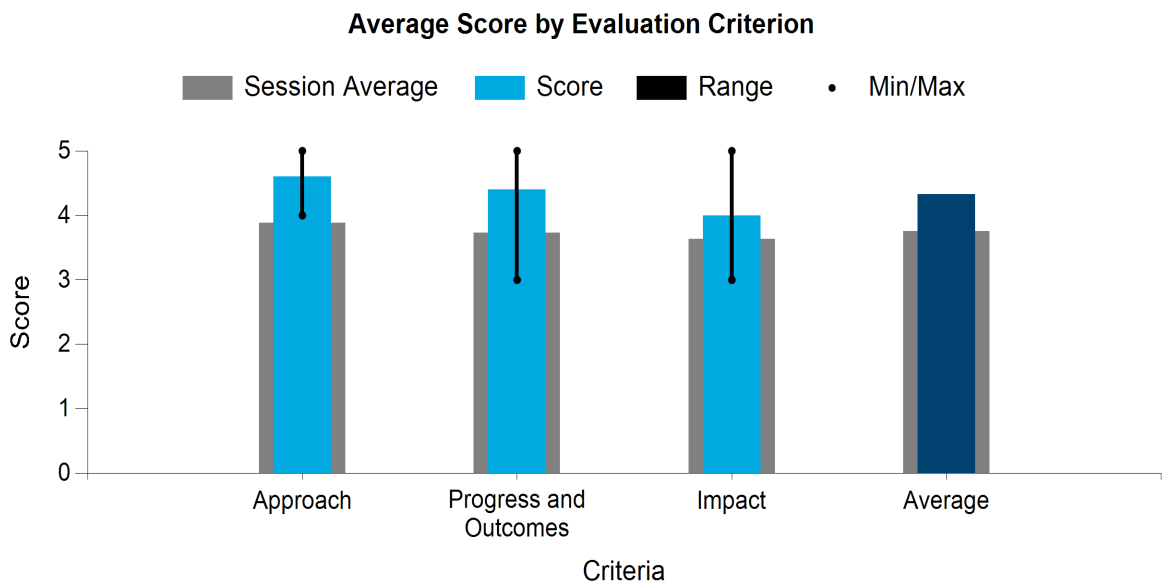
ACCELERATING POLYKETIDE SYNTHASE ENGINEERING FOR HIGH-TRY PRODUCTION OF BIOFUELS AND BIOPRODUCTS

University of California, Berkeley

PROJECT DESCRIPTION

WBS:	2.5.3.207
Presenter(s):	Jay Keasling
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2023
Total Funding:	$3,125,741.00

Polyketide synthase (PKS) enzymes have a modular, deterministic logic that holds the potential to act as a flexible chemical factory for the biological production of a huge diversity of valuable small-molecule compounds. However, engineering a custom PKS to produce a specific desired product currently requires years of trial and error, for reasons that remain poorly understood. In this project, we have developed a rapid, high-throughput DBTL cycle for PKSs and demonstrate its utility for production of material precursors. The objectives are to (1) develop a rapid, high-throughput DBTL cycle for PKSs that will enable production of a large number of unnatural, organic molecules on demand at high TRY; (2) demonstrate the utility of the PKS DBTL cycle to produce three molecules: one commodity chemical (caprolactam or valerolactam) and two novel material precursors (caprolactam or valerolactam derivatives); and (3) demonstrate the utility of the PKS DBTL cycle to increase the TRY of one molecule (caprolactam or valerolactam). In this project, we have successfully demonstrated our high-throughput PKS DBTL pipeline and have biologically produced valerolactam and several other novel nylon monomers.



COMMENTS

- The use of the well-understood PKS pathway to enable production of billions of potential molecules is an interesting approach with considerable potential. This research aims to improve the ability to create PKS pathways to targets without relying on extensive trial and error, the current state of the art. By utilizing ML and simulation tools, the thinking is that functional PKS pathways can be found more quickly. This research has demonstrated the ability to rapidly produce a wide range of pathways for testing and validation, allowing a faster development process. However, the process still feels a bit "brute force," and it is unclear whether the learnings from the experimental setups are being passed back to ML models to improve their performance and efficacy. Ideally with more runs and data, the number of PKS candidate pathways that fail would be reduced, while the performance of pathways would also increase. Folding in tools like AlphaFold may be helpful in advancing the research. The impact of this approach is still limited by low overall performance (<1-g/L titers at lab scale), but this research may show a path to generating significantly more data to better train ML models and rapidly improve learnings to increase performance.

- Strengths:
  - Engineering PKSs offers enormous potential for bioproduction of chemicals with diverse but precisely defined structures. However, PKSs are notoriously difficult to engineer due to their complicated structures and folding issues. This team has obtained substantial success in expressing novel polyketides. The ability to build and test 100 PKSs in 9 months is impressive, considering the previous state of the art (one PKS for one Ph.D. in 5 years to complete).
  - The team has made excellent progress, achieving most milestones.
  - Production of four lactams, including three novel nylon precursors, was achieved. This result proved the possibility of building and testing novel polymer precursors from PKS libraries.
- Weaknesses/areas for improvement: N/A.
- This project was started in 2020 and is nearly completed. The goal of the project, essentially "develop a high-throughput DBTL cycle for PKS engineering, and test it by building a PKS to make the nylon monomers caprolactam, valerolactam, and novel derivatives," fits perfectly with the ABF mission to further synbio to produce industrially relevant molecules, and in this case has the bonus of harnessing the diversity of enzyme function to create new molecules. The project is making an array of valuable products, including several novel plastic (nylon) monomers with potentially better properties. They are using a much better host than the organisms that have PKS enzymes in them for faster growth and faster engineering.
- The project is ambitious to build an entire pipeline for high-throughput engineering and screening, which will be useful for many projects for a long time. The project will be very successful and meet its milestones and goals. It was very refreshing to see all the milestones listed and their state of completion. This needs to be required for all projects and AOP funding. They were honest in early struggles and failures. Industry is going to be more reluctant here to show struggles and failures, making the milestone list important. There was some legitimate concern about the difficulties and lack of progress midway through the project, but the project team overcame them and was ultimately successful.
- Also, all FOA and DFO reviews going forward should have an impact slide clearly stating benefits to the ABF and the U.S. bioeconomy.
- The project has been very successful based on meeting the ABF's and BETO's missions: "We have confirmed production of valerolactam and three additional novel nylon precursors with PKSs with titers from 1 to 10 mg/L … We have demonstrated that our build pipeline can build hundreds of PKSs at once in high throughput."
- This is overall a very strong project. The presentation did a great job at showcasing the project goals, milestones, and how milestones have been met. I appreciated their details on the diversity, equity, and inclusion (DEI) components of the work. I would also recommend that all presentations be required to

show milestones and their achievement of them. I would suggest that they should show all milestones at least in the appendix. While the eventual impact of developing PKSs as a biosynthetic pathway tool is large, the current project titers are still rather low (despite improvements from the state of the art), and further development will be needed.

- This projects seeks to design ML tools that enable successful prediction of PKS design, which would ultimately lower the barriers to PKS engineering and improve the efficiency of the DBTL cycles for those biosynthetic pathways that use a PKS. This approach represents a significant improvement relative to trial-and-error methods that are currently in use for novel PKS design. The management plan provides for regular meeting between all teams, and individual teams meet as needed. However, there is no indication of specific ABF personnel participating in the research program. Risk and mitigation plans are provided. One risk that should also be considered includes successful PKS gene synthesis and protein folding, but insufficient substrate throughput to detect and accurately identify the resulting product. It is also unclear how novel PKSs are being evaluated from the standpoint of product formation. For example, is product formation assessed for an *in vivo* process, or are enzymes purified and challenged with a variety of starter units? A commendable plan is in place to increase the diversity of project participants and to improve the development of young scientists by allowing them to take ownership of their assigned tasks. The project has made good progress. ClusterCAD has been shown to successfully demonstrate an automated approach to PKS design. Results have been disseminated in one peer-reviewed paper, and additional manuscripts are planned. ClusterCAD is available to the ABF and to the community at large. Quantitative end-of-project milestones are not likely to be met by the project end date. The impact of the project is jeopardized by modest PKS substrate throughput, which would limit applicability in the performance-advantaged materials space due to low TRY values. The impact is likely to be more significant when applied to identification of complex novel structures, which would include higher-value specialty chemicals and the pharmaceutical space. Methods for improvement of the catalytic properties of PKS enzymes should also be considered.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The use of the well-understood PKS pathway to enable production of billions of potential molecules is an interesting approach with considerable potential. This research aims to improve the ability to create PKS pathways to targets without relying on extensive trial and error, the current state of the art. By utilizing ML and simulation tools, the thinking is that functional PKS pathways can be found more quickly. This research has demonstrated the ability to rapidly produce a wide range of pathways for testing and validation, allowing a faster development process. However, the process still feels a bit “brute force,” and it is unclear whether the learnings from the experimental setups are being passed back to ML models to improve their performance and efficacy. Ideally with more runs and data, the number of PKS candidate pathways that fail would be reduced, while the performance of pathways would also increase. Folding in tools like AlphaFold may be helpful in advancing the research. The impact of this approach is still limited by low overall performance (<1-g/L titers at lab scale), but this research may show a path to generating significantly more data to better train ML models and rapidly improve learnings to increase performance.

- Response to Reviewer 1: Thank you for your helpful comments and suggestions. As you mentioned, this project was initially “brute force,” but with a goal of collecting enough PKS data to make future projects possible with much less trial and error. As our successfully producing strains/designs were only achieved recently, we did not yet have enough diverse examples of working designs to train our ML models until now. At present, we are just completing a large “build” round, which will provide enough positive working examples to inform ML models that require on the order of hundreds of examples. We are using a wide array of “features” to describe each design, including features computed from AlphaFold structures as you suggest. Now that we have working strains, we are also working to optimize metabolism and growth conditions to improve TRY and have already identified several bottlenecks that will allow us to increase production titer substantially.

- Comments: Strengths: (1) Engineering PKSs offers enormous potential for bioproduction of chemicals with diverse but precisely defined structures. However, PKSs are notoriously difficult to engineer due to their complicated structures and folding issues. This team has obtained substantial success in expressing novel polyketides. The ability to build and test 100 PKSs in 9 months is impressive, considering the previous state of the art (one PKS for one Ph.D. in 5 years to complete). (2) The team has made excellent progress, achieving most milestones. (3) Production of four lactams, including three novel nylon precursors, was achieved. This result proved the possibility of building and testing novel polymer precursors from PKS libraries. Weaknesses/areas for improvement: N/A.

- Response to Reviewer 2: Thank you for your supportive comments.

- Comments: This project was started in 2020 and is nearly completed. The goal of the project, essentially "develop a high-throughput DBTL cycle for PKS engineering, and test it by building a PKS to make the nylon monomers caprolactam, valerolactam, and novel derivatives," fits perfectly with the ABF mission to further synbio to produce industrially relevant molecules, and in this case has the bonus of harnessing the diversity of enzyme function to create new molecules. The project is making an array of valuable products, including several novel plastic (nylon) monomers with potentially better properties. They are using a much better host than the organisms that have PKS enzymes in them for faster growth and faster engineering. The project is ambitious to build an entire pipeline for high-throughput engineering and screening, which will be useful for many projects for a long time. The project will be very successful and meet its milestones and goals. It was very refreshing to see all the milestones listed and their state of completion. This needs to be required for all projects and AOP funding. They were honest in early struggles and failures. Industry is going to be more reluctant here to show struggles and failures, making the milestone list important. There was some legitimate concern about the difficulties and lack of progress midway through the project, but the project team overcame them and was ultimately successful. Also, all FOA and DFO reviews going forward should have an impact slide clearly stating benefits to the ABF and the U.S. bioeconomy. The project has been very successful based on meeting the ABF's and BETO's missions: "We have confirmed production of valerolactam and three additional novel nylon precursors with PKSs with titers from 1 to 10 mg/L … We have demonstrated that our build pipeline can build hundreds of PKSs at once in high throughput."

- Response to Reviewer 3: Thank you for your supportive comments. We are glad that our presentation framework was effective in communicating both the challenges and accomplishments of this project.

- Comments: This is overall a very strong project. The presentation did a great job at showcasing the project goals, milestones, and how milestones have been met. I appreciated their details on the DEI components of the work. I would also recommend that all presentations be required to show milestones and their achievement of them. I would suggest that they should show all milestones at least in the appendix. While the eventual impact of developing PKSs as a biosynthetic pathway tool is large, the current project titers are still rather low (despite improvements from the state of the art), and further development will be needed.

- Response to Reviewer 4: Thank you for the positive comments and feedback. At the time of our presentation, our success in producing valerolactam and three additional novel nylon precursors was relatively recent. As described in our comment to Reviewer 1, after successful proof-of-concept production, we shifted much of the project to optimizing our PKS designs, growth conditions, and host metabolism. We have recently discovered that a key pathway precursor is being rapidly diverted to other metabolic pathways, and we are optimistic that our current efforts to divert this flux toward our nylon precursor will result in substantial titer improvement. We have made substantial progress in improving TRY and have a clear path forward for further improvement. We believe the learnings from this project will also enable accelerated TRY improvements for other PKS projects in the future.

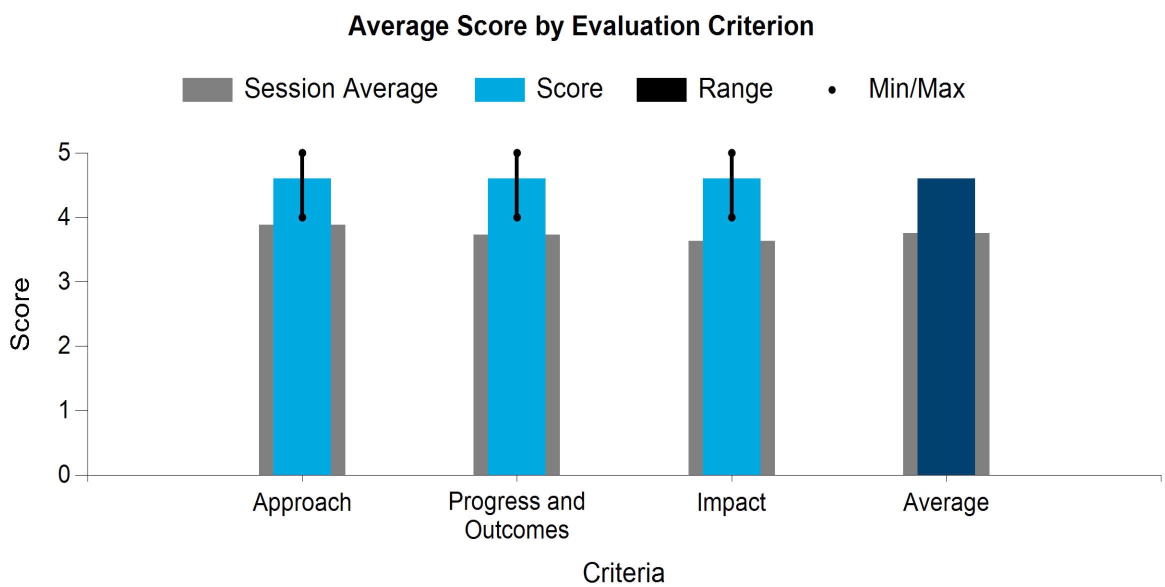
- Comments: This project seeks to design ML tools that enable successful prediction of PKS design, which would ultimately lower the barriers to PKS engineering and improve the efficiency of the DBTL cycles for those biosynthetic pathways that use a PKS. This approach represents a significant improvement relative to trial-and-error methods that are currently in use for novel PKS design. The management plan provides for regular meetings between all teams, and individual teams meet as needed. However, there is no indication of specific ABF personnel participating in the research program. Risk and mitigation plans are provided. One risk that should also be considered includes successful PKS gene synthesis and protein folding, but insufficient substrate throughput to detect and accurately identify the resulting product. It is also unclear how novel PKSs are being evaluated from the standpoint of product formation. For example, is product formation assessed for an *in vivo* process, or are enzymes purified and challenged with a variety of starter units? A commendable plan is in place to increase the diversity of project participants and to improve the development of young scientists by allowing them to take ownership of their assigned tasks. The project has made good progress. ClusterCAD has been shown to successfully demonstrate an automated approach to PKS design. Results have been disseminated in one peer-reviewed paper, and additional manuscripts are planned. ClusterCAD is available to the ABF and to the community at large. Quantitative end-of-project milestones are not likely to be met by the project end date. The impact of the project is jeopardized by modest PKS substrate throughput, which would limit applicability in the performance-advantaged materials space due to low TRY values. The impact is likely to be more significant when applied to identification of complex novel structures, which would include higher-value specialty chemicals and the pharmaceutical space. Methods for improvement of the catalytic properties of PKS enzymes should also be considered.

- Response to Reviewer 5: Thank you for your supportive comments and constructive feedback. We agree that it would have been useful for us to include a slide outlining which ABF personnel were involved in this project. Briefly, we have a host construction (build) team lead by Dr. Chris Johnson at NREL, an ML (learn) team led by Dr. Phil Laible at ANL, an ML (learn) team led by Dr. Hector Garcia Martin at LBNL, a proteomics (test) team led by Dr. Chris Petzold at LBNL, and a metabolomics (test) team led by Dr. Jon Magnuson at PNNL. Our PKSs have been evaluated for product formation *in vivo* using liquid chromatography/mass spectrometry. Thus far, we have detectable levels of product production *in vivo* for a number of our PKS designs, but it is indeed possible that some strains are catalytically active yet remain below limits of detection. For purposes of this project (optimizing these strains and creating ML models), we believe it would still be appropriate to categorize these PKS designs as expressed/folded proteins that are effectively catalytically inactive. Our Peer Review presentation was presented relatively shortly after producing our first successful designs, but we have subsequently identified and corrected some significant metabolic bottlenecks that allowed us to achieve large improvements in TRY, as well as some changes to our PKS designs themselves that improve catalytic activity, and we are optimistic that we will continue to improve TRY in the remaining months of the project. We agree that further research into optimizing PKS catalytic activity would be valuable here, especially in light of the extremely high TRY obtained in laboratory conditions with some natural PKSs.

DEVELOPING MULTI-GENE CRISPRA/I PROGRAMS TO ACCELERATE DBTL CYCLES IN ABF HOSTS ENGINEERED FOR CHEMICAL PRODUCTION

University of Washington

WBS:	2.5.3.212
Presenter(s):	Carol Rhodes; James Carothers
Project Start Date:	10/01/2019
Planned Project End Date:	12/31/2023
Total Funding:	$2,269,966.00



COMMENTS

- This is a core project that builds capabilities for the ABF that can be useful and applicable to a potentially wide range of industrial users. By developing new CRISPR activation (CRISPRa) and interference (CRISPRi) tools in two ABF host strains (CRISPRa to activate/maximize the production pathway, and CRISPRi to inhibit side pathways to other products), the team is building up the ABF library of information and tool set to apply similar approaches to other organisms in the future if needed for a different engagement. The work in this study validated the ability to build complex, multi-gene programs using CRISPR and applied this knowledge to 4-aminocinnamic acid production. The feedback loop, particularly on the ML side, is a further interesting factor in this research. However, the degree to which the feedback loop was closed and the level of enhancement achieved through the use of the ML tool was not well validated. Further cycles and improvements driven by the ML tool would be helpful in validating the ability of ML to shorten development times by reducing required cycle counts.

- Strengths:

  - Engineering multi-gene activation in non-model organisms to guide metabolic flux is an important tool to industrial biomanufacturing but has not been well developed. This team demonstrated successes in developing these tools.
  - The team used a combination of mechanistic modeling and an ML model to address the large combinatorial space of multi-gene programing; the approach is highly innovative and effective.
  - The PI developed a straightforward method to measure DBTL cycle efficiency. The method makes it very clear to quantify their progress and impact. More than 30% DBTL cycle time reduction was achieved. This can be a good model for the other ABF teams to follow—developing similar methods to quantify their DBTL efficiencies.
  - The team has achieved all the proposed milestones on time and demonstrated the build of six guides in 5 days, which is impressive.
  - Multiple high-impact publications resulted from this project.
- Weaknesses/areas for improvement: N/A.
- This is overall an academic and research and development (R&D) program that has large potential to help the field of synthetic biology and therefore U.S. biomanufacturing. For this reason it fits with BETO's mission. This work clearly fits well with the mission of the ABF. Thank you for Slide 14 showing all tasks and progress toward them. The project is clearly making good progress and has a high likelihood of being successful.
- This is a very relevant project that leverages the ABF's skills and expertise. The development of CRISPRa/i tools is useful for the synbio field and can open up new methods for gene expression tuning. The project has proceeded mostly on schedule and met several main milestones and deliverables, though from the later slides, it appears that less progress has been made on the second host and on the production of 4-aminocinnamic acid in *P. putida*. The current production levels are also very small (in the micromolar range), hence my lower score on the impact category. There is likely still a lot of development needed before there is strong impact for the production of the molecule of interest.
- Funded in response to the 2019 multi-topic FOA, work completed under this project appropriately responds to the area of interest that includes development of tools for use in the ABF that show increase in DBTL efficiency and production of data sets that enable the ABF learn methodology. The key metric was a 30% increase in efficiency in DBTL cycle time relative to the state of the art in the same organism. An ambitious plan was devised to create CRISPR-Cas expression tools capable of bacterial gene activation and inhibition followed by demonstration in two ABF hosts. The initial plan was to implement these tools in *P. putida* and *A. baylyi*, although a verification team seems to have recommended maximizing learning in the *P. putida* system at the expense of work in *A. baylyi*. This was a sound recommendation. The project has achieved good progress in creating and evaluating efficient new activation/inhibition tools for *P. putida* that should be applicable to other ABF organisms possessing basic genetic engineering tools. Publication of several manuscripts in high-impact journals ensures good visibility, particularly for an academic audience. Project strengths are as follows. Although it was frustrating that no information was provided in advance, the presentation slides are clear and informative. Project roles and milestones were well articulated. Definitions for gene activation and DBTL efficiency are provided, which enables measurement of progress toward quantitative milestones. Plasmid-based genes were activated in the range of 8–32 times, and genome-based genes were activated 1–29 times. Variability in the same gene activation is not a problem given the ability to quickly assess multiple constructs. Gene repression varied from 1–25 times. DBTL efficiency increased more than 30%. Project weaknesses are as follows. Although it was stated that the number of multi-gene CRISPRa/i

assessed simultaneously does not impact product formation, insufficient evidence was provided to support this conclusion. The choice of 4-aminocinnamic acid as the model system for assessment of their tool relegated product formation to exceedingly low concentrations (maximum 0.6 mM, about 0.1 mg/L). I would prefer to see the tool assessed on a well-defined pathway that affords higher product concentrations. This would enable a larger product range and rationalization of the impact of higher and lower gene expression. Future experiments in bioreactors should be reconsidered given the time frame remaining and the modest concentrations of 4-aminocinnamic acid produced.

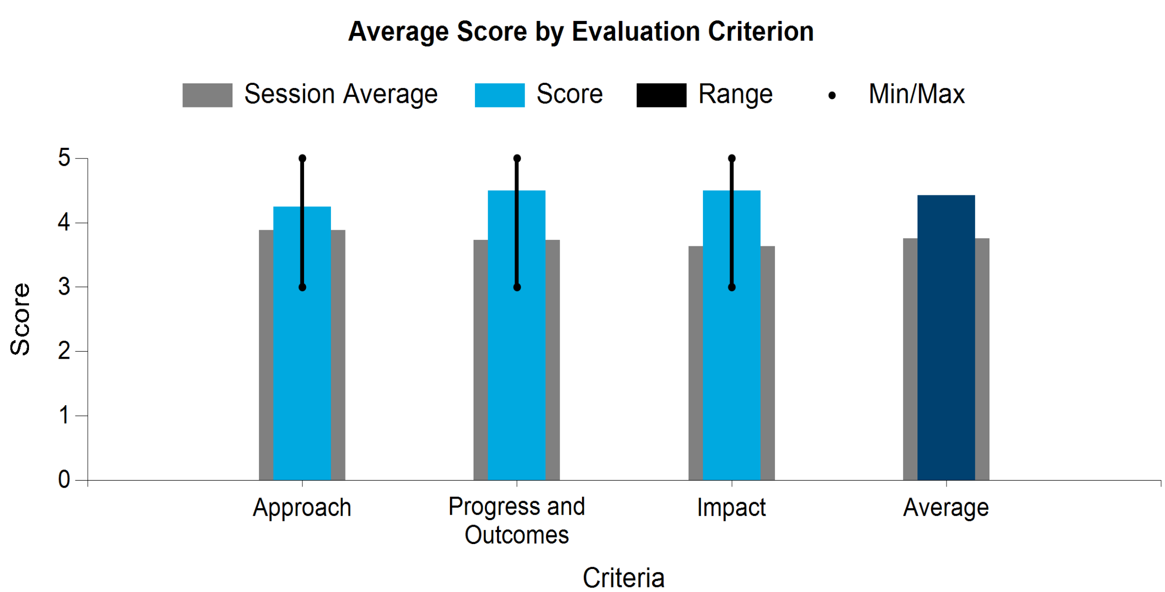
ABF DFO WITH C16 BIOSCIENCES

Sandia National Laboratories and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.707
Presenter(s):	John Gladden; Karthikeyan Ramasamy; Katarina Younkin; Michele R Jensen; Di Liu
Project Start Date:	02/20/2020
Planned Project End Date:	02/01/2024
Total Funding:	$1,449,000.00

Palm oil is the most widely used vegetable oil in the world; however, its production causes a variety of issues, including environmental damage and increased greenhouse gas (GHG) emissions. The motivation of the project is to overcome these issues by developing alternative palm-oil-producing approaches by engineering microbial-derived oils with equivalent properties. In this project, C16 Biosciences partners with the ABF to engineer *R. toruloides*, an ABF host, to produce mid-chain fatty acids and fatty alcohols as an alternative to products derived from palm kernel oil. The main challenge is that these chain lengths are particularly rare in nature and are not a naturally abundant fraction of microbial lipids. Here we leverage tools, knowledge, and capabilities previously developed in the ABF on *R. toruloides* and design a number of strategies to (1) engineer the fatty acid synthase, (2) bridge bioconversion gaps, and (3) address pathway bottlenecks. We further implemented functional genomics and multi-omic analysis to address these challenges. We have achieved our go/no-go milestone by reaching production of over 5% mid-chain fatty acids and fatty alcohols as a proportion of overall lipids or fatty alcohol profile. This project would enable C16 Biosciences to establish *R. toruloides* as a platform to produce a wide range of oleochemicals as a sustainable alternative to palm kernel oil, as well as to promote CO_2 emissions reduction and sustainable biomanufacturing.



COMMENTS

- C16 is developing a palm oil alternative using synbio processes. ABF tools are helpful to C16 in identifying strains and pathways to produce mid-chain fatty acids that can be optimized for its product and process. The ABF was successful in generating strains capable of producing the target lipids, and is currently in the process of working to better understand the bioconversion gaps that limit further production. Decreased degradation of product is also targeted through further gene identification and strain design. The current results appear to require further optimization in order to produce commercially viable results, and it is not clear how ongoing work to optimize the current strain will yield the performance increases needed, although some detail was likely not provided in these slides due to IP concerns.

- Overall, this is a great project for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. The work in this proposal clearly advances the capabilities of the ABF, national labs, and BETO.
- The presentation lists several milestones that were achieved and go/no-go criteria in FY 2022. Presumably the project is going well, but next time, put all milestones and status (and percent complete if not complete). It's hard to judge without this info. Very good impact slide clearly stating the benefit to the ABF and the U.S. bioeconomy.
- This project is an excellent example of how core ABF work can be leveraged for commercial applications. ABF's prior work with *R. toruloides* helped enable the success of this project. The question posed leveraged ABF strengths in difficult strain engineering and metabolic-based discovery. The impact of the work on C16 and the overall palm oil industry is well articulated.
- The project between C16 Biosciences and the ABF seeks to engineer *R. toruloides* to produce mid-chain fatty acids and fatty alcohols as an alternative to palm kernel oil. The project leverages ABF *R. toruloides* expertise and multi-omic capabilities. The three-pronged experimental approach includes engineering Type II fatty acid synthase, identifying bioconversion gaps, understanding the mechanism, and eventually alleviating product degradation. This is a challenging project, but the plan is sound and the project timeline fortunately extends for 3 years. Functional genomics and metabolomics are in place as a mitigation strategy for unknown biochemical gaps that may be identified in the biosynthetic pathway and to guide strain development to reduce product degradation. Specific DBTL tasks were assigned, although communication plans were not provided. DEI was not addressed. Significant progress has already been achieved. Several iterations of fatty acid synthase engineering were evaluated, one of which provided an approximate tenfold increase in the relative level of mid-chain fatty acids compared to the control. Product concentrations were not reported, however. Although experimental details are limited, it seems that heterologous expression of one protein has increased mid-chain fatty acid product at least sixfold. Feeding studies and functional genomics have identified potential gene candidates that may be involved in product degradation. Given the additional 1.5 years on the project timeline, the prospects for additional advancements are high. As mentioned, product concentrations have not been indicated, so it is difficult to assess commercialization potential. It seems that the technical advances already achieved would justify venture investment in C16 Biosciences, should that be their goal.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the positive evaluation and feedback of the project. As the reviewer suggested, we did not provide some technical details due to IP concerns. Our ongoing work focuses on (1) further engineering the fatty acid synthase based on our first two rounds of design and testing results, (2) identifying and bridging bioconversion gaps to enable and improve mid-chain product synthesis, and (3) addressing product degradation. We have clear research plans to optimize yields of current strains, with milestones and objectives to address these areas. We thank the reviewer for the suggestion, and we will be sure to put all milestones and their completion status next time. Regarding communication plans, we hold monthly meetings to discuss progress and next steps and have action items clearly laid out for each team. In addition, the project uses a shared team drive to share data, protocols, quarterly reports, presentation slides, and meeting follow-up discussions. We also hold meetings in smaller groups to discuss focused topic areas as needed. DEI is very important and integrated to the project, including team composition, creating an environment for discussion to be inclusive for feedback from team members and leadership. We did not report product concentrations due to potential IP concerns. In that regard, C16 Biosciences has clear objectives on product concentrations to meet their commercialization plans.

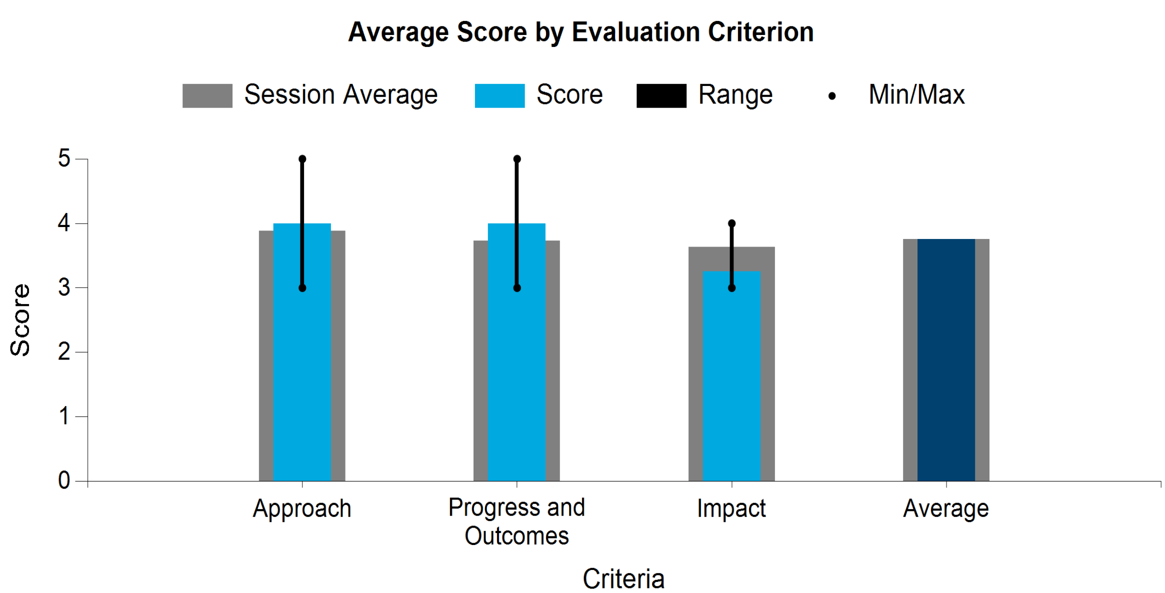
ABF DFO WITH THE UNIVERSITY OF DELAWARE AND WASHINGTON UNIVERSITY IN ST. LOUIS

Lawrence Berkeley National Laboratory and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.708
Presenter(s):	Deepti Tanjore; Katy Christiansen
Project Start Date:	02/26/2020
Planned Project End Date:	09/30/2023
Total Funding:	$500,000.00

The nonconventional yeast *Yarrowia lipolytica* is a promising biomanufacturing chassis well suited for production of oleochemicals and terpenoids, including biofuels such as limonene and bisabaline and other valuable chemicals of the carotenoid family. Scale-up of these processes, however, has been marred by phenotypic changes, such as loss of titer (or titer instability). This problem is exemplified by an engineered ß-carotene-producing strain that was developed as a platform for the production of b-ionone (https://doi.org/10.1186/s12934-018-0984-x) as part of a collaboration between co-PI Tang and Arch Innotek, a St. Louis biotech startup. In brief, the mevalonate pathway was optimized by enhancing flux from acetyl coenzyme A (CoA) to terpene precursors by overexpressing several upstream mevalonate pathway enzymes (push) and by reducing flux (block) toward squalene synthesis. Then, we overexpressed carB and carRP via genome integration to pull flux from geranylgeranyl diphosphate to ß-carotene, achieving approximately 4 g/L using benchtop bioreactors. The ß-carotene strain was further engineered by overexpression of a novel carotenoid cleavage dioxygenase, resulting in ß-ionone fermentation (approximately 1 g/L). However, when moving those engineered strains to larger bioreactors, cell performance significantly dropped. This problem has catalyzed the current collaboration between PI Blenner and co-PI Tang to investigate the nature of titer instability in this b-carotene strain as a model to understand more broadly the factor that led to cellular heterogeneity during cell line development and scale-up.



COMMENTS

- Understanding performance loss during organism scale-up is an important topic that can help enable future work by helping strain designers and process engineers optimize organisms and conditions for performance at scale. In this research, multiple hypotheses for performance loss during scale-up are presented and tested experimentally. The design of experiments utilizes amber systems to enable testing of a variety of growth conditions quickly. As of the time of the presentation, early results had demonstrated titer loss as a function of generation and culture conditions, providing useful data to further analyze (ongoing) and better understand mechanisms associated with performance loss. The applicability of this research may be limited to a set of conditions and a single organism, limiting impact. However, further experimentation with other hosts or comparison against other academic data may help draw learnings applicable more broadly.

- This is a great project overall for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. The work advances the capabilities of the ABF, and at the same time, the partner gains knowledge and access to capabilities it does not have in-house.

- The execution of the work plan appears to be going well from what was on the slide. Next time, put all milestones and status (and percent complete if not complete). It's hard to judge without this info. Also, all FOA and DFO reviews going forward should have an impact slide clearly stating benefits to the ABF and the U.S. bioeconomy.

- The overall work plan and approach is not the best approach to solve the problem. This is advice to the partner, not the ABF. The ABF is doing what the partner is asking them to do. Looking at Slide 11, I'd say there is, practically speaking, no difference in stability (instability). The relatively small shifts in instability aren't going to matter in a real-world manufacturing setting. Clearly the population is going to zero production pretty quickly, with a cliff at Day 2. No amount of media tweaking is going to solve that problem. There are other fundamental issues at play. The genomic sequencing is the obvious place to start. You probably could have just focused on one media condition. Even if the genetic rate of mutation might change in different conditions, that knowledge is not helpful or applicable to solve the massive instability. Clearly any media condition is leading quickly to zero production.

- Focus on the genetic mutations, and think about other fundamental issues that could be leading to such strong selection to shut down production. Also, try to add a kill switch for anything that shuts down production (i.e., addiction circuit that the ABF has developed for other projects). Sometimes you don't need to understand a problem to fix it.

- This project addresses important questions for biomanufacturing around the causes of cell heterogeneity and declines in performance across fermentation scales. The scientific approach presented is reasonable and leverages ABF capabilities. There have been several fermentation rounds completed. However, given that the project started in 2021 and several fermentation rounds have been done, I find the lack of data around any potential gene candidates concerning at this stage (the project is slated to end in September). As a result, the overall impact of the work is not as easy to gauge; however, elucidating the mechanism of decline in performance under larger-scale fermentation is a key problem for the synbio field and worthy of resources.

- The partnership between Washington University in St. Louis, the University of Delaware, and the ABF seeks to link multiple macroscopic causes (O_2, mixing, and shear stress) to the genetic instability and metabolism (i.e., product formation) of *Y. lipolytica* in a concerted fashion. The project leverages ABF omics expertise (proteomics and metabolomics) to understand the root causes of strain instability and production instability for this promising biomanufacturing chassis. Several hypothetical causes are presented. The ambitious experimental plan called for implementation of fermentation at an ABF site and included several variations in what appear to be challenging culture conditions. Problems encountered in fermentations (drained reactors, foaming issues, and unusual mixing dynamics) were overcome but likely slowed progress. Risks and mitigation strategies were not provided. Responsibility for various data collection was assigned without indicating what communication plans were in place. DEI plans were not described. Loss of productivity was observed, as expected. Omics analysis has commenced on various samples. The project has two additional quarters before completion. The end-of-project milestones were overly ambitious and are not likely to be met. It is not clear from the presentation if multiple strains with varying gene expression were cultured, making it difficult to understand how optimal levels of gene expression will be determined. Whether strain engineering strategies will be evident from omics data remains to be seen. This project would have benefited from a tighter experimental plan—for example, selecting a specific culture condition that brings about a change in productivity/strain stability (pH, dilution, and O_2) and analyzing replicates at two values.

PI RESPONSE TO REVIEWER COMMENTS

- RESPONSE: Thanks for the comments. We agree that the study on other hosts can be useful. However, due to limited resources and challenges in this study, we cannot investigate other hosts. We look forward to continued investment from the ABF (and NSF) to support the importance of the work noted.

- RESPONSE: We thank the reviewer for their comments. We want to clarify that the goal of this project was not to solve the problem of instability, but to study it. It would be a company's justified approach to solve instability; however, we are not a company, and our interest is to understand *how* instability arises. We strongly feel that the ABF's capabilities are most useful for generating fundamental knowledge rather than solving low-hanging problems. We are still awaiting further data, but sequencing data suggest that something other than point mutations are at play. We are still analyzing the omics data and genome sequences. We hope to get more insights this summer. Moreover, we have some interesting results (e.g., use oil extractive fermentation process) that may improve strain stability by alleviating burdens and stresses. We'd never know this if we didn't focus on understanding the problem. We will be much more successful in fixing the problem once we develop the understanding.

- RESPONSE: Our project has been significantly delayed due to COVID. In 2021, the bioreactor facility was not fully operational, and all omics analyses and services are very slow. Another issue is the supply chain that delayed the purchases of chemicals and lab supplies. To continue this work, we have applied for an NSF-ABF grant to continue this project and resolve strain stability problems.

- RESPONSE: In this study, we had various bioreactor operation problems because long-term chemostat culture is always challenging. Additional repeated tests have been performed to overcome this problem. We had pre-meetings to coordinate project work and have monthly meetings to update on progress and make any necessary adjustments. The University of Delaware, Washington University in St. Louis, and ABF teams are meeting monthly to discuss the work plans and risk mitigation strategy. Also, we have collected various samples and are waiting for the omics results from ABF labs. We hope to get more understanding once these samples are analyzed. DEI plans, while valuable, are not a requirement of this project; nevertheless, we still demonstrated a commitment to DEI. A Ph.D. student, Alyssa Worland, has worked with the ABF lab for 9 months. She has accumulated rich experimental skills and data analysis experience. Moreover, an undergraduate student (Millie Savage) from Lincoln University (a historically Black university) is working at co-PI Tang's lab at the Washington University in St. Louis to help with yeast culture and data analysis this summer. Such student training is a part of workforce development for female and minority students. We have proposed to build strains with varying levels of gene expression and stability for the NSF/ABF project, a mechanism that better (at all) resources the academic partners. We hope this reviewer remains enthusiastic about this direction. We agree that the research plan could have been tighter. We did eventually come to this position, and finished with a tight set of conditions on the last runs.

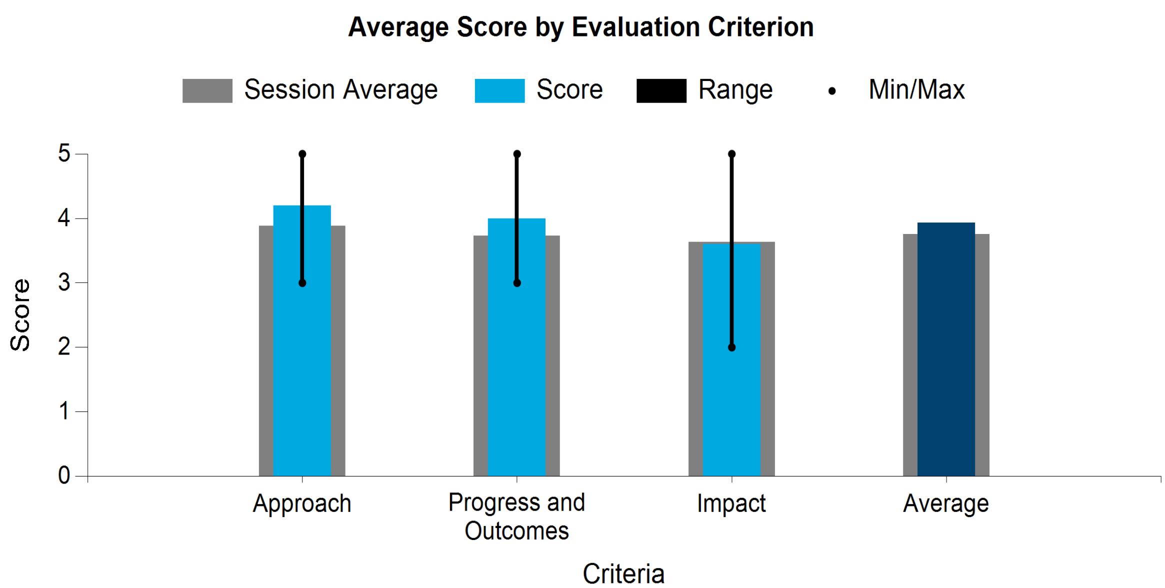
ABF DFO WITH ENDURO GENETICS

Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, and National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.709
Presenter(s):	Deepti Tanjore; Katy Christiansen
Project Start Date:	03/05/2020
Planned Project End Date:	07/29/2023
Total Funding:	$500,000.00

A major challenge to industrial development of new bioprocesses is scale-up. Engineered production strains experience significant selective pressures caused by metabolic burden and toxicity of heterologous overexpression. This selective pressure promotes growth of low- or non-producing cell variants, and thus leads to production decline at scale. Enduro Genetics is a startup that uniquely and directly addresses the challenge of cellular culture heterogeneity. Enduro has pioneered an analytical algorithm based on next-generation sequencing to uncover and quantify genetic heterogeneity throughout the different stages of a fermentation (https://doi.org/10.1038/s41467-018-03232-w) and is working with industrial companies to investigate the culture heterogeneity that arises in their processes. In this DFO project, the goal is to understand the causes of heterogeneity, especially in large bioreactor runs. We will also apply customized gene circuits to prevent loss in productivity in the ABF strains.



COMMENTS

- Scaling is a particular challenge in biological systems, as larger reactors have a tendency to select for organisms that are nonproductive. In order to overcome this limitation, this research looks to couple the production gene with a key survival/growth gene in the organism. The approach is potentially applicable to a wider range of organisms and targets. Preliminary results show that engineered strains are outperforming wild-type strains by a significant margin at 300-L scale. Fermentation studies will validate the approach further. Learnings from this study can be used by the ABF for other hosts and targets that are facing scaling challenges.

- Strengths:
  - The team has identified essential genes that can be used in *P. putida* for selection of stable producing strains.
  - Early evidence was obtained and showed that Enduro's strain outperformed the wild-type strain at 300 L.
- Weaknesses/areas for improvement:
  - Because Enduro is a Europe-based company, it is not clear how this project can benefit the U.S. bioeconomy.
  - The connection between work done in *P. putida* at NREL and *B. subtilis* at ABPDU is unclear.
- This is a great project overall for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. Enduro's value proposition to the bioeconomy and biological manufacturing through fermentation is very large. Strain instability is a major problem all synbio companies have to overcome, and having off-the-shelf tools to fix it would be enormously helpful. The work advances the capabilities of the ABF, and at the same time, the partner gains knowledge and access to capabilities it does not have in-house.
- The execution of the work plan appears to be going well from what was on the slide. Next time, put all milestones and status (and percent complete if not complete). It's hard to judge without this info. Also, all FOA and DFO reviews going forward should have an impact slide clearly stating benefits to the ABF and the U.S. bioeconomy.
- This project addresses a highly relevant problem in bioprocessing. The lessons learned and tools developed for this will have impact beyond the specific project. The project demonstrated a successful increase in the production of the target molecule at 250 mL. It was not clear why the 300-L results were still pending if three out of the four campaigns at that scale have been completed. The project is slated to end in September 2023, but no work on *P. putida* was presented or appears to have been done yet, which raises some questions on the feasibility of achieving the full project goals.
- The project between Enduro and ABF aims to address culture heterogeneity in large-scale fermentation by coupling cell growth to production. The approach includes concept demonstration with Enduro-prepared *Bacillus* strains and porting the technology into *P. putida*. The project leverages ABF expertise in *P. putida* engineering, fermentation process development and scale-up, and genomics. Seven essential genes in *P. putida* have been targeted, for which three constructs are ready for insertion and four of which remain under construction. Three *Bacillus* strains have been cultured at 250-mL scale at ABPDU. Risk management, communication plans, and DEI were not provided. For the *Bacillus* strains analyzed, product signal is amplified in the range of 9- to 14-fold over wild-type at 250-mL scale. Product identity and concentrations are not provided. Deep sequencing results are not provided. Two quarters remain before project completion. It is not possible to determine commercial potential currently. It was reasonable to select as many as seven *P. putida* targets to evaluate the concept, but extending the project to 3 years would have enabled a more thorough evaluation of the technology in *P. putida*.

PI RESPONSE TO REVIEWER COMMENTS

- RESPONSE: We thank the reviewer for taking the time to review us and provide feedback. We look forward to contributing our learnings for ABF to use in the future. We plan to publish at least one paper from this work.

- RESPONSE: The project will benefit the U.S. bioeconomy by creating joint learnings in a strong background within fermentation scale-up—an important field to the U.S. bioeconomy. By integrating work from both sides of the Atlantic, it is expected that the U.S. bioeconomy will be able to leverage advances in Europe. For the work done in *P. putida*, Enduro's technology will be applied to a U.S. strain development project. The work in *P. putida* at NREL uses the same underlying technology for product addiction as in *B. subtilis* at ABPDU, thus testing the technology in two different systems and stages of development.
- RESPONSE: Thank you for the comments and suggestions. We will make sure to follow them going forward.
- RESPONSE: For *Bacillus*, at the time of submission, there were some questions on whether minor medium differences between the runs at 300 L precluded direct 1:1 comparison. Further, it appeared that one run at 300 L might have been subject to at least partial contamination. This is currently being investigated. For *P. putida*, as reported in our presentation, strain construction is nearly complete, and we anticipate initial strain evaluation to commence soon. Following that, downselected strains will be scaled up to evaluate strain stability, which we expect to be able to complete by the end of the project. This project start was delayed due to COVID, so we expect to extend until December, if necessary.
- RESPONSE: Due to the very limited amount of time allotted to presenting these projects, we were not able to include risk management. Communication and DEI are broadly relevant to the ABF, and as such, were presented elsewhere. We agree that the project may have benefited from a longer time frame, but budgetary constraints favor shorter collaborations, and we believe we are on track to complete this project in the time we have.

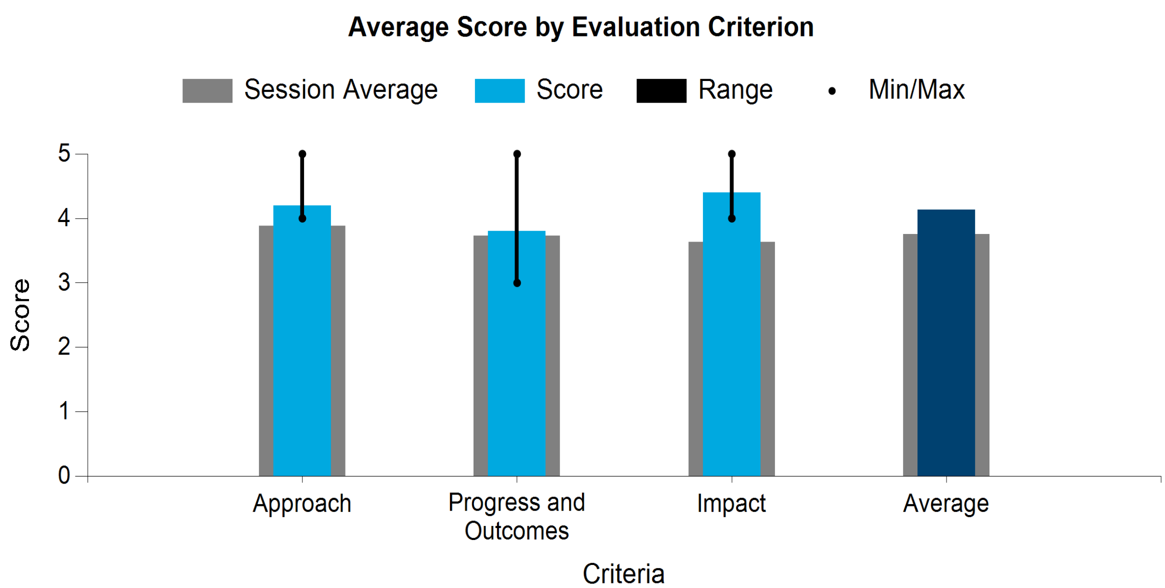
ABF DFO WITH SUPERBREWED FOOD

Los Alamos National Laboratory, Oak Ridge National Laboratory, and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.711
Presenter(s):	Adam Guss; Karthikeyan Ramasamy; Michele R Jensen; Tim Theiss
Project Start Date:	02/24/2020
Planned Project End Date:	05/05/2024
Total Funding:	$1,400,000.00

A major limitation of traditional anaerobic fermentation processes is the low mass yields of products due to the decarboxylation of pyruvate to acetyl-CoA. Most products have a maximum theoretical carbon yield of 66%. To help overcome this inefficiency, Superbrewed Food has developed a novel fermentation platform called MixoFerm, combining sugar fermentation with the addition of additional electrons in the form of H_2. This allows theoretical yields to approach 100% carbon yield. Strains have been engineered to produce isopropanol using this approach, but the resulting strains are unstable. In this project, we are investigating the mechanism(s) of strain instability and decreasing performance to help understand the phenomenon and devise strategies to overcome it. We are also developing biosensors that can detect the presence of isopropanol and control the expression of an essential gene, enabling the selection of strains with improved isopropanol production. Together, these approaches will result in the generation of enhanced isopropanol-producing bacterial strains and provide insight into mechanisms of strain instability.



COMMENTS

- This research is aimed at using ABF expertise to further optimize the performance of a strain for Superbrewed Food that makes isopropanol. The approach uses a biosensor circuit in order to detect strains producing the product of interest, with a goal of using the sensor to identify strains with higher performance, which can then be isolated. A further effort to link the biosensor to survival should drive evolution toward strains of higher performance. This project is now in flight, with fermentation runs completed and results sent for further analysis at the national labs. Results are pending for whether targets can be identified that improve performance. If successful, this research will point toward a potential optimization pathway that would be helpful for other users as well.

- Strengths:
    - This project aims to address strain instability during isopropanol production, which is a common problem in microbial fermentation that leads to diminished performance. Knowledge learned from this project may be applicable to other bioproduction systems.
    - The combination of sequencing and omics analysis may reveal insights into the mutation mechanism.
- Weaknesses/areas for improvement:
    - This project seems like it is just getting started; not much progress was reported.
    - The project aims to address cell-to-cell variations in fermentation, but no single-cell-based analysis technique was proposed.
- This is overall an excellent use of ABF technology and expertise to advance the bioeconomy and help a smaller company with infrastructure it does not have. It advances both the ABF and the company. It's great to see the impact slide for projects clearly stating benefits to the ABF and the U.S. bioeconomy. This should be required on all FOA and DFO slides going forward.
- An addiction switch is a very good idea and is likely to work. The only criticism is that sometimes you don't need to fully understand the problem if you have a way to fix it, like in the addiction switch. Some of this might be overkill; just try the addiction switch first and see if it fixes your problem sufficiently.
- Also, next time, put all milestones and status (and percent complete if not complete).
- This is an interesting project that leverages ABF's skill and capabilities. The development of biosensors to track production outputs is likely to be useful in other projects and applications, particularly for anaerobes. Though the project only started last year, I was surprised that there was not any substantial data presented; it would appear the project may be behind schedule.
- The partnership between the ABF and Superbrewed Food seeks to understand the cause of and identify solutions to strain instability that occurs over time in the anaerobic Superbrewed Food process for isopropanol production. The approach leverages ABF genomics, proteomics, metabolomics, and biosensor development expertise. Anticipated challenges/risks are the difficulty of working with anaerobic organisms and the fact that omics data obtained from bulk culture samples or from individual colonies may not reveal the cause of instability. One risk mitigation strategy to be pursued includes construction of a biosensor to enable selection of improved strains. This work has not yet been initiated. Communication between team members occurs monthly. DEI plans were not specifically addressed. The project is in Q3 of a 2-year project, so progress is difficult to assess, although strains have already been cultured and omics work is underway. The project impacts for all partners, including Superbrewed Food, ABF, and the U.S. bioeconomy, were clearly and accurately stated. Assessment of commercialization potential is inappropriate at this point in the project timeline.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for the helpful comments. Initial work was slowed due to a contamination event in the bioreactor, but that has now been fixed and work is proceeding. For single-cell work, molecular methods typically rely on extensive polymerase chain reaction amplification, which is known to skew some results. Therefore, we are initially focusing on (1) bulk culture sequencing and measurements to understand general trends, and (2) sequencing of colonies derived from single cells in the bioreactor population to look at genomic changes that occurred in individual members of the population. If need be, we will consider trying single-cell approaches to gain more information.

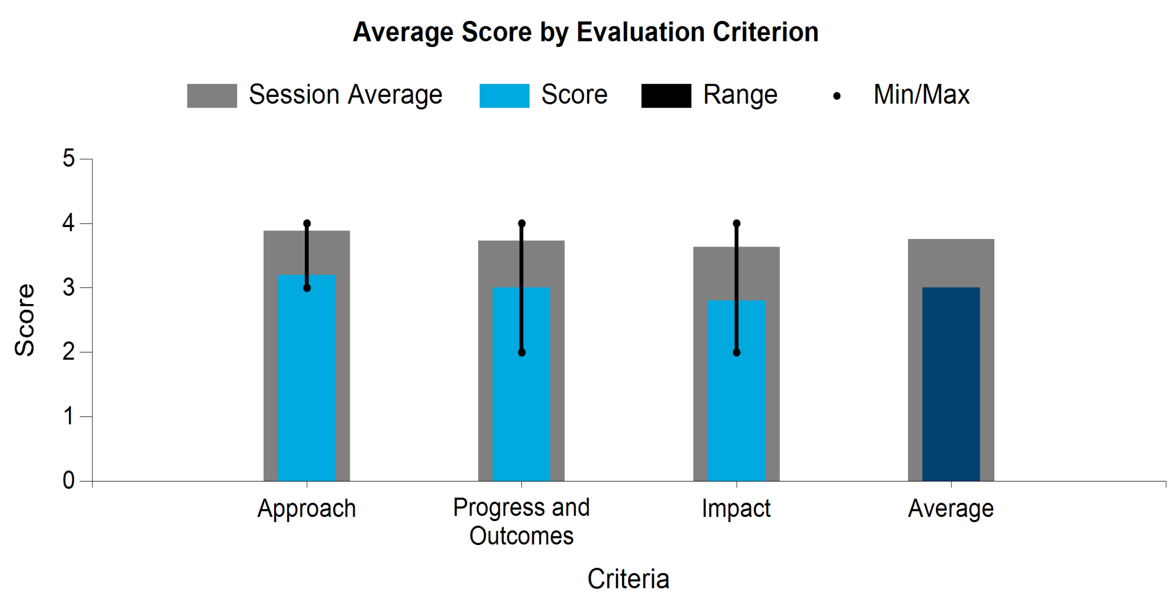
ABF DFO WITH KALION INC.

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.712
Presenter(s):	Laura Hollingsworth; Megan Krysiak; Michelle Reed; Violeta Sanchez i Nogue
Project Start Date:	04/02/2020
Planned Project End Date:	10/22/2022
Total Funding:	$425,000.00

Kalion Inc. is an industrial biotechnology manufacturer of high-purity chemicals from biomass, including glucaric acid, to be used in the industrial, material, and pharmaceutical markets. The project goal is the application of ML in conjunction with high-throughput cultivations and metabolomics to understand and overcome two different challenges: (1) improve glucaric acid productivity (the rate of production slows considerably after 48 hours, which limits the overall productivity that can be achieved in the process); and (2) decrease its production costs (components from complex media are necessary to achieve robust production). Through a series of experiments, a set of metabolites contained in rich media that improved performance were identified using metabolomics, high-throughput cultivations in bioreactors, and ML-friendly experimental designs. It was found that the substrate feeding strategy was the potential major driver to enhance bacterial performance of glucaric acid production. The major industrial impacts from this project are improving the production process technology, as well as advancing infrastructures and workflows (where ML approaches in conjunction with high-throughput cultivation and metabolomics are used) to improve the analyses by making them more rapid and comprehensive.



COMMENTS

- The ABF worked with Kalion to improve strain performance of glucaric acid production, primarily through changes to media. Given the complexity of the media and difficulties untangling the impacts of various media components, a structure experimental design was used to perform rapid media screens, with the intent to use data as part of ML training. The results of the experiments identified some key media components, primarily sugar concentration, that impact final titer. The experiments did not seem to produce any surprising results, and the ML feedback loop was not clearly closed, so it is unclear how the ML tool was utilized in the experimental process. The use of this ML tool to predict applicable media was not discussed.

- Strength: The team benefited from the high-throughput cultivation and metabolomics analysis tools to analyze glucaric acid production in Kalion.
- Weaknesses/areas for improvement:
  - The discovered results—higher glucose concentration leads to higher product titer—are mostly expected, and thus have limited scientific impact.
  - Only different media compositions were analyzed; the project can further benefit from ABF's strain engineering capabilities.
  - It is not clear what the proposed milestones are and how well the team has achieved these milestones.
- This is a great project overall for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. It's not clear from this slide deck what the value proposition is to the bioeconomy of glucaric acid; the assumption is that a company would not be going after it if there was not good TEA. It is not clear what the demand from the chemical industry is.
- Next time, put all milestones and status (and percent complete if not complete). It's hard to judge without this info. Also, all FOA and DFO reviews going forward should have an impact slide clearly stating benefits to the ABF and the U.S. bioeconomy. This project is especially hard to evaluate as there was no mention of milestones or progress toward them. There has been progress and learning on media optimization and metabolomics work.
- The work in this proposal clearly advances the capabilities of the ABF, and at the same time, the partner gains knowledge and access to capabilities it does not have in-house.
- The ABF implied that the BioLector high-throughput fermentations have a lot of variation, which makes it hard to conclude data and use for artificial intelligence. After years of trying to prove the usefulness of these instruments, the company I work for has officially shut down all work on these systems for that reason. They are too unreliable and can't get good replications, among a lot of other technical issues. The ABF should consider getting rid of them and investing in more 250-mL Ambr tanks for moderate-throughput fermentations.
- The presentation of this project was rather confusing. There are two stated goals: improving productivity after 48 hours and finding less complex media that can achieve similar results. There are no results or lessons learned presented for the first goal. On the second goal, the slides put forth confusing information. In Slide 4, it is not clear whether myo-inositol was being added to the media. Also, glucose is not identified in the list of 14 relevant metabolites, so it is not clear why that is the focus of later work as opposed to other sugar sources such as mannose, which is identified. The graph on Slide 5 does not have a legend for colors, and as such is basically impossible to interpret. The title states that only the 2a sugar group saw an increase in titer, though the results appear nearly identical to those from glucose (and other treatments). The increase in titer from increasing glucose shown on Slide 5 is very mild: A tenfold increase in glucose leads to less than a twofold increase in titer. It is not clear whether having a media so rich in glucose would be any better than the current media that Kalion is using. The impact of the project on Kalion's practices or any future work they might do in line with project goals is not discussed.

Concluding that a microbe will make more product when fed more sugar seems like a very obvious result. Overall, this project was pursuing a very basic question and delivered meek results.

- The project between Kalion and the ABF seeks to apply ML and metabolomics to improve glucaric acid productivity and decrease production costs. One challenge/risk provided by the project team is the possibility that scaling to 2-mL bioreactors for media screening could limit productivity and product profile resolution. No mitigation strategy was provided, and there was no indication that product profiles between 2 mL and 0.5 L were compared. No information was provided regarding project management, communication, or DEI. I have several reservations about the experimental plan and data analysis. Glucaric acid production was demonstrated in 0.5-L bioreactors in several rich media. Presumably these media were not supplemented with myo-inositol. Metabolomic results are reported (volume not specified) for media supplemented with myo-inositol, which is two steps removed from glucaric acid. Decreased concentrations of metabolites when myo-inositol is converted to product are not necessarily representative of metabolites when glucaric acid is synthesized from glucose. In a different experiment, it was concluded that glucaric acid production improved when a group of sugars was added to the media; the data shown do not support this conclusion. A training set was generated from a particular experimental campaign to increase learning, but I see no evidence of ML to alter media, culture conditions, etc. It seems that insufficient resources were available to complete the experiments originally planned. Although project continuation may yield useful additional data, at this time commercialization potential is not evident. The impact of this project for ABF tools/resource development was not evident.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' comments. Because the project ended in February, we did not include the completed milestones, but we recognize that would have helped the reviewers. Over the course of this project, some research questions tangential to the main project goals arose, and given the time and budget constraints, we decided to prioritize efforts toward those that could be of immediate benefit for Kalion while advancing ABF's infrastructure and workflows.

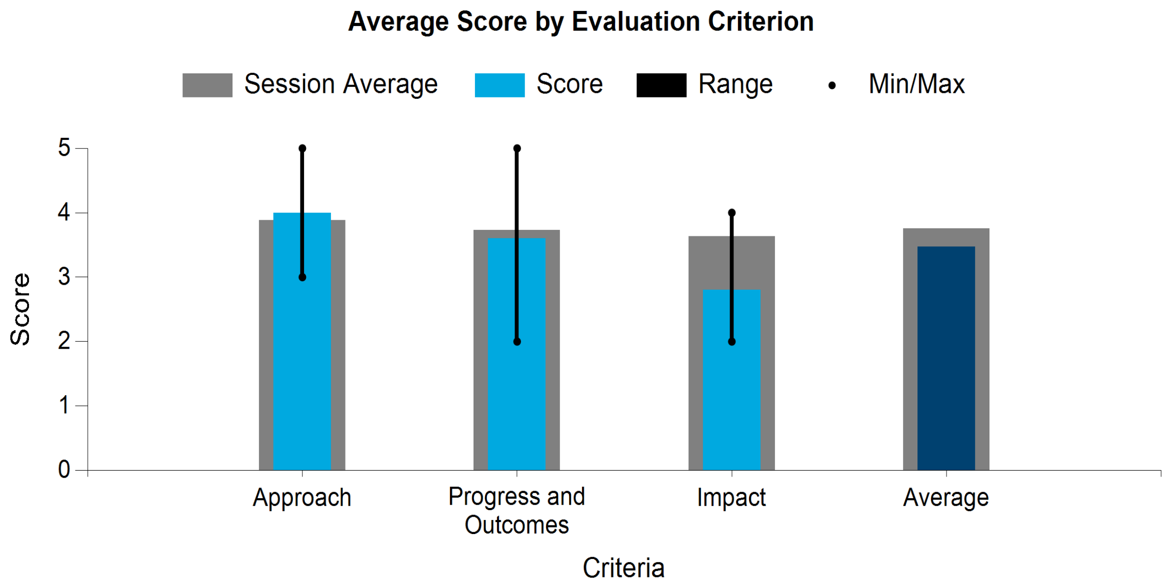
ABF DFO WITH INVAIO

National Renewable Energy Laboratory and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.713
Presenter(s):	Jon Magnuson; Katarina Younkin
Project Start Date:	03/23/2020
Planned Project End Date:	01/01/2022
Total Funding:	$410,000.00

This project is a partnership between Invaio, with their pioneering platforms for identification and development of active biologics, and two national labs (NREL and PNNL) in the ABF who are applying their strengths in fungal genetic engineering and fermentation scale-up to the expression of Invaio's valuable antimicrobial peptide (AMP) against a bacterial pathogen of citrus. Currently, the widespread use of biologics in crop protection is severely hampered by the lack of available tools for their mass production. This project is focused on developing an efficient bioprocess to produce and secrete the AMP in an ABF protein/peptide production host. A few viable hosts were examined for tolerance to the AMP. *Aspergillus niger*, which produces products in the generally regarded as safe category, was selected for expression of the heterologous AMP. AMP production has been verified by targeted proteomics using internal peptide standards, and culture optimization efforts continue to maximize titers. Developing the precursor to a scalable production process for this AMP is beneficial for Invaio as a foundation for further development and commercialization of this AMP, and is beneficial for the ABF by building a platform strain for production of other peptides and proteins, as well as procedures to approach the development of other protein production hosts.



COMMENTS

- This project represents a good use of ABF resources, wherein a target product/molecule is identified and the ABF is brought in to help develop the biologic tools to generate the molecule of interest. In this case, the ABF used its expertise to find a suitable strain, engineer the strain for molecule production, and then begin optimizing that strain. Progress is ongoing, with performance targets below desired levels. The muted performance of the strain at current scales puts the strain far from commercial viability and limits impact. Further positioning by the ABF to demonstrate pathways to commercially relevant TRY levels is recommended.

- Strength: This project benefits from the fungal production strains developed at the ABF. *Aspergillus niger* was shown to be the best AMP tolerance strain.
- Weaknesses/areas for improvement:
  - Current AMP titers and yields are way too low. AMP is less than 0.1% of total proteins produced by the best host. Its impact to commercial AMP production is very limited.
  - Only media optimization was discussed to improve AMP production. There was no mention of the use of any genetic strategies to improve AMP titer.
  - The project lacks preliminary TEA. It is unclear whether bioproduction of AMP is economically viable given the measured AMP toxicity.
  - The use of a large peptide fusion may result in a low carbon yield.
  - This project does not seem to align with BETO's mission on GHG emissions reduction or bulk chemical/SAF production.
- Objective: Develop a high-yield, cost-effective, large-scale fermentation bioprocess to produce an AMP with Invaio; collaborate with the team at Invaio to develop an expression/secretion host for peptides with antimicrobial action.
- Very good alignment with the goals of the ABF to advance industry and the bioeconomy. Not so much aligned with BETO on SAF and decarbonization, and that is OK. ABF should be supporting the U.S. bioeconomy to advance new products for a more sustainable planet as its mission.
- Very good; the project showed all milestones and reported on progress. They said there were tight timelines and a small budget, so it's impressive what they were able to accomplish. Also, all FOA and DFO reviews going forward should have an impact slide clearly stating benefits to the ABF and the U.S. bioeconomy.
- The path to commercialization is on track, but it's still pretty early stage (technology readiness level [TRL] 4). This is why "Impact" got a 4.
- This was a straightforward project that leveraged ABF capabilities; however, the alignment to BETO priorities and goals is not very clear. It also did not have as much of a potential impact of technology development as other ABF DFOs. The project end is set as April 27, 2023, and several tasks were still rather uncomplete at the time of Peer Review (Milestones 3 and 4). The impact of the work was not well explained. What is the application of this peptide? The intended market size? What is it replacing? Only agriculture is mentioned in an early slide, but no details are provided. As such, judging the impact is difficult.
- The partnership between the ABF and Invaio developed a sound approach to use ABF fungal hosts for expression of an AMP. This approach leveraged ABF fungal genetic engineering for heterologous protein expression, proteomics, and process development/scale-up expertise. The team appropriately mitigated anticipated risks by assessing host sensitivity to AMP and constructing multiple (eight) transgenic strains in two different fungal species. Communication mechanisms and frequency between the ABF and Invaio were not addressed. DEI approaches were not addressed. Good progress was made on generating and evaluating strains, modifying media, and detecting product. Unfortunately, product concentrations were

quite modest (0.33 mg/L). Whether the detected product was unadulterated gla1-AMP was not addressed, although identical sequence to AMP was listed as a project must-have. The end-of-project milestone to conduct 100-L bioreactor cultivation is not warranted given current product levels. Significant improvement (103-fold) in AMP expression must be realized before meeting the low end of product concentration stated in the end-of-project milestones. Without these improvements, commercialization prospects cannot be assessed.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank all the reviewers for their constructive comments and feedback. One reviewer recommended that all ABF "funding opportunity" project reviews have an impact slide clearly stating benefits to the ABF and the U.S. bioeconomy. We appreciate the comment and will emphasize such impacts more in the future. The potential impact to the U.S. bioeconomy from the Invaio project stems from the need for additional methods to target plant pathogens and protect crops. Biological antimicrobials and pesticides have the potential to decrease the use of more toxic chemical agents and pathogen resistance that often accompanies the extensive use of such agents. The initial development of a fungal process for expression of the AMP in this project provides a foundation for further strain and process development and future commercialization. For the ABF, the expression vector and genetically modified fungal strain developed within this project has the potential to be a chassis for production of other peptides and proteins (including enzymes) of high relevance to biofuel, bioproduct, and biomaterial production. As noted by many of the reviewers, this project is not aligned with BETO's current focus on SAF. The year that this project was proposed predated that emphasis, but admittedly, AMPs are not products that fit into the commodity chemical realm. The economic and sustainability impact of biologicals would be more indirect in avoidance of waste and monetary losses due to crop failures, repeated applications of pesticides to kill the insect carriers of the bacterial plant pathogen, destruction of diseased trees, etc. Both TEA and LCA would be instructive regarding those impacts in the case where AMPs were successfully employed for citrus greening disease prevention and treatment.

- The project is aligned with the ABF's goal to reduce the time and cost to market of bioproducts, and to accelerate microbial strain and process development for industrial deployment. Production of a soluble and secreted AMP was a significant step forward from previous biotechnology development for this AMP. The scientific challenges encountered were very instructive for future peptide/protein bioprocess development. We appreciate the reviewers' comments noting the significant challenges and progress in this project. Producing an AMP in a microbe was certainly a high-risk task, and that was noted in the proposal. To mitigate that risk, Task 1 focused on addressing that immediately by selecting the best host available, with a decision point in that regard. The ABF has received positive feedback from Invaio, which noted the progress made in peptide expression vector and strain development, detection of the AMP, and titer increases through genetic modification and bioprocess optimization. The reviewers noted that despite the progress, there is still a need for further improvement. The ABF and the Invaio team recognize the need for significant increases in AMP titer before moving forward with significant scale-up and commercialization. The smaller-scale (0.5–2-L) bioreactor work was used to assess performance gains that could be achieved by moving from small tube and flask cultures to a more realistic bioprocess environment without the expense of a large bioreactor run. Multiple approaches were discussed with Invaio on paths forward, including additional genetic modification strategies and bioprocess development. Those could be the foundation of future work, but the limited project resources remaining will be focused on peptide purification and efficacy testing to demonstrate proof of principle for the initial process developed in this project. IP protection will be further discussed with the company, and then we intend to publish results in a peer-reviewed journal.

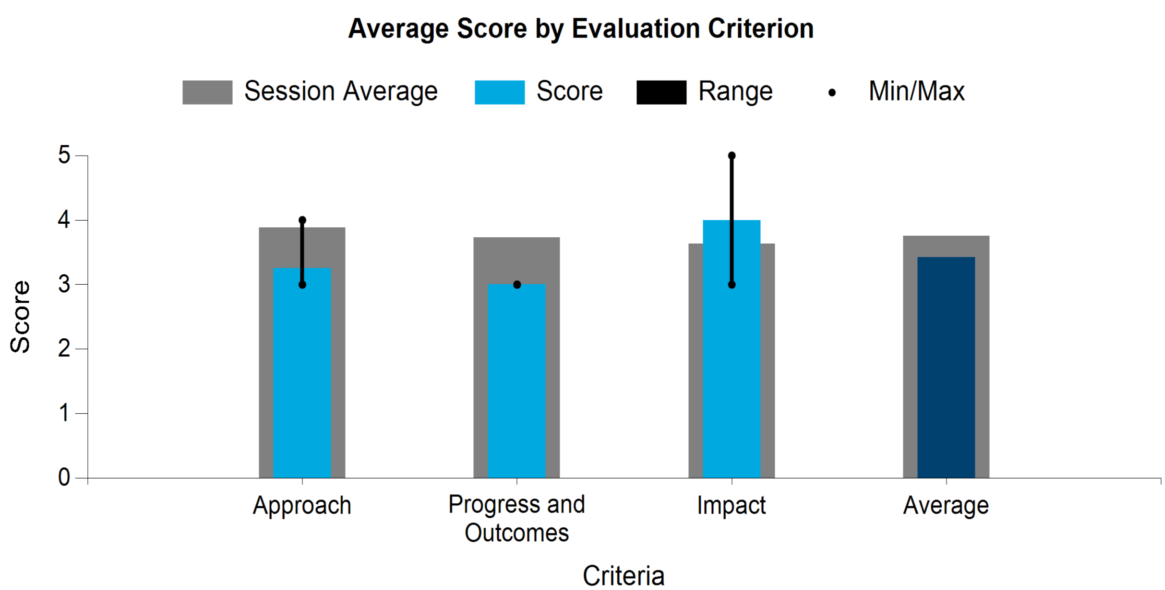
ABF DFO WITH DANIMER

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.714
Presenter(s):	Gregg Beckham; Michelle Reed
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2023
Total Funding:	$500,000.00

This ABF DFO project with Danimer Scientific focuses on the development of a strain and a corresponding bioprocess to convert bio-based feedstocks to mixed-composition polyhydroxyalkanoates (PHAs). Danimer Scientific produces PHAs today at industrial scale in proprietary strains and for many applications where bio-based, biodegradable materials are advantaged. The project team consists of NREL to lead the strain engineering efforts, PNNL to conduct systems biology experiments that will inform further strain engineering, and Danimer to conduct bioprocess development and materials development. To date, we have onboarded Danimer strains and demonstrated successful engineering thereof. We anticipate conducting systems biology studies in spring 2023. Overall, the impact of this DFO project could be improved material properties accessed through the DBTL cycle for designer PHA production.



COMMENTS

- Although this project is nearing the end of its award window, there is very little information provided in the presentation to inform the review. IP concerns are limiting disclosure for this project. In general, the production of PHA formulations with new and interesting material properties is an impactful goal that can lead to new products and materials with superior characteristics to legacy alternatives. The ABF's familiarity with the technology suite should enable learnings to the benefit of Danimer. The progress on milestones is unclear, as is the impact of the PHA formulations identified and synthesized.

- This is a great project overall for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. The value proposition of PHAs is assumed but not stated clearly. A lot of PHAs are not great for plastic replacement. The goal says, "Working to develop new PHA formulations that have not been reported in the literature and that could lead to new material properties for PHAs," presumably to improve the ability of PHAs to be useful as a real replacement for plastics. Again, assumed but not clearly stated. A clearer impact slide as it relates to BETO and the bioeconomy goals should be included.

- Next time, put all milestones and status (and percent complete if not complete). It's hard to judge without this info. This project is especially hard to evaluate as there was no mention of milestones and progress toward them. There has been progress and learning listed, but I'm not sure how much of the work is on track. I understand a company needs to keep their work more secret. You can list milestones just as numbers and give a percent completion and on-track status.
- Overall, PHAs are an important market, and the brief description of the approach appears straightforward. However, there was very limited substance in the information shared about this project. The project began in 2021 and it's a few months out from completion, yet no real data or results were shared. It is difficult to evaluate the progress and impact in this case. Even if this lack of information is from company proprietary information reasons, at least the overall milestones and progress should be shared.
- The project between Danimer and the ABF seeks to develop designer PHAs in an industrially relevant host to enable scale-up. Based on end-of-project milestones, the goal is to achieve PHA composition to within 10% of a targeted composition of 75% C4 and 25% C8, C10, and/or C12. Strain engineering is taking place in Danimer strains, which were successfully onboarded. Parallel pathways are being implemented in *P. putida* KT2440, which is extensively used by ABF. Very few details are provided to enable assessment of the experimental approach or progress. Scores given for approach and progress/outcomes will be relatively low, but this is out of a desire for consistency across project review. The impact of the project assisting in development of a strain that will ultimately be used in a commercial process is what ABF should be striving to routinely achieve. Danimer's leveraging of ABF expertise in iterative strain engineering (design/build) combined with omics characterization (test/learn) is an appropriate use of national lab resources to accelerate development of bioeconomy products. Knowledge of Danimer's strain capabilities and quantitative milestones expands ABF expertise, which will be applicable to future projects.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the understanding from the reviewers that we cannot disclose the full findings of this project. As the reviewers note, this is work toward improving PHA material properties, and we are on track to complete most of the project deliverables, but there will be outstanding questions remaining to be addressed in follow-up work.

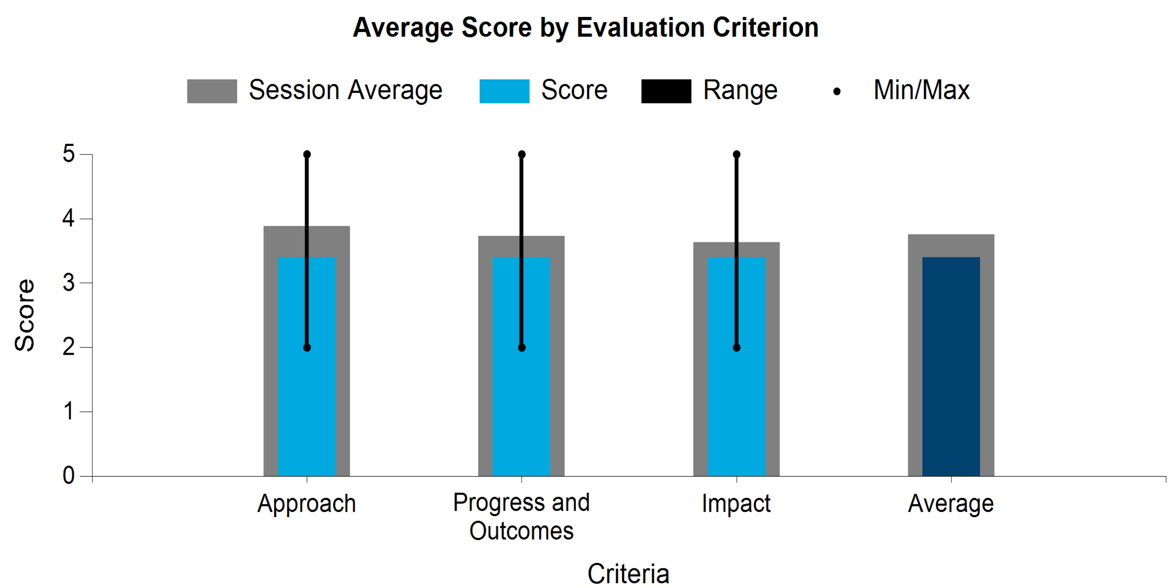
ABF DFO WITH PYRONE

Sandia National Laboratories and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.718
Presenter(s):	John Gladden; Karthikeyan Ramasamy; Katarina Younkin; Michele R Jensen; Alberto Rodriguez
Project Start Date:	01/27/2021
Planned Project End Date:	12/01/2023
Total Funding:	$600,000.00

The use of fatty acids as substrates for microbial fermentation can be an alternative to valorize lipid-containing waste streams by converting them to bioprivileged compounds such as triacetic acid lactone (TAL). Pyrone Systems Inc. partnered with ABF members at SNL and PNNL to build and optimize engineered yeast strains for biosynthesis of TAL from fatty acids. Fatty acids represent a direct source of the polyketide metabolic precursor, acetyl-CoA, and the yeast *Candida viswanathii* has the ability to metabolize different fatty acids by beta-oxidation. We engineered *C. viswanathii* to promote the compartmentalization of fatty acid degradation and TAL biosynthesis pathways in the peroxisome, as part of a strategy to increase product yields. TAL-producing strains were subjected to adaptive laboratory evolution to improve growth and production rates in the presence of oleic acid, and isolates with faster growth than the parental strain were identified. A multi-omic characterization of the generated strains will enable the identification of potential bottlenecks and new targets for process optimization.



COMMENTS

- This project seeks to create TAL from fatty acids using a yeast host. The project is in its early phases, and has started with a focus on evolving the host to improve performance characteristics. At the current stage of research, a pathway was identified and utilized in a host, and some comparison studies were run to understand media impacts on performance. Most open questions remain, with work ongoing to better understand the impacts on performance and to optimize the strain for further rounds of optimization.

- Strength: TAL seems to be a high-value platform chemical that has multiple applications.

- Weaknesses/areas for improvement:
  - The team used adaptive lab evolution for strain engineering, which is too old a technology and does not reflect the state-of-the-art strain engineering capability of the ABF. The method is not targeted and thus not effective, as seen from the results.
  - The current TAL titer is only 6 mg/L, which is too far away from the team's final goal of >5 g/L. It is hard to imagine the proposed approach will lead to a thousandfold enhancement during the second half of their project. The impact on commercial production of TAL from this project is very limited.
  - The current TAL titer is also too low compared to previous published results.
- This is a great project overall for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. The value proposition was stated and had impact slides clearly stating benefits to the ABF and the U.S. bioeconomy. The work in this proposal clearly advances the capabilities of the ABF, and at the same time, the partner gains knowledge and access to capabilities it does not have in-house.
- Next time, put all milestones and status (and percent complete if not complete). It's hard to judge without this info. This project is especially hard to evaluate as there was no mention of milestones and progress toward them. The slides do show a lot of technical progress and learnings; it's just not possible to judge if they are on track or not.
- This project addresses a straightforward but difficult challenge and adequately leverages ABF capabilities to deliver promising results with direct impact to industry and advance bioproduction processes generally. While the project seems on track to meet the 5-g/L target, having already seen 5 mg/mL titers in their strains, there may be limitations to reproducing those titers at higher fermentation volumes. This risk is not mentioned explicitly and may limit the eventual impact of the project for Pyrone.
- Pyrone Systems is partnering with ABF to build and optimize engineered *Candida viswanathii* strains to synthesize TAL from renewable fatty acids. The approach calls for three experimental activities: (1) engineering the yeast strain to preserve acetyl-CoA and malonyl-CoA in the peroxisome to enable TAL synthesis; (2) adaptive laboratory evolution experiments revolving around high growth on fatty acids and exploration of supplemental carbon sources; and (3) characterizing the evolved strain by genome sequencing and multi-omics to discover new targets for strain improvement. Tasks have been assigned to the various partner organizations, but no indication of communication plans is provided. No risk assessment with corresponding mitigation plans is provided. The project is in the third quarter of a 2-year timeline. Some progress has been made. Two strains were generated that are incapable of growth on oleic acid as a sole carbon source and synthesize TAL (maximum concentration reported 10 mg/L). Two approaches to adaptive laboratory evolution were initiated, and some media assessment has been performed to maximize product formation. However, I have strong reservations and questions about the experimental approach. What genetic modification tools are in place for the selected organism? Is this strain on the list of onboarded ABF strains? Does ABF or Pyrone Systems have expertise in engineering this organism? Although adaptive laboratory evolution is emerging as an important strain engineering tool, it is best applied on organisms for which there is a foundation of knowledge, engineering tools, etc., which enable the combination of random and rational engineering. Also, if the TAL-synthesizing strain does not grow on fatty acids, as indicated, why would adaptive laboratory evolution for a strain with superior growth on fatty acids improve TAL production? It would seem this means acetyl-CoA is exiting the peroxisome to enable cell growth. The end-of-project milestone calls for a strain that produces 5–10 g/L of TAL, which requires a thousandfold increase relative to current TAL production. Finally, is there a

reason why fatty acids are selected as feedstock rather than sugars? Strains that synthesize more than 1 g/L of TAL from glucose have been reported. Would improving glucose to TAL be a better approach?

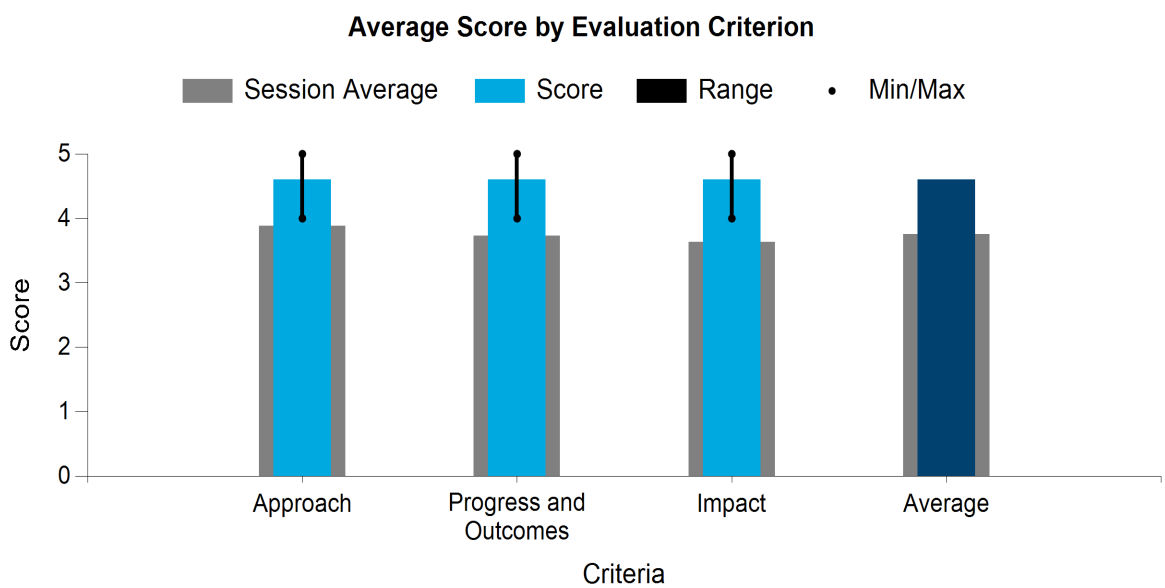
ABF DFO WITH TECHNOLOGY HOLDING INC.

Los Alamos National Laboratory, National Renewable Energy Laboratory, and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.719
Presenter(s):	Gregg Beckham; Karthikeyan Ramasamy; Michele R Jensen; Michelle Reed
Project Start Date:	03/11/2021
Planned Project End Date:	12/01/2023
Total Funding:	$1,400,000.00

This ABF DFO project with Technology Holding and partners focuses on the development of both a strain of *Pseudomonas putida* KT2440 and a corresponding bioprocess to convert cellulosic sugars to beta-ketoadipic acid, which can be used in performance nylons and polyesters. Our approach follows the DBTL cycle, wherein we have transferred learnings from muconic acid production in *P. putida* to develop a glucose- and xylose-utilizing beta-ketoadipic acid production strain. This strain achieves 65 g/L of beta-ketoadipic acid at 0.7 g/L/h and a Carbon mol yield of 0.40. We are currently onboarding arabinose utilization as well. To identify nonintuitive strain modifications as well, we are deploying a beta-ketoadipic acid biosensor and building randomly barcoded transposon insertion sequencing (RB-TnSeq) libraries and gene overexpression libraries in beta-ketoadipic acid production strains. Moreover, we are using global metabolomics and other systems biology tools to identify off-target pathways. Lastly, we are scaling up beta-ketoadipic acid production to kilogram-scale production for Technology Holding for evaluation in performance polymers with their partners.



COMMENTS

- This project aims to develop a new strain for the production of a chemical precursor, beta-ketoadipate. This molecule can be used to produce bio-based fibers like nylon and polyester. The ABF was well suited to perform this work given prior work on strains with similar metabolic pathways, and utilized that knowledge to develop a functional strain with apparently commercial-relevant performance metrics. Small quantities of product have been produced, and further scaling is ongoing to generate more product for testing by end users.

- Strengths:
  - The team used a combination of the ABF's most recent tools (e.g., product sensors, RB-TnSeq) and strains (*P. putida*) to produce b-ketoadipate from hydrolysate, representing a good leverage of ABF capabilities.
  - Substantial progress has been made in a short period of time, indicating the team is highly efficient in delivering results and reaching milestones.
  - Extremely high titer and yield were reported, demonstrating both the impact of ABF technology and the process commercialization potentials.
- Weaknesses/areas for improvement: N/A.
- This is a great project overall for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. The value proposition was stated and had impact slides clearly stating benefits to the ABF and the U.S. bioeconomy. The work in this proposal clearly advances the capabilities of the ABF, and at the same time, the partner gains knowledge and access to capabilities it does not have in-house.
- Next time, put all milestones and status (and percent complete if not complete). It's hard to judge without this info. This project is especially hard to evaluate, as there was no mention of milestones and progress toward them. There clearly has been progress and technical advancements, but it's impossible to say how well overall the project is on track.
- This project is another great example of appropriately leveraging the ABF's prior work and expertise to address an industry-relevant problem. The ABF's prior *P. putida* and muconic acid work has enabled faster progress and more ambitious goals for this project. The combination of TnSeq, adaptive laboratory evolution, and biosensor development helps ensure project success and pulls across ABF expertise. The project has already delivered test material and appears on track to meet the final 1-kg goals.
- This project leverages an extensive database of knowledge and expertise that the ABF has accumulated related to a particular biosynthetic pathway in *P. putida* to produce a new performance-advantaged bioproduct, beta-ketoadipate. Multiple ABF tools will be brought to bear to improve the TRY. Because ABF personnel are literally the global leaders in developing this pathway, I have no doubt the experimental approach is well considered. Given the challenges of demonstrating applications for new materials, Technology Holding will benefit from strain development efforts at the ABF.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the positive feedback. In terms of milestones, this project is on track, and we have successfully met all of our milestones.

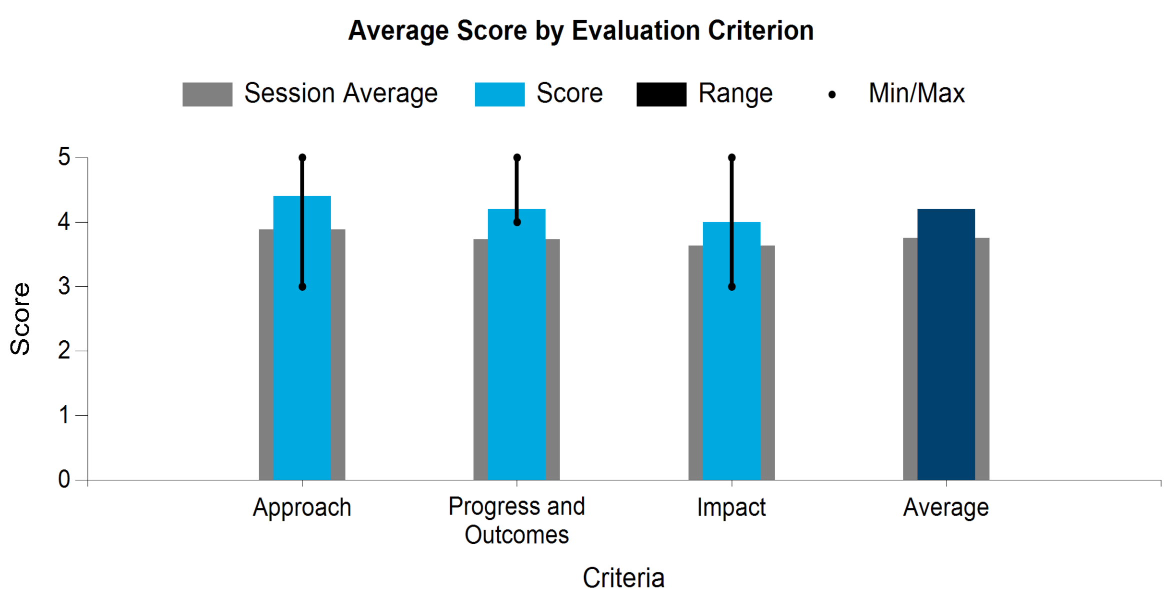
ABF DFO WITH IMICROBES

Los Alamos National Laboratory, National Renewable Energy Laboratory, and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.3.720
Presenter(s):	Eric Sundstrom; Karthikeyan Ramasamy; Katarina Younkin; Michele R Jensen
Project Start Date:	03/11/2021
Planned Project End Date:	12/01/2023
Total Funding:	$1,000,000.00

Bioconversion of gaseous feedstocks enables efficient production of fuels, chemicals, and materials from a variety of waste feedstocks, including electrochemical intermediates, syngas, landfill gas, biogas, and flared natural gas. At present, metabolic engineering, laboratory bioreactor equipment, commercial manufacturing facilities, and professional expertise within the biomanufacturing industry are heavily focused on heterotrophic processes, with minimal support available for the growing number of companies exploring gaseous feedstocks. This limitation is particularly acute for aerobic gas fermentations, which require stringent attention to process safety and dynamic control of multiple gas feeds. This project seeks to address these challenges by leveraging ABF capabilities in bench-scale gas fermentation, process scale-up, high-throughput proteomics, and deep learning to accelerate strain and process development for aerobic gas fermentations. In particular, we will work closely with our industry partner, Industrial Microbes, to improve production of the renewable polyethylene substitute poly(3-hydroxy)propionate (P3-HP) from ethane gas, targeting a threefold improvement in TRY over the initial project baseline. Initial laboratory results have established a performance baseline and harmonized TRY and proteomics data for P3-HP production between the Industrial Microbes and LBNL fermentation laboratories. This research effort will accelerate deployment of renewable polymer production from waste gas feedstocks via direct deployment with Industrial Microbes, while building generalizable capabilities within the ABF to rapidly improve performance and predict process scalability for aerobic gas fermentations.



COMMENTS

- The primary impact of this project is developing capabilities at the ABF and ABPDU to perform gas fermentation at lab and pilot (300-L) scales using flammable gases that create process complexities. Such a capability is likely to be useful to any innovator planning to explore gas fermentation technology, as the complexity of the system (from a design and operations perspective) makes a third-party test platform particularly attractive. This project has a clear and logical approach to execution, with an initial focus on tech transfer and reproducing results demonstrated by iMicrobes, and later stages aimed at scaling up and improving TRY over baseline. The project is nearly on schedule, achieving close to its ±15% target on performance versus the iMicrobes baseline; however, most of the heavy lifting lies ahead in scaling this process up to 300 L with 3× improvement on TRY.

- The impact of this project is unknown at the current review point, as the larger pilot reactor has yet to be validated against the baseline performance. Demonstration of performance at pilot scale will validate the ability of the ABF to scale gas fermentation processes, and demonstrated follow-on interest from iMicrobes or other gas fermentation innovators will validate the impact of this new capability.

- Strengths:

  - The combination of multiscale process engineering, high-throughput proteomics, and deep learning is a powerful tool. The team leverages this unique capability from ABF.

  - Conversion of ethane to P3-HP is challenging in its process. This team will leverage the capability of ABPDU to address this issue.

  - The team consists of highly capable PIs with complementary expertise.

- Weaknesses/areas for improvement:

  - (Not a weakness) this project has recently started; there are not many results to review.

  - *E. coli* does not seem to be a good host for this conversion. Methane monooxygenases are notoriously difficult for engineering. There have been many failed attempts to functionally express these enzymes in *E. coli*. The team is suggested to consider alternative methylotrophic hosts.

- This is a great project overall for the ABF. It fits very well into the mission of the ABF to support industry and advance the bioeconomy. The value proposition was stated and had impact slides clearly stating benefits to the ABF and the U.S. bioeconomy. The work in this proposal clearly advances the capabilities of the ABF, and at the same time, the partner gains knowledge and access to capabilities it does not have in-house.

- The project is new, and first goals are not due yet. The slides do list project goals. Still, a table of milestones and progress toward them should be included. They did state 80% achievement of the first goal.

- This project leverages ABF gas fermentation capabilities and prior genetic engineering work in *P. putida* to address a relevant challenge for an industry partner. The project approach is straightforward and rational. The goal of using ML to better understand and predict scale-up performance will have implications and impact beyond the project and is a good synergy between the ABF's expertise and industry needs. The project appears to be on track and has seen successful progress thus far.

- This collaboration seeks to leverage ABF bioprocess development, proteomics, and ML to create a predictive model for bioconversion of ethane into P3-HP. Project strengths include clearly defined tasks assigned to the project participants. The project was initiated in October 2022, but good progress has been made with regard to technology transfer from iMicrobes to ABPDU. This project will enable ABPDU to advances its safety protocols, equipment, and foundational knowledge for utilization of gaseous feedstocks. There are multiple weaknesses in the project plan. The project does not appear to include a strain development component, and no information was provided regarding gene/pathway expression, induction, etc. With that in mind, it is not clear how proteomic data based solely on bioprocess changes will be utilized to develop predictive models and, more importantly, to improve the process to obtain higher TRY. No risks were included in the presentation, which makes me question whether ample thought was given to how the project plan might be disrupted and what strategies will be followed to keep the project on track. The connection between the stated final product, P3-HP, and the final project goal to demonstrate 300-L ethanol scale-up is also not clear.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for their thoughtful comments. We heartily share their enthusiasm for the impact this project can provide, both specifically for production of P3-HP from ethane, and more broadly for predictive scale-up of aerobic gas fermentation processes. The reviewers are correct that heterologous expression of the methane monooxygenase has been notoriously difficult to achieve! Industrial Microbes has solved this problem as part of their core technology suite and has already demonstrated methane monooxygenase rates in *E. coli* sufficient to support commercial production of P3-HP. The benefits of working in *E. coli* as opposed to native methanotrophs include acceleration of DBTL cycles, utilization of mixotrophic metabolism, and reduction of scale-up risk. Use of *E. coli* enables rapid deployment of processes that would be extremely challenging in methanotrophs, including conversion of ethane and carbon dioxide to P3-HP. We note that the project does include a strain development component at Industrial Microbes, which will iteratively leverage fermentation data to target scale-up-relevant improvements in the production strain. Microbial response to bioprocess changes is specifically targeted for this project because of the complex biosynthetic pathway, which requires high flux of oxygen, CO_2, and ethane to the conversion host; management of ethanol concentrations as a key intermediate; continuous pH control; and carefully managed fed-batch supply of glucose for cell growth. Given these parameters, evaluation of strain performance under scale-up-relevant conditions is impossible to replicate outside of bioreactor trials.

- ABF funding provides a unique opportunity for Industrial Microbes to access key national laboratory capabilities in gas fermentation, allowing them to assess bioprocess robustness and response to perturbation at an early stage of development. The resulting proteomics data will identify changes to the strains, including increases in stress response proteins, pathway protein degradation, relative expression of pathway proteins, and increases in insoluble protein diagnostic during the culturing under variable conditions. These results will be utilized alongside standard fermentation metrics to inform strain development efforts. While not explicitly described due to the brief presentation format, we have conducted extensive risk analysis and mitigation as part of the project scoping and execution. We have deployed parallel development of the higher-risk ethane-to-P3-HP conversion process alongside the lower-risk ethanol-to-P3-HP conversion process to ensure progress is not halted if the higher-risk pathway encounters technical challenges early in the research effort. We note that the 300-L scale-up effort will target P3-HP production from ethanol feedstock, as ethanol is a key intermediate generated from biological ethane oxidation. This scale-up result will be used by Industrial Microbes alongside bench-scale ethane fermentation data to achieve pilot- and commercial-scale P3-HP production from ethane. In addition to mitigation of feedstock risk, extensive technology transfer and harmonization of fermentation and analytical protocols were conducted to minimize risk associated with site-to-site variability. We are excited that the project is on track, and we look forward to sharing more comprehensive results at the next BETO Peer Review.

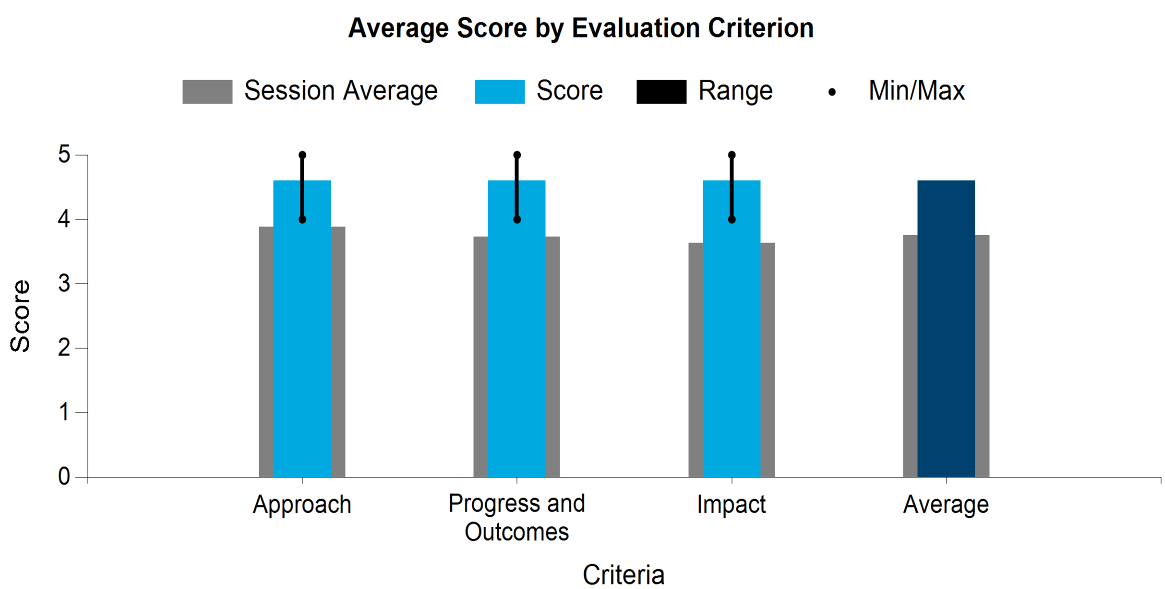
A TWO-CHAMBER GROWTH AND PRODUCTION SYSTEM FOR ROBUST CONTINUOUS BIOPROCESSING

Pow Genetic Solutions Inc.

WBS:	2.5.6.201
Presenter(s):	Ouwei Wang; Shannon Hall; Maggie Stoeva
Project Start Date:	10/01/2019
Planned Project End Date:	06/30/2023
Total Funding:	$3,108,303.00

PROJECT DESCRIPTION

The current bioproduction process, (fed-)batch fermentation, is repetitive and serial in nature, with each batch having to regenerate the biocatalyst, which has fundamentally limited the effectiveness of biomanufacturing. Replacing this system with a continuous process would minimize equipment downtime, increase volumetric productivity, and drastically reduce operating and capital expenses, paving the way for "high-yield, low-cost" biomanufacturing. The project team has developed a process that overcomes genetic drift and contamination, the major challenges of continuous biomanufacturing. We solve these two problems by combining three emerging technologies: (1) the introduction of a highly controllable and economical genetic switch technology that minimizes genetic drift and enables efficient decoupling of growth from production, and (2) an economical biocide/biocide-resistant system to prevent biological contamination during prolonged continuous fermentation, using (3) a two-chamber fermentation process to physically separate growth from production. This process has been implemented in Visolis's patented mevalonolactone production system at the 2-L scale, with contamination-free run times >500 h and ~3× increases in productivity over fed-batch. The process has been scaled to 30 L and is being optimized for maximum productivity. Our TEA confirms the "capital-light" promise of the platform and informs on future scale-up and deployment strategy.



COMMENTS

- Pow.Bio has developed a novel continuous fermentation approach that utilizes some biological tricks to separate growth from production while enabling a straightforward contamination control system.

Progress in this research is aimed at scaling the process to larger reactors and tech transfer to the ABPDU to run the two-stage continuous fermentation process. Overall goals for performance at various scales have been reached, and the continued scaling of this technology will enable higher performance for a variety of product targets. Further TEA work is recommended to better position this technology against other continuous fermentation approaches, and further discussion on the limitations of this technology, particularly around the products and molecules that can allow for a separation of growth and production in the host, would better clarify the potential impact of this technology.

- Strengths:
    - The use of cheaper inducer and contamination control is innovative and can improve process economics.
    - The developed two-chamber fermentation technology showed a substantial improvement in accumulated product amount and productivity (but not yield). The team obtained a high productivity of 2 g/L/h for 72 hours at 30-L scale. This result is very impressive.
    - All proposed milestones were achieved with satisfactory progress.
    - TEA showed that continuous fermentation has substantial benefits compared to fed-batch fermentation; thus, the developed technology may have a major impact on improving biomanufacturing economics.
- Weaknesses/areas for improvement:
    - Tech transfer of the two-chamber fermentation system to ABPDU failed. It is not clear how to address this issue. Scale-up fermentation seems to be the only connection of this project with the ABF.
    - The contamination control system may not work if the production pathway is mutated while the selection gene (chlorite dismutase) is not. This can happen at a high probability because the pathway is often much larger (easier for mutation) than the selection gene.
- Continuous fermentation is clearly a benefit to U.S. bio-based manufacturing. The value proposition here is clearly laid out. Impacts to the bioeconomy are clearly stated (that was very nice to see). Their approach overall is good. I just don’t know how universal it will be to many different types of microbial hosts. Also, many other companies and facilities do run continuously, or close to continuously. For many systems, you need some cell growth to keep the cells healthy and generate intermediates for catabolic processes. Overall, this technology could be very helpful and useful, and it is definitely in line with BETO’s and ABF’s missions, although their uniqueness seems overstated.
- Chlorite and chlorite dismutase is a very novel and potentially very useful tool to control contamination in industrial manufacturing fermentations, which is a big problem. I am dubious of their claims that there are no regulatory issues around chlorite usage. Having residual chlorite could mean very substantial changes and added cost to waste disposal of fermentation broth—for example, the practice in Brazil of spraying vinasse (fermentation broth) on cane fields as fertilizer. The tool could still be very useful, but again, the universality of the approach might be limited.
- The slides show all three go/no-go decisions, which is very good to see laid out. Still, a table of all milestones and progress toward them is needed for an accurate review, and going forward this should be requested for all projects from BETO. Industry can just list them numerically if they can’t give details.

- Clearly this project has made a lot of progress and is advancing biomanufacturing in the United States. They should consider now working with BioMADE to increase the TRL.

- This was a highly successful project (all milestones met) with a high relevance and impact for the overall bioeconomy. Developments that enable the use of continuous fermentation will be highly needed in order to scale the bioeconomy. This project leveraged ABF and ABPDU expertise well and was able to advance their technology.

- Project participants devised a multitiered approach to demonstrate a robust, contamination-resistant continuous production system. This process will be used to synthesize mevalonolactone, a platform molecule of one of the partners. The approach addresses several issues that increase biomolecule production costs by combining an inexpensive and tightly regulated genetic switch, an economical method to address reactor contamination, and a two-chamber design that separates bacterial growth and biomolecule production. Project participants and their corresponding expertise are provided, but defined tasks are neither listed nor assigned to participants. Communication and technical transfer between Pow.Bio and ABPDU are facilitated by their physical proximity, but communication frequency is not indicated. Several risks are provided, although the mitigation strategies were not necessary given the successful execution of the project. No plan was provided to address DEI on the project. Quantitative production goals (rate and duration of productivity) from cellulosic sugars have been achieved on a 2-liter scale. Additional experiments confirmed successful contamination control, co-consumption of C5 and C6 sugars, and good plasmid stability. Additional experiments are in progress to achieve the quantitative goals for product formation from cellulosic sugars on a 30-liter scale. This approach has a high potential for successful scale-up, potentially to commercial scale. The product is described to have the potential to address a market size totaling $10 billion, although the status of catalysis required to obtain end products is unknown. The potential impact (8-fold increase in product, 4.4-fold decrease in production cost) is striking. Utilization of this technology on other biomolecule products targeted by the ABF is worthy of exploration.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their comments and agree that further expanding the scale and use cases of our continuous technology will greatly benefit the U.S. bioeconomy. Several comments are addressed in more detail below.

- "Tech transfer of the two-chamber fermentation system to ABPDU failed. It is not clear how to address this issue. Scale-up fermentation seems to be the only connection of this project with ABF. The contamination control system may not work if the production pathway is mutated while the selection gene (chlorite dismutase) is not. This can happen at a high probability because the pathway is often much larger (easier for mutation) than the selection gene." We would like to reiterate that the tech transfer of the two-chamber system to ABPDU has not failed. On the contrary, we have initiated the process, and ABPDU has already successfully replicated the growth chamber, run as a turbidostat. We have developed a tech transfer package and will be initiating a run at ABPDU in the coming weeks. We anticipate no real risk in their ability to successfully execute the project (as we have done so in-house multiple times already), and we are located close to the ABPDU and will be available on-site for troubleshooting. In regard to the contamination control system (i.e., chlorite and chlorite dismutase), it is decoupled from mutations that may occur in the production pathway. To clarify, chlorite/chlorite dismutase may be used to prevent or treat contamination in either chamber. Separately, in order to prevent mutation/loss of the production pathway, we have taken a two-pronged approach: (1) growth occurs in the absence of production, and hence there is no selective pressure on the pathway to mutate, and (2) growth is limited in the production chamber, and hence, even if a single microbe mutates the production pathway, this will not affect productivity of the system as a whole since outgrowth of this microbe is prevented.

- "Their approach overall is good. I just don't know how universal it will be to many different types of microbial hosts. Also, many other companies and facilities do run continuously, or close to continuously. For many systems, you need some cell growth to keep the cells healthy and generate intermediates for catabolic processes. Overall, this technology could be very helpful and useful, and it is definitely in line with BETO's and ABF's missions, although their uniqueness seems overstated." We agree with the reviewer that it is critical to determine the translatability of our platform, and have already initiated industry partnerships to develop a two-chamber continuous system for protein production in yeast. We plan to further expand our host repertoire in the coming months. In regard to other facilities running continuous fermentation, we would like to make the distinction between our process and theirs; we are running a mesophilic *E. coli* process, where a high-value molecule has been engineered into the host background. In terms of what we have seen in industry, continuous fermentations (1) rely on extreme conditions (pH, gas fermentation, and ethanol production), (2) are for the production of ethanol or mixed-culture biomass (naturally contamination-resistant, and no danger of mutation/production biomass), or (3) rely on expensive, single-use materials (i.e., pharma). In these cases, the risks of contamination and pathway loss are minimal (there is no engineered pathway). Hence, we uniquely solve the barriers to the adoption of continuous processes for synbio more broadly (i.e., loss/mutation of the production pathway, and contamination of non-extreme processes). Finally, we agree that a certain flux through central metabolism is needed for robust production. However, to date, our team has demonstrated this continuous platform process with bacterial and yeast hosts, with product classes from organic acid to a food protein (growth-coupled).
- "I am dubious of their claims that there are no regulatory issues around chlorite usage. Having residual chlorite could mean very substantial changes and added cost to waste disposal of fermentation broth—for example, the practice in Brazil of spraying vinasse (fermentation broth) on cane fields as fertilizer. The tool could still be very useful, but again, the universality of the approach might be limited." Chlorite is generated naturally by perchlorate-reducing bacteria in nature, and we have an enzymatic system in place to remove chlorite. The challenge we are facing is actually how to maintain a non-zero chlorite concentration in the tank.
- "Further TEA work is recommended to better position this technology against other continuous fermentation approaches, and further discussion on the limitations of this technology, particularly around the products and molecules that can allow for a separation of growth and production in the host, would better clarify the potential impact of this technology." We thank the reviewer for this comment and plan to expand our TEA alongside our planned further scale-up. As mentioned above, we are also expanding into additional hosts and processes to confirm the wide applicability of our platform.
- "Project participants and their corresponding expertise are provided, but defined tasks are neither listed nor assigned to participants. Communication and technical transfer between Pow.Bio and ABPDU are facilitated by their physical proximity, but communication frequency is not indicated. Several risks are provided, although the mitigation strategies were not necessary given the successful execution of the project." The full proposal, intermediate validation, and quarterly reports include task assignment; we will make sure to include the full list of tasks, milestones, and assignees for future presentations at BETO Peer Review. Pow.Bio and ABPDU communicate regularly as part of BETO progress update meetings, and during tech transfer have been in close, weekly communication. The main outstanding risk mentioned is tech transfer to the ABPDU. To mitigate this risk, we (1) scaled up successfully in-house and (2) initiated the process several quarters prior to the milestone run. The final risk is maintaining our productivity using cellulosic hydrolysate as a feedstock; we have confirmed that fed-batch tanks result in productivity comparable to that with glucose.

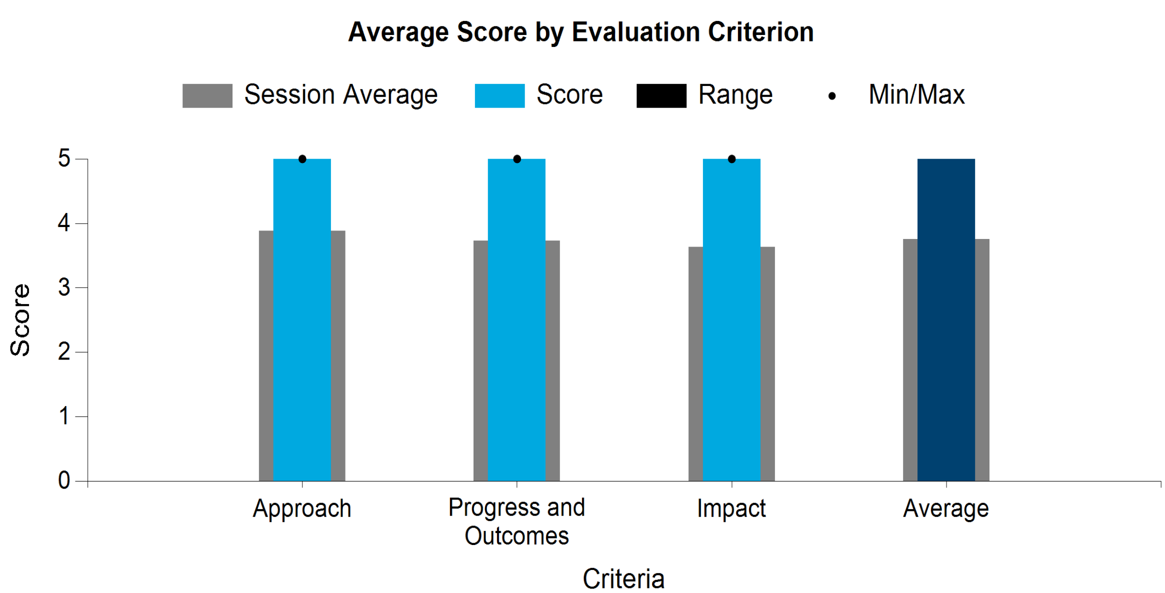
LBNL ABPDU SUPPORT

Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	2.6.1.101
Presenter(s):	James Gardner; Deepti Tanjore; Katy Christiansen
Project Start Date:	07/13/2010
Planned Project End Date:	09/30/2022
Total Funding:	$6,216,319.00

The ABPDU, as part of LBNL, was authorized in 2009–2010 and commissioned in late 2011 as a shared community resource to provide process optimization, prototyping, development, and piloting and scale-up services to the biofuels and bioproducts research and development community, including industry, academia, and the national labs. Over the past 10 years, the ABPDU has performed exemplary process science research, leading to multiple publications in high-impact-factor journals (see “Research” at abpdu.lbl.gov). Through collaborations with a diverse set of partners (see “Collaborations” at abpdu.lbl.gov), the ABPDU staff has identified key areas for process development research that will benefit the biofuels and bioproducts community and accelerate commercialization of bioprocesses. This AOP details four tasks that not only continue ABPDU operations, but also build on previous experience and generate public data in areas that directly align with BETO’s program priorities: (1) ABPDU Operations, (2) Learning from Data for Predictive Scale-up of Biofuel Technologies, (3) Biomanufacturing Using Gaseous Feedstocks (supporting the development of SAF, renewable diesel, and coproducts), and (4) Capital Upgrades. The process research and optimization work that the ABPDU conducts brings value to the entire biofuels and bioproducts community and provides high-visibility examples relevant to the BETO mission.



COMMENTS

- The ABPDU is an impressive organization that makes an outsized impact on the synthetic biology space vis-à-vis its funding levels and staffing. The organization provides a critical service to startups and established companies alike looking to advance their ideas beyond TRL 1 and test new theories or approaches. The leadership at the ABPDU has built a unique and hard-to-replicate capability that is well tuned to the needs of the industry. It is clear that ABPDU leadership (1) listens to the “voice of the customer" to ensure that their offerings meet the demands of industry and (2) is committed to continually updating and evolving their offerings to remain relevant in a rapidly evolving field. The ABPDU is especially impressive for the ways in which it makes impact outside its own walls: Their commitment to workforce development through seeding trained laboratory experts throughout the industry is commendable, as are their digital products and collateral to share learnings, tools, and tricks with the community at large.

- The ABPDU has proven through its impact on follow-on funds the level of industry growth enabled by the asset, and this proof point confirms the appropriateness of the approach and strategy.
- The challenge for the ABPDU moving forward will be in supporting further innovation in the industry and evolving their tool set and capabilities within a constrained staffing and budgetary picture. Further direct governmental support would very much be welcome to allow the ABPDU more flexibility to invest in staff, operations, and capabilities to broaden its functionalities for the industry. Downstream processing, in particular, is an often overlooked area of process development early in technology scale-up, and further capabilities in this space would further enhance the ABPDU portfolio. Much of the ABPDU demand prior to the last 12 months came from word-of-mouth, and although ABPDU has begun to invest in more advertising and outreach, measurement of the impact and reach of those strategies will be needed to properly refine and target the message. This work should be expanded: The ABPDU has a unique capability to serve as a funnel to other organizations (governmental or otherwise) that can take the next step in the scale-up journey with ABPDU clients. Forming relationships with these organizations and developing a scale-up pipeline will further drive impact at ABPDU, enabling their client companies to access scale-up support and complementary tools (such as TEAs) to further their technical innovations.
- Strengths:
  - The ABPDU team has made impressive achievements over the past 2 years. They have been working with a large number of partners from both industry and academia on a wide range of strains and processes.
  - The ABPDU team has highly efficient management under the leadership of Deepti Tanjore. This has made the ABPDU highly productive during the past few years. This is reflected not only by delivering impressive results in various projects, but also in interacting with and servicing different partners, outreach activities, and communications to the public, as well as collecting feedback.
  - The team has made efforts to address previous panels' comments on promoting public awareness of the ABPDU.
  - The ABPDU managed to keep a short contracting time; this should be set as a good model for the other ABF teams to learn from and shorten their CRADA times.
- Weaknesses: None.
- The ABPDU was really a shining example of a BETO-run organization after a really challenging set of days reviewing the ABF. The ABPDU has brought in many outside partners and is a sought-after capability. The leaders are doing an excellent job bringing in partners and money and continuing to increase awareness in industry of the ABPDU and its capabilities. They said they could contract in a matter of a few weeks, which is impressive, and ABF needs to follow that example. The website is very informative (if a bit wordy, and could use a little improvement there), but overall has great videos, standard operating procedures, and content. The ABPDU continues to expand its technical capabilities and expertise. It's also doing a great job in DEI.

- Really, there isn't much else to say here. Don't mess with what is going well. The leadership team should be highly recognized for their work and excellence and retained at all costs. Don't mess with what is clearly working.
- In the next review, don't leave this for the last session on the last day, but put it with the ABF reviews.
- Overall, the ABPDU serves its mission effectively. The management of the ABPDU works well and can deliver on a variety of industry projects in a timely and reasonable manner. Communication and outreach by the ABPDU are standardized and coordinated and also include a variety of mediums. Industry perceptions of the ABPDU are favorable. The ability to execute strategic partnership project contract vehicles instead of relying solely on CRADAs greatly increases the effectiveness and appeal of the ABPDU for industry. The ABPDU website is straightforward and accurately conveys their capabilities. The use of case studies highlights their success, capabilities, and diversity of industry partners served. Training programs address both workforce development in the bioeconomy and recruitment of minorities into STEM fields.
- While the industry listening day appears to have been successful and generated useful feedback, it would have been good to know how many of the attendants had worked with ABPDU in the past and how many were new ABPDU engagements. I would recommend targeting at least a 50/50 breakdown for future listening sessions to better understand what capabilities and resources could bring more industry partners to the ABPDU as opposed to just serving current partners better. I love that the ABPDU makes short, useful bits of code available for use on their website. This is a great example of working in good faith with industry partners and facilitating technology for the bioeconomy. The ABPDU has also done a great job at considering the overall impact of their work and tracking those outcomes (e.g., the information shared on Slide 33).
- Internally, it is evident that the ABPDU is carefully considering how to improve their equipment management and safety, as well as the retention and satisfaction of their staff. Hiring a program manager to alleviate administrative burden and allow for more mentorship time by PIs is a great example of an insightful intervention that has both scientific and DEI benefits.
- The two tasks that were presented, microbial image analysis and gas fermentation, are relevant and will have a high impact for industry. Tracking culture health and response during fermentation processes is challenging, and the imaging platform could be a very useful tool for addressing this. This is a worthwhile endeavor and a good example of challenges that should be tackled by the ABPDU and national labs, as it may be too risky/costly for industry to do. If this effort does yield reliable methods for correlating cell phenotypes with culture performance, the impact would be substantial. However, the likelihood of success is perhaps rather low given the range of biological variability; any insights gained may be limited to specific species/conditions and not generalizable. This is not a reason to not pursue the work, but simply something to keep in mind for realistic evaluation of the potential project impact. The development of gas fermentation capabilities and development of strains that can use C1 feedstocks for growth is well in line with BETO priorities around decarbonization and the use of waste feedstocks. The development of these resources will undoubtedly have a positive impact on industry partners and on the bioeconomy more generally.
- The industry projects presented showed a wide breadth of use of ABPDU resources and had substantial progress and success. Most projects also address key BETO priorities such as lignocellulosic biomass conversion, SAF production, and bioplastics.
- In summary, the ABPDU appears to be functioning well and is conducting internal projects that leverage national lab strengths and that will have wider applications for the bioeconomy. External partner projects are well aligned with BETO and DOE priorities and have shown appropriate success and progress.

ABPDU management appears strong, external engagement mechanisms have been successful, and expansions of outreach are well planned.

- The ABPDU is a valuable component of the ABF, and investments in its operation add a positive multiplier to the bioeconomy. The ABPDU began operations in 2012, which is approximately 5 years earlier than the ABF *in toto*. If the new strategic plan results in an ABF that is as productive and service-oriented as the ABPDU, which I am confident is possible, the bioeconomy will be well served by this public investment. In addition to providing standard scale-up services to produce product, the ABPDU interfaces with strain improvement (i.e., via metabolic samples produced at scale) and downstream processing evaluation. These are valuable de-risking activities. ABPDU staff also participate in tool development (predictive scale-up, microbial imaging, and use of gaseous feedstocks) for use on future projects. It would be easy to attribute ABPDU success to a high barrier to entry for bioprocessing needs, which is not really the case for strain development. However, engagement with 75 organizations more likely indicates the ABPDU is doing many things well, both for its partners and for the bioeconomy. They are customer- and potential-customer-oriented. They provide extensive information about their capabilities and educational materials on their website, in quarterly newsletters, and on social media. Their industry days are well attended, which means their customers are invested in ABPDU improvement. Their training of interns and inexperienced scientists is valuable from a DEI perspective and for expanding the bioeconomy talent pool.

PI RESPONSE TO REVIEWER COMMENTS

- RESPONSE: We thank the reviewer for taking the time to review and provide comprehensive feedback. We appreciate their effort. We do agree that, to evolve further, the ABPDU has to provide unique cutting-edge tools that will advance state-of-the-art capabilities available to enable novel synbio and other fermentation-based technologies. Based on feedback from industry, for the past couple of years, we have been keen on developing capabilities such as the self-driving bioreactor and gas fermentation. With substantial internal LBNL funds (approximately $1 million), we were able to get the gas fermentation capability to a stage where we started to collaborate with industry partners on process development. With BETO funding, we are working toward delivering these capabilities to the industry. We look forward to pursuing similar projects in downstream processing, as suggested by the reviewer. We agree with the reviewer that we need to develop metrics to measure the impact of our communication and outreach activities. We are working on this topic.

- RESPONSE: We thank the reviewer for their valuable time. We very much appreciate the feedback and look forward to responding to any further questions or comments.

- RESPONSE: We thank the reviewer for their effort in reviewing us and providing valuable feedback. We agree with the reviewer that our website could use fewer words. We are working on this topic and hope to have new content on our website by the end of FY 2023.

- RESPONSE: We thank the reviewer for their generosity in spending time reviewing us and providing comprehensive feedback. We agree with the reviewer that the imaging project is low TRL and thereby tricky. We are looking at this problem in a few different ways, and this particular project is helping us define the problem much better. For example, realizing that real-time sampling of live cells from a bioreactor is unavailable as an off-the-shelf capability was a significant development for us. Similarly, we want to understand the limitations of artificial intelligence/ML applications in this space. We plan to develop a more robust project from these initial studies.

- RESPONSE: We thank the reviewer for sharing their limited time in reviewing us and providing comments. We agree that strain engineering poses a different contracting challenge than bioprocessing needs. As we generate IP through development of novel fermentation equipment and pursue collaborative research work with industry, the ABPDU will face similar challenges. We have been relatively successful in executing a few funds-in CRADA projects in the past couple of years and are hoping to take this approach for future early-stage projects as well.

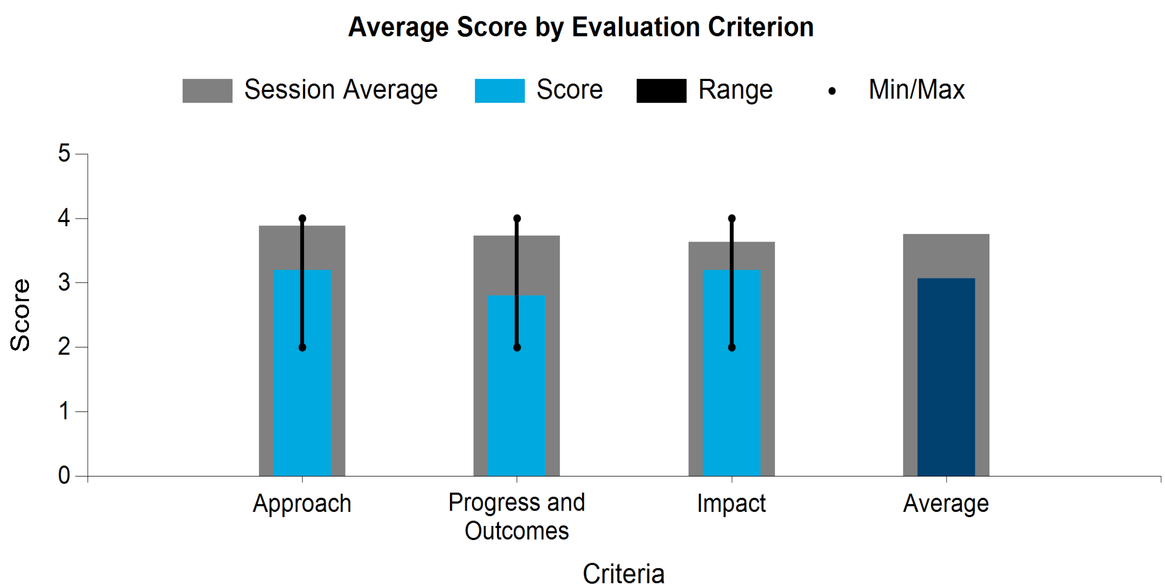
ABF INTRODUCTION AND OVERVIEW

Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	ABF1
Presenter(s):	Katy Christiansen; Nathan Hillson
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022
Total Funding:	$20,000,000.00

The ABF, a consortium of seven national labs, has operated since 2016, with the goal to enable biorefineries to achieve 50% reductions in time to bioprocess scale-up. The ABF's relevance is that it has been a $20-million/year public infrastructure investment that increases U.S. industrial competitiveness, with impacts including the reduction of technical barriers for industrial and academic partners; increased access to broadly enabling engineering biology infrastructure, precluding the need for industry to reestablish metabolic routes and hosts; and a greater diversity of publicly available microbial hosts. Top challenges for the ABF have been leveraging past collaboration learnings with future collaborators, predictive scale-up and method transferability, and the intellectual framing of strategic beachheads (metabolic intermediates). The ABF's outcomes have included the development and deployment of technologies enabling commercially relevant biomanufacturing, with technical accomplishments spanning demonstrations of bioprocess improvements across microbial hosts and metabolic targets, the establishment of strategic beachheads and the development of TEA/LCA approaches to assess them, the onboarding and development of microbial hosts, and bioprocess scale-up. This presentation focuses on the ABF up until September 2022, with a subsequent set of presentations covering the ABF from October 2022 to date.



COMMENTS

- The ABF utilized multiple presentations to document their past performance and journey in developing a new strategic plan for the next funding cycle. These presentations grew off each other, and as a result, it is difficult to separate them as required in this review process. Instead, I have used the "Strategic Plan" presentation to provide feedback on the future plan, and have used the presentations related to specific past activities to review past performance. Please look there for my comments.

- Strengths:
  - Overall, the ABF team has been making satisfactory progress on their proposed projects. They have met the milestones and demonstrated the transfer of the 3-HP pathway and tools between different hosts (proposed five molecules/tools, achieved seven). These successes have proved the value of ABF technologies in potentially reducing DBTL cycles and bioprocess scale-up time for industrial partners.
  - Several ABF core teams demonstrated high titer/rate bioproduction of chemicals, such as muconate and 3-HP.
  - Collaborations with industry clearly demonstrated that ABF has empowered U.S. industry in biomanufacturing development.
- Weaknesses/areas for improvement:
  - Although efforts were made to improve the dissemination of ABF's capability, further improvements are needed to better serve the biomanufacturing industry. This includes updating the strains and tools information on HObT and publicizing the website soon. Right now, the database is still not available to the public.
  - The wide adoption of ABF tools (mostly omics, ML, and the ABPDU) by industrial partners and success on the malonyl-CoA/3-HP pathway are exciting. However, it is somewhat disappointing that the only beachhead used by industry is malonyl-CoA. Given the size of past support, multiple beachhead molecules are expected to benefit society.
- Most scores were moderate for judging impact on previous goals because there was a balance of very low scores and some high scores. Low scores because (1) nearly all DBTL goals were not met, (2) management structure was not sufficient to lead the ABF to success, and (3) there was poor industry outreach/engagement, as well as not engaging the IAB effectively. High scores for overall a lot of solid work advancing synthetic biology, delivering on several projects that advance U.S. capabilities, and advancing industry to be impactful. Also good plans for addressing DEI.
- Good:
  - Better tools for tracking DBTL, and showed DBTL cycle data for results of transferring one molecule pathway to a different host. Hit the Q4 2021 milestone: "2X efficiency improvement in automated DBTL engineering cycle unit operations compared to FY22Q2_DBTLI_R1 non-automated baseline efficiencies demonstrated."
  - Key milestones (Slide 25) and impact (Slide 27) show a lot of good progress was made in the last 3 years developing the tools and infrastructure to advance synthetic biology in the United States and help BETO's goals to decarbonize the chemical industry.
  - Hit the metric set earlier to "demonstrate transferability of ABF technologies and ability to accelerate bioprocess development."
  - ABF metabolic map depicting beachheads was added to the website (it should not have taken until after the 2021 Peer Review to do this).
  - Challenge noted: "Our lack of ability to predict how a process will scale, or how well a method can be transferred across facilities, may limit the impact of our research and development efforts." It's true that tech transfer and replication of process/results between sites is challenging and often hard.

This is part of scale-up and can take a lot of time and effort to work through. It's good that the ABF is recognizing this as a challenge, and it's not insurmountable. It takes time (money) and people dedicated on both sides to work through the differences. Usually it's best to send people from one facility to another to understand firsthand and help each other solve the problems.

  - The ABF's interaction with different consortia is good and noted. They should always be looking to partner with and benefit from other consortia.
  - The new emphasis on DEI is very good.

- Better, and could still use improvement:
  - It's good that the ABF is starting to capture some DBTL. I think it's a mistake to abandon all DBTL metrics going forward. Revise the DBTL goals to be more realistic and relevant. Still have a goal to reduce the DBTL cycle or even parts of DBTL that make the most sense, are the most commonly used, or are the biggest bottleneck. It doesn't have to be every capability and every tool. A metric could be time needed to finish one complete experiment and learn from it (per tool or per instrument), and focus on making those individual unit ops more efficient. Drop wall time versus clock time. What matters is how long it takes you to learn from an experiment. If there is some large downtime (let's say you need to ship samples from one site to another, and that takes weeks), then that is part of your cycle time and something to target to be more efficient. Focus on gaining efficiencies and improving the infrastructure already in place.
  - The ABF states that the "Capabilities section of ABF website was updated, and ABF began providing capabilities webinars," but the website could still be improved to be clearer in what the ABF can offer (e.g., services, tools, HObT) with examples and videos. The ABPDU should be the gold standard for websites. Sit down with the ABPDU and learn from what they have done.
  - "Beachhead development/selection was informed by industry, and one example is a collaboration project that leverages acetyl-CoA/malonyl-CoA beachheads." It's good that the beachheads got some traction, but overall it seems to have either not been of interest to much of industry, or it was not advertised to industry well. It's good the ABF is not pursuing beachhead strategy anymore.
  - I don't understand the challenge that says, "Only portions of past collaborative data or learning methods that do not reveal the underlying primary data may be available." The ABF should reserve the right to learn from all data and projects from all work done in the ABF. Learning is different from using propriety information. If the ABF is saying they don't have access to past data (data are not stored properly), that is a big issue that needs to be addressed going forward.
  - Slide 28 (how impact is disseminated): It's definitely an improvement over 2021. However, publications is not a good metric for impact. It's what academics see, but it doesn't correlate with progressing real-world changes or what BETO wants to see. What matters are the number of licenses, offtakes, manufacturing or pilot samples produced, or companies spun out from technology.

- Bad:
  - Slide 7 says "ABF's HObT now publicly provides information about onboarded host organisms." The host onboarding done in the ABF is one of the greatest benefits the ABF has provided (or could provide) to industry. First, the HObT website is literally inaccessible from the ABF website. This is puzzling and disappointing. Also, if you know how to find the HObT website, it has no useful information other than the species and publications listed. There is no explanation of what

the different tiers mean, what tools are available, or the general status of the strain. The explanation for why this was not listed on the website was that this was not ready for the public yet. Work (money) needs to be allocated to getting this website up to date (parts, tier explanation, and protocols) to make sure the money already spent is not wasted, and this incredibly useful work done by ABF can be accessed and used by the public. This should have been done years ago (let alone by the end of 2022).

  - Overall DBTL cycles were not met, and for reasons that are still not clear, were said to be hard to measure/quantify. It really isn't that hard to quantify how long it takes to go from one step to another, or from the start of an experiment to when data are returned.

- Approach: The ABF's approach has advanced the state of the art and has produced innovative results in the past 2 years. However, the cohesiveness of the work in advancing toward a common goal was not evident. The presentation mentioned a gaps analysis resulting from industry engagement but provided no learnings from that effort (in this or any of the later presentations). It would be highly beneficial to map the ABF's efforts onto a comprehensive overview of the bioeconomy and more strategically target where the ABF can have an undue impact for advancing the bioeconomy relative to academia, industry, etc. That kind of strategic oversight should be what the management plan is focused on, and I'm not sure I see sufficient evidence that this is the approach that the ABF has taken. This concern was also mentioned in the 2021 Peer Review report. In that context, the management of the ABF appears too disjointed, with individual PIs pursuing work of interest to them as opposed to collectively driving toward a common vision that integrates into a larger road map of bioeconomy technology gaps. The slide on DEI efforts lacks specific metrics (e.g., number of speakers, number of target poll participants, number of presentations).

- Progress and outcomes: Some of the projects presented show solid progress and outcomes. For instance, fungal and yeast demonstrations showed production of a variety of molecules and much higher than the 1-g/L targets. Serine recombinase-assisted genomic engineering for host onboarding is a promising new method for enhanced genetic transformations, though it is not clear from the presentation the time frame corresponding to those accomplishments. The partnership with NSF to allow more minority-serving institutions to leverage the ABF is an exciting and positive accomplishment. A few milestones were labeled as complete but upon digging did not exactly meet the stated descriptions. For instance, the ABF listed as completed: "Bring a total of at least 15 microbial hosts to at least Tier 1, and provide corresponding information, resources, and tools via publicly accessible ABF HObT website." The resources described are not in fact available on the HObT website, as was pointed out during the Peer Review. This website was discussed in the 2021 Peer Review and does not appear to have been made more accessible since that time. It was also evident from discussions during the Peer Review that there is a lack of industry engagement and that the IAB is not properly utilized by the ABF.

- Impact: Overall, the ABF met their end-of-project milestones for the 2021–2023 AOP period (those listed in the key milestones and quad chart slide).

- The ABF has published a lot of scientific papers on the conducted work; however, they should diversify the dissemination of information to other mediums. For instance, blog posts and videos should be available on the ABF website to share fundamental insights gained from ABF work that may not be publication-ready, or negative results that may not be of interest to journals but can nevertheless advance knowledge about synbio and biomanufacturing processes.

- The number of licensed technologies seems quite low relative to the number of inventions, with only two licenses versus 36 patents, records of inventions, and software disclosures. One aspect that may be limiting licensing of ABF technologies is the degree of applicability of the work, as well as the presence/absence of continued support for the tools, especially in the case of software technologies. The bandwidth/feasibility of software support should be considered in the development on any new software tools intended for licensed use.

- ABF leadership provides five activities that encompass the technical approach: (1) demonstration of ABF capabilities via DBTL infrastructure, demonstration projects, and metabolic beachheads; (2) use of TEA and LCA; (3) onboarding of industrially relevant host organisms; (4) integration of bioprocess scale-up as a test capability; and (5) industry engagement and outreach. Identification of these activities is indicative of sound scientific merit; however, this summary will not specifically review whether these activities were adequately executed. Each activity will be judged individually in the reviews that follow. No management plan for successful implementation of these activities was provided, which leads me to believe the current management structure is not as strong as it should be. Who takes ownership, provides ultimate oversight, and possesses final decision-making authority for each activity? A multi-site biofoundry funded with public resources requires a defined management structure with strong leadership willing to set priorities and distribute resources (financial, technical, and human). Leadership by consensus is ineffective and results in delayed decision-making. Multiple risks were identified with appropriate mitigation strategies; however, failure to describe a management structure is itself a risk that needs to be addressed. Communication and collaboration mechanisms between the different activities were not provided in this specific presentation, but extensive interactions with lab leaders over the course of the review revealed strong professional relationships among these principals, which appears to provide adequate internal communication. Twelve DEI-related activities were listed as completed, in development, and/or ongoing. These activities were spread over current staff, future workforce development, minority-serving institutions, and compliance with the Americans with Disabilities Act (ADA). Specific metrics related to DEI should be developed and reported on in future peer reviews to monitor progress in this regard. Both progress/outcomes and impact for each activity will be reviewed on an individual basis in the reviews that follow.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the extensive, thoughtful, and helpful comments that the reviewers have provided (and the time and effort that went into them), both for this particular presentation and for all following ABF-related presentations. As the reviewers have noted, our presentations flowed from one to another, which made it difficult for the reviewers to fully compartmentalize their feedback on a per-presentation basis. Several reviewer comments were provided verbatim across multiple presentations. Our approach in responding has been to address comments as they arise, and rather than replicating our (same) responses across presentations, to instead refer the reader to our previous responses. While more detailed responses can be found below (and in our responses for subsequent presentations), we thought it would be helpful to make several high-level responses here. The ABF and BETO teams worked intensively and extensively together during the recent ABF strategic and implementation planning activities, and the ABF is committed and fully bought-in to its new direction and is excited to support BETO in achieving its ambitious goals for 2030.

- Host onboarding and development activities will continue within the ABF, as directed by industry and other partners in collaboration projects. We will continue to make improvements to the ABF website and specifically to our HObT web application to better depict our capabilities. As part of our capability benchmarking activities (which will help prioritize ABF development efforts and enable business development and technology transfer), the ABF will continue to consider DBTL-related metrics.

- We have changed from a consensus-driven management approach to the lead PI (with BETO support) having and exercising decision-making authority. A new strategic implementation lead will help ensure that all work in the ABF remains aligned with its strategic and implementation plans, and that work is not disjointed. The ABF is continuing on its path to becoming more of a “customer”-facing entity, with the establishment of new business development co-leads, upcoming changes to how the ABF interfaces with its advisory board, and increasing amounts (>50% by the end of FY 2025) of its resources dedicated to collaboration projects.

- The ABF has contributed (and is contributing) to multiple product/process commercialization efforts, several of which are building off of established ABF beachhead molecules. Regarding the HObT website, we agree that HObT will be useful to the public and further the ABF's impact and dissemination of its accomplishments and capabilities. HObT itself has not been published, nor has the ABF Host Tier system, and the functionality that permits only public sharing of publicly disclosed (and not prepublication) information regarding experiment data, strain, and sequence information has not been implemented yet. For these reasons, as discussed at the Peer Review, we have not yet promoted HObT (e.g., linking from the ABF website). Once these issues are resolved (target date Sept. 30, 2023), we will more prominently promote HObT. The capabilities associated with each tier, and the progress made within each tier for each organism, is (in fact) publicly accessible now. We are excited to make the rest of the public information accessible through HObT as quickly as possible.

- Regarding the observation that only beachhead (malonyl-CoA to lipid products) has been used by industry thus far in collaboration projects, we note that ß-ketoadipic acid is being worked on with an industry partner in a DFO project (protocatechuic acid beachhead), as are PHAs (acetyl-CoA beachhead). We have also had several companies express interest in 3-HP through both aspartate and malonyl-CoA beachheads via their proposals into the competitive ABF funding opportunity. As discussed in the Peer Review, challenges regarding DBTL metrics (and the reasons behind them) were part of the reason for the strategic redirection of the ABF toward more measurable goals. We agree with the reviewers that we should not abandon all DBTL metrics going forward. DBTL metrics will be used internally within the ABF when prioritizing opportunities for improvement (including new capability development), and as part of our capability benchmarking activities.

- Regarding the management of the ABF, until 2023, decisions across the seven national labs in the ABF consortium were predominantly made through consensus-driven approaches and processes, which, as discussed, have their limitations. Starting in 2023, the ABF's lead PI (with support from BETO) will have authoritative decision-making control, in line with reviewer suggestions, along with updates to the org chart that show clearer lines of hierarchy. Regarding the ABF not using its IAB as effectively as possible, a prominent component of the restructuring exercise—and ongoing discussions between industry engagement efforts, BETO management, and, in the future, ABF business development—is to better define the roles and goals of having an advisory board and tailoring interactions and utilization efforts of the board for these outcomes. We welcome these changes and improved interactions, as they will be needed as industrial collaborations intensify.

- Regarding the ABF's ability to learn from all projects (internal and collaborative), this is not a data management issue, but rather a concern that models trained on data could be reverse-engineered to reveal the underlying proprietary training data. There are a number of means of mitigating this risk, but it remains an important risk to be cognizant of and work with collaborators to address. Regarding individual PIs within the ABF pursuing disjointed work, we now have an ABF strategic implementation lead, who will monitor activities for continued unified alignment with the ABF strategic plan. Regarding the need for the ongoing support of ABF software tools to drive licensing efforts, it is expensive (i.e., a high opportunity cost) to maintain software. The ABF seeks commercial solutions where possible. For essential software for which there is no commercial solution, the ABF continues development, support, and maintenance. The ABF prefers to license software to companies that will themselves take on the support and maintenance of the software for its customers. The ABF agrees that a lack of future obligated support for its (nonessential or where a commercial solution is available) software could negatively impact licensing, but in these instances, the costs to the ABF would exceed the benefits of the licensing.

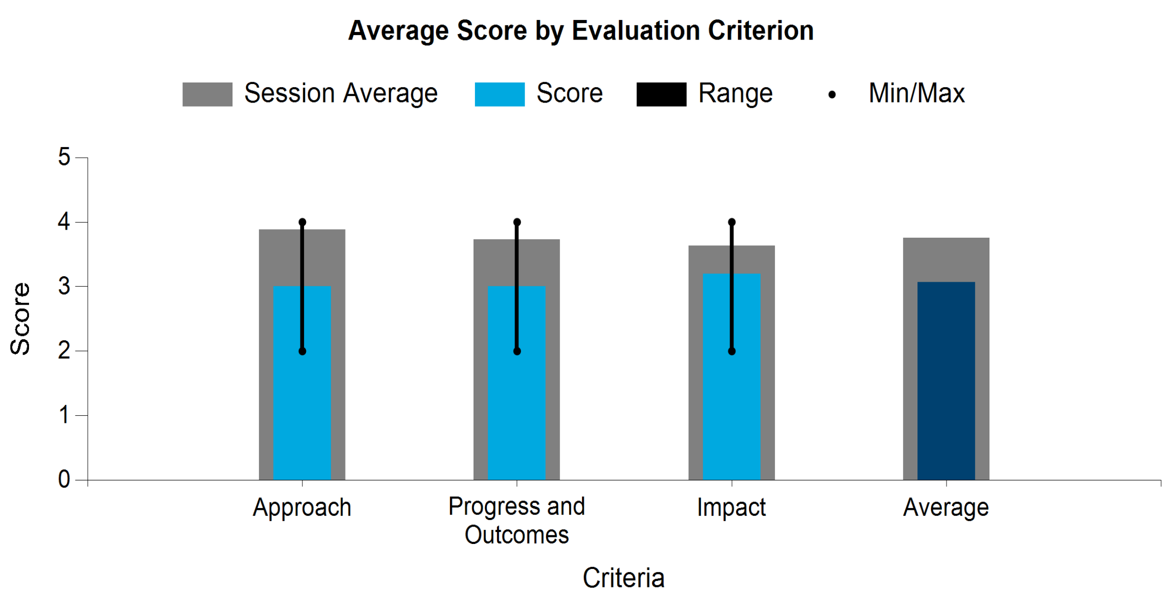
ABF FUTURE STRATEGY – IMPLEMENTATION PLANS

Lawrence Berkeley National Laboratory, National Renewable Energy Laboratory, Sandia National Laboratories, and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	ABF10
Presenter(s):	Gregg Beckham; John Gladden; Jon Magnuson; Katy Christiansen; Nathan Hillson
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

In January 2023, the ABF began to develop the implementation for its recently completed strategic plan. Implementation planning was completed in March 2023, including sets of milestones to go along with the goals and deliverables described in the strategic plan. The relevance of developing the implementation plan is that it ensures that ABF planned activities for FY 2023–2025 meet BETO's budget allocation and are consistent with a path likely to accomplish the deliverables established in the BETO-approved revised ABF strategic plan. The impact of establishing the implementation plan is primarily the resumed operations of a reimagined DOE ABF, with consequential impacts including industry-partnered commercialization paths to SAF and renewable biochemicals with significant carbon dioxide equivalent (CO_2e) reducts, as well as benchmarked ABF capabilities demonstrating substantial operational performance gains. The top challenges of completing the implementation planning process are maintaining team morale and interpersonal relationships; developing a transparent, inclusive, and equitable activity prioritization process; and supporting broadly enabling tools. The outcome of this activity is to develop a budget-constrained implementation plan that largely accomplishes the deliverables established in the ABF strategic plan and gracefully breaks from the status quo to preserve capabilities and relationships as best as possible.



COMMENTS

- The ABF utilized multiple presentations to document their journey in developing a new strategic plan for the next funding cycle. These presentations grew off each other, and as a result, it is difficult to separate them as required in this review process. Instead, I have used the "Strategic Plan" presentation to provide feedback on this presentation as well. Please look there for my comments.

- Strengths:
  - Use of go/no-go to downselect bioconversion systems in SAF and biochemicals is an effective approach to allow the ABF to focus their resources.
  - It is critical for the ABF to continue developing new tools/capabilities to keep them as the leader in biofoundries. Several proposed new capabilities are innovative and have a lot of scientific merits.
  - The use of genome-scale screening tools and artificial intelligence/ML-guided approaches can effectively enhance TRY metrics of target biochemicals.
- Weaknesses/areas for improvement:
  - There is a list of tools proposed to be developed. It is not clear whether these tools were selected by their impacts to industrial biomanufacturing or because these are ongoing projects in ABF PI labs. It is also not clear what criteria were used to select these tools as targets. Some of these tools are more specific to individual projects rather than general tools that can benefit the broader biomanufacturing industry. For example, protein structural modeling to change substrate specificity and improve thermostability seems to be specific to the thermophilic ethanol production project.
  - The FY 2024 milestone for alkane SAF is to measure baseline TRY. It is unreasonable to take a year to just complete baseline measurement. The FY 2025 milestone is set to achieve the final target of 75% theoretical yield. It is unlikely to achieve such a big transition from baseline TRY to final deliverable in just 1 year. If it is possible, it would suggest that the FY 2025 milestone was set too low. Additionally, specific approaches to reach 75% theoretical yield are lacking.
  - It is not clear how the 500-kiloton CO_2e reduction will be measured. This number is associated with titer, yield, and scale of each conversion system. Will this number be demonstrated through scalable production? If not, this number is meaningless, because any bioconversion system multiplied by a huge imaginary scale value can potentially reach 500-kiloton CO_2e reduction. It is not clear how this milestone can be evaluated by FY 2025.
- These comments are the same for the ABF Future Strategy (1) Strategic Plan; (2) Goals, Milestones, and Deliverables; and (3) Implementation Plans:
  - The ABF and BETO have both struggled for years with how the ABF fits in with BETO's mission. This struggle is still ongoing. While it's clear the ABF needs new direction, management, and goals, at the same time, BETO needs to decide whether or not it's going to support an outwardly facing biofoundry focused on supporting synthetic biology. BETO was absolutely correct in calling out the ABF's failures to deliver on previous goals and forcing a reorganization of the ABF. That being said, the ABF was founded with a vision to support and advance synthetic biology in the United States, both for industry and at the national labs. This has frankly never seemed to fit well with BETO's overall mission statement in the past. However, with the Biden administration's call to decarbonize the chemical industry, ABF finds itself more aligned with BETO than in its previous history. My recommendation is for BETO to support the ABF consortium as it was intended—namely, to be outwardly facing, heavily engaged with industry, and providing services to all U.S. research efforts (industry and academia) to advance synbio goals and develop America as a leader in bioproduction of the molecules our world needs. This means changing the current

focus of the ABF away from some of their core work and putting funds back to supporting external partners and ABF infrastructure.

- I recommend the ABF revise their goals in the current strategic plan. This is not going to be something the ABF (and maybe BETO) wants to do. However, the current strategic plan is not well thought out in some areas, and seems to overcorrect and try to appease perceived BETO unhappiness. It's much better to spend another few months rethinking and replanning than waste $45–$60 million over the next 3 years.

- Specifically, the core SAF targets seem out of scope with the ABF's mission and put in to appease BETO. First, the economics of SAF from lignocellulosic sugars is never going to work. Not unless BETO is OK relying on massive government subsidies for SAF, far more than the current subsidies. It's not possible to be economically viable to make SAF currently from cheap sugar cane, using a terpene strain that has near-maximum theoretical yield and a very simple and cheap purification process. The extra costs of lignocellulosic sugars only make the economics worse. The ABF should get clarity from BETO on what level of subsidy is OK to assume if they are going to pursue this path. Second, instead of the ABF trying to guess what would be the best SAF molecule for them to develop, they should be engaging with the big industry players to understand what they want, if there is any overlap between what is needed/wanted, and what the ABF/synbio can help develop. The ABF and BETO need to be brutally honest here, and if the economics of hydrocarbon production from cellulosic sugars is not going to be the most economically viable route to SAF, then don't work on this in the ABF. With regard to the consolidated bioprocessing (CBP) work proposed by the ABF, the CBP is very high risk and high reward. I don't know enough about the challenges of CBP to know if the ABF is adequately addressing the risks, and therefore the probability of success. I do think the CBP work overall is aligned with BETO and is in the national interest to fund at the national labs. It is this kind of "blue sky" visionary work that industry won't do because of the risk, cost, and timelines involved. This is where government funding of basic science can push development of new technologies. That being said, should this work be done in the ABF? Again, I cannot judge that because little detail was given on why the ABF thinks they are best suited to do this work.

- Assuming some or all of the proposed SAF work is dropped from the ABF strategic plan, what should they do with the money? Some recommendations (in rank order): (1) Continue to host onboarding work, which we learned was cut completely. This is my number 1 recommendation for the money. The host onboarding is one area that ABF and BETO funds can really make a difference to advance new technologies and develop new strains to enable new chemicals and pathways at better costs. This is expensive and time-consuming, and often industry is reluctant to take it on. If they do develop a unique microbe, they will keep it strictly proprietary. Host onboarding should pick a small number of microbes that have very different properties, would access very different feedstocks or fermentation abilities, and are likely to be tractable genetically. Then, develop them to a high TRL rating to make them really useful. I have a lot to say about the apparent lack of progress on the HObT website since 2021 and the lack of helpful information to the U.S. research community from this work when reviewing this part of the ABF presentation. Regardless, if further work on host onboarding is done, there must be funds allocated to bring the website up to date and make the tools developed useful to the public, or BETO can consider a lot of that work and money wasted. (2) Develop another chemical target, if there is another one as developed and with clear TEA and CO_2e reduction benefits. (3) Put more money to partner-facing projects (FOAs) that support BETO's goals and will also support industry and commercial realization of BETO's goals.

- Several aspects of the technical targets had not yet been worked out by the time of the BETO review in April. Given that the ABF had 4–5 months already to replan, this is surprising and disappointing. The tools section of the strategic plan is not well thought out at all. They have not come up with criteria to even choose which tools to benchmark, or how to conduct benchmarking. It seems like no one wanted to give up their pet project, and with no one really in charge, they are having a hard time figuring out what to pursue further. It is good to not spend time and effort trying to build a capability that is already publicly available that people can access. DOE/BETO/national labs should focus on offering capabilities or research tools that are not available or that industry is not going to do. However, I caution that the ABF should not throw out a capability or tool even if it is measured to be not as good as something already out there. It might be that the ABF provides a different benefit that makes the tool/capability useful to researchers and industry. For example, an ABF capability might be almost as good as something already commercially available, but ABF might be cheaper, more accessible, or offer more capacity to a limited service. The ABF needs to figure out their criteria and how they are going to benchmark tools immediately and complete the assessments as soon as possible. In the current plan, it looks like this will not be done until the end of 2025.

- Lastly, I think it's a mistake to abandon all DBTL metrics going forward. Revise DBTL to be more realistic, but still have a goal to reduce the DBTL cycle (or even parts of DBTL that make the most sense, are the most commonly used, or are the biggest bottleneck). It doesn't have to be every capability and every tool. The team can measure time needed to finish one complete experiment and learn from it (per tool or per instrument), and focus on making those individual unit ops more efficient. Drop wall time versus clock time. What matters is how long it takes you to learn from an experiment. If there is some large downtime (let's say you need to ship samples from one site to another, and that takes weeks), then that is part of your cycle time and something to target to be more efficient. Focus on gaining efficiencies and improving the infrastructure already in place. There is some acknowledgement of this in the strategic plan; under tool milestones it says, "Operational performance gains of significant impact demonstrated for at least 2 ABF benchmarked technologies."

- The ABF said there was large interest from chemical companies for the proposed 3-HP and muconic acid targets. (I know from my own company that industry is very interested in muconic acid to make nylon.) These two core projects are much more aligned with the capabilities the ABF has built, have a high chance of success, and align with BETO's goals. These two projects should definitely continue and are a good change from the beachhead approach, which for whatever reason did not appear to get much industry traction.

- The shift in emphasis to bring in more external money (FOA and DFO) and have >50% of the ABF's budget committed to external partnerships by 2025 is a good change of direction and furthers the goals of the ABF to support industry and other research to translate lab work to real-world changes in decarbonization and reducing CO_2. It's going to be very challenging to achieve a significant increase in industry money into the ABF in the near future, especially if contracting takes a year. It will take time to get >50% of the ABF's budget committed to external partnerships and reach an average of more than fivefold oversubscription for the ABF's funding opportunities. The 2024 milestone to have two funds-in projects means the ABF needs to land those partnerships in a few months if contracting is going to take a year. Also, the length of time to contract must be improved. The ABF needs to redo its approach to IP and how it contracts projects to de-risk bringing in more industry partners and money. BOTTLE has worked out a very clear IP management plan that allows different levels of industry access to any IP developed. There is an option for industry to keep all the IP (and the national labs then get a higher percent royalty fee). The ABPDU also has worked out smooth contracting and IP understandings that allow them to contract in a few weeks, and industry does not have to share IP if it does not want to. The ABF should have developed something like this years ago.

- There was no mention of how the ABF will measure reduction of CO_2e in their partner projects. Given the ABF's track record regarding an inability to quantify metrics, this does raise concern.
- The ABF revised management plan is significantly better than the old management structure. The one area that still needs to be changed is for the lead PI to be solely accountable and responsible for running the ABF. There should not be any decision by committee. The ABF needs a 100% dedicated full-time employee running it. This person should be an "outsider" with no emotional connection to the past 6 years of the ABF. The executive committee reports to and advises the ABF PI but does not make decisions. It's clear that the ABF has really suffered from decision by committee and a lack of someone whose job is 100% running the ABF.

- Approach: The ABF has strong capabilities and expertise to target the proposed targets.
- Progress and Outcomes: Go/no-go industry interest gates for the four molecules will be highly important. Beyond just go/no-go, incorporating industry feedback into what alternative molecules, pathways, and approaches should be pursued by the ABF will be critical. It will also be extremely important to request feedback from diverse industry sectors, not just synbio or synbio-adjacent players. There are a lot of new capabilities listed under new development (Slide 12). It is not clear how these capabilities will be developed given the focus of core funding on the four molecules. During previous sessions it was stated that new software tools will not be developed, yet several are listed here, and the plan is not clear. If the plan is to develop these as part of funds-in projects, this is highly risky since the funds-in projects may not be interested in developing or paying for specific tools that are not directly related to the work.
- Progress/outcomes and impact are given neutral scores of 3 because this is a review of plans rather than progress. Implementation plans to achieve milestones related to tools, SAF, and biochemicals are sound, with acknowledgement that details are necessarily sparing. Technical excellence demonstrated in previous performance periods lends confidence that progress will be made in these areas, assuming management takes an active role in reorienting research objectives across the ABF scientific enterprise. Going forward, partnerships carry the greatest risk to the new strategic plan, but few details were provided as to how the stated milestones will be achieved. Three activities are provided to achieve milestones: actively engage industry to develop and promote adoption of ABF processes/technologies, develop new IP management plans to enable efficient licensing, and demonstrate/measure ABF's impact on and contribution to biomanufacturing. Without specific actions to be taken and without demonstrated prior success in this area, it is difficult to feel confident that partnership goals will be achieved. As a reminder, expediting partnership agreements and formulating IP management are complicated by the ABF distributed model.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback. We responded above for the "ABF Introduction and Overview"; "ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads"; "ABF Past Accomplishments – Industry Engagement, Outreach, and Management"; "ABF Past Accomplishments – TEA/LCA"; "ABF Past Accomplishments – Host Onboarding and Development"; "ABF Past Accomplishments – Process Integration and Scale-Up"; "ABF – Lessons Learned and Introduction to Future Plans"; "ABF Future Strategy – Strategic Plan"; and "ABF Future Strategy – Goals, Milestones, and Deliverables" presentations. As stated above for the "ABF Introduction and Overview" presentation, we reiterate our appreciation for the extensive, thoughtful, and helpful comments that the reviewers have provided (and the time and effort that went into them), for this particular presentation and for all previous ABF-related presentations. While more detailed responses can be found in our responses for previous presentations, we thought it would be helpful to repeat several high-level responses here. The ABF and BETO teams worked intensively and extensively together during the recent ABF strategic and implementation planning activities, and the ABF is committed and fully bought-in to its new direction and excited to support BETO in achieving its ambitious goals for 2030. Host onboarding and development activities will continue within the ABF, as directed by industry and other partners in collaboration projects. We will continue to make improvements to the ABF website and specifically to our HObT web application to better depict our capabilities. As part of our capability benchmarking activities (which will help prioritize ABF development efforts and enable business development and technology transfer), the ABF will continue to consider DBTL-related metrics. We have changed from a consensus-driven management approach to the lead PI (with BETO support) having and exercising decision-making authority. A new strategic implementation lead will help ensure that all work in the ABF remains aligned with its strategic and implementation plans, and that work is not disjointed. The ABF is continuing on its path to becoming more of a “customer”-facing entity, with the establishment of new business development co-leads, upcoming changes to how the ABF interfaces with its advisory board, and increasing amounts (>50% by the end of FY 2025) of its resources dedicated to collaboration projects. The ABF has contributed (and is contributing) to multiple product/process commercialization efforts, several of which are building off of established ABF beachhead molecules.

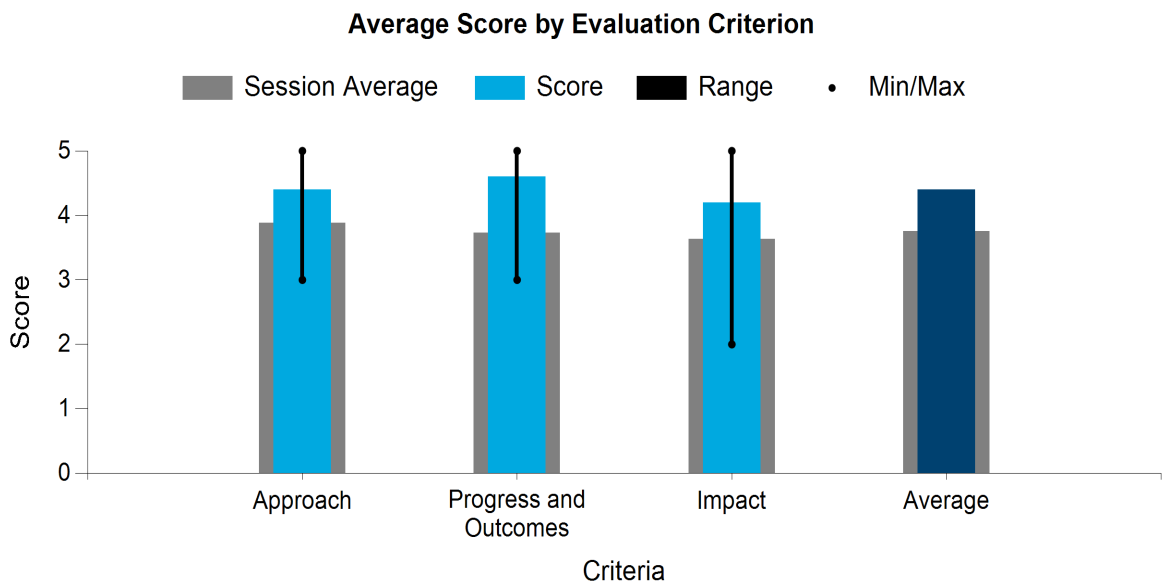
ABF PAST ACCOMPLISHMENTS – PROCESS INTEGRATION AND SCALE-UP

Lawrence Berkeley National Laboratory and National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	ABF11
Presenter(s):	Davinia Salvachua; Deepti Tanjore; Katy Christiansen
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

The main objectives of the Process Integration and Scale-Up (PISU) task were to produce lignocellulosic hydrolysates, screen microbial strains, and develop bioreactor cultivation processes to improve product TRYs. In the past 2 years, we developed bioprocesses for (1) muconate production by engineered *Pseudomonas putida* and (2) terpene production by *Rhodotorula toruloides*. In addition, we evaluated *P. putida* as a host for the production of various value-added compounds. The PISU task has also been involved in the production of targeted compounds at larger scales for industry and other DOE-BETO-funded projects to test downstream product recovery processes and analyze material properties. We also demonstrated better utilization of traditional real-time data for in-line process control, and we are now working toward using imaging as an approach to better understand bioreactor performance.



COMMENTS

- Scale-up is a critical step in bringing new products and strains to market. Understanding the challenges in scale-up, and in particular understanding what issues are likely to appear at larger scale that are not manifested in lab-scale experiments, is critical to ensuring R&D efforts in the lab will have applicability at commercially relevant scales. It is therefore important for BETO to have scale-up of technologies as a goal, and for the various research groups and consortiums under BETO to communicate and share knowledge and best practices. It is less obvious that these activities should live at the ABF. Where scale-up is most useful and applicable at the ABF is in understanding the performance of the various strains in its catalog at a variety of scales. By understanding the various trends of different organisms as they are grown in progressively larger reactors, the ABF can better guide industrial partners on the best strains to utilize for commercial applicability; they may not be the best-performing strains at the lab scale.

- This context informs the approach and impact scoring for this activity. The approach presented is centered around the idea of developing this type of knowledge by understanding experimental results at different scales and optimizing processes for different hosts at larger scales to improve TRY. The demonstrated successes and activities appear to be more one-off, however, and there doesn't seem to be a coordinated scale-up strategy for the various hosts in the library. Impact is low for this reason, and because there does not seem to be a way for scaling issues at still larger scales (beyond those offered by the ABF) to be fed back to the team at the ABF. It is important for the ABF to follow partners after they outgrow ABF capabilities in order to close the feedback loop from outside the ABF on scale-up learnings (e.g., 100-L to 100,000-L reactor sizes) that can further help optimize the lab-scale testing and experimental work done by the ABF.

- As a result, the scale-up activity at the ABF is at a crossroads. One path forward focuses on more scale-up testing across hosts using AOP funds to better understand the ABF strain library and the behavior of each host at various scales. This work would then inform host selection for new product development. The other path limits scale-up activities to DFO or funds-in uses where scale-up is a critical part of the research opportunity. This pathway may begin to overlap with efforts at ABPDU or BioMADE, and so coordination with other groups in orbit with the ABF is important to ensure ABF funds are spent on the tools and capabilities where the ABF has the most specialized knowledge and potential for impact. Being a scale-up partner may not be the best use of ABF funds if other organizations that operate at the 100–5,000-L scale are better placed to take hosts and products identified at the ABF to the next TRL stage.

- Strengths:

  - The PISU team has made excellent progress. All proposed milestones were delivered on time.

  - Extremely high TRY was obtained for multiple conversion systems, including production of muconate, ß-ketoadipate, and 3-HP from various carbon sources. Muconate production was scaled up to 150 L, and high titer was achieved at this scale. These results are very impressive.

  - The PISU team has also demonstrated collaborations with industry and academia, proving their values in facilitating the U.S. bioeconomy and the scientific society.

- Weaknesses/areas for improvement: N/A.

- Overall, the work done in the PISU is highly relevant to many aspects of the ABF. Scale-up is hard; ask anyone who's done it. It's imperative to do scale-up work to advance the TRL of any project, whether industry or national labs. As the PISU team states, the work is also necessary to give better, more realistic parameters to the TEA/LCA teams for their modeling. The most important aspect of any synbio project is to generate material to have for actual application testing and understanding the impurity profile. ABF is encouraged to generate representative samples as soon as possible (in PISU) to accelerate downstream purification and applications testing.

- The work on oxygen uptake rate in fermentation is very important, and it's good to see that being implemented. That should be considered standard on all fermentations for the ABF. This is routine in industry.

- Several milestones were reached successfully. It's not clear if this is all the milestones (feedback to BETO for all projects to list all milestones and percent completion on them).

- Scale-up is one of the biggest challenges for the bioeconomy. As such, the work done under this task is highly relevant for advancing the U.S. bioeconomy. The work that was presented does address many important challenges, such as understanding cell heterogeneity and its impact on fermentation performance across scales. The media development tools are also a highly relevant and potentially impactful contribution and could be expanded to better account for the expected performance under lower-carbon-intensity media feedstocks. One shortcoming I see in the approach is that the experiments and data from fermentation runs do not appear well integrated into other aspects of the DBTL cycle. For instance, how might design or build considerations impact eventual performance across scales? This could be a highly impactful question that the ABF is well suited to solve. The dissemination of the work done could use improvement. For instance, the media optimization tool could/should be accessible through more than just publications (e.g., through a web app or other interactive mechanism).
- The PISU team continues to perform well, meeting a diverse number of ABF needs. It takes strong technical and organization skills to successfully operate over the range of bench scale (2 mL) through pilot scale (9,000 L) for various organisms. Their Pilot City Internship Program for high school students is a creative addition to DEI initiatives that exposes students to real-world STEM professional opportunities at a point early enough to influence selection of an educational path.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback, some of which was responded to above for the "ABF Introduction and Overview"; "ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads"; "ABF Past Accomplishments – Industry Engagement, Outreach, and Management"; "ABF Past Accomplishments – TEA/LCA"; and "ABF Past Accomplishments – Host Onboarding and Development" presentations. In terms of interactions with BioMADE for scale-up, we note that we are planning to have a joint funding call that will be pursued with BioMADE in the future. We also note that the ABPDU is not the only scale-up facility in the ABF—NREL's Integrated Biorefinery Research Facility can scale to 9,000 L. In terms of feedback loops with industrial partners, we are certainly interested in feedback from industrial partners, but this is not our decision to make; stated differently, we rely on connections to DFO partners after the award to provide this feedback, and we will consider a mechanism in the funding opportunity process going forward where this can be included. In terms of generating samples for separations, purification, and downstream testing, we fully agree, and we are doing this again for several target compounds in the FY 2024 time frame in collaboration with the performance-advantaged bioproducts projects in the BETO portfolio. In terms of milestones, all PISU milestones were met and delivered in a timely fashion. In terms of integrating scale-up into the DBTL cycle, we agree that this is an excellent opportunity that we are not fully taking advantage of, and we will work to improve this going forward. With regard to a coordinated scale-up strategy for hosts, the PISU task produces hydrolysate for fermentation and conducts bioprocess development of ABF hosts in bioreactors at multiple scales. To this end, we tested multiple ABF hosts at bench and pilot scale. In the past 2 years, we demonstrated multiple target-host combinations across bench to pilot scales, delivered lignocellulosic hydrolysate, developed several new bioprocess tools, and enabled DFOs and other consortia.

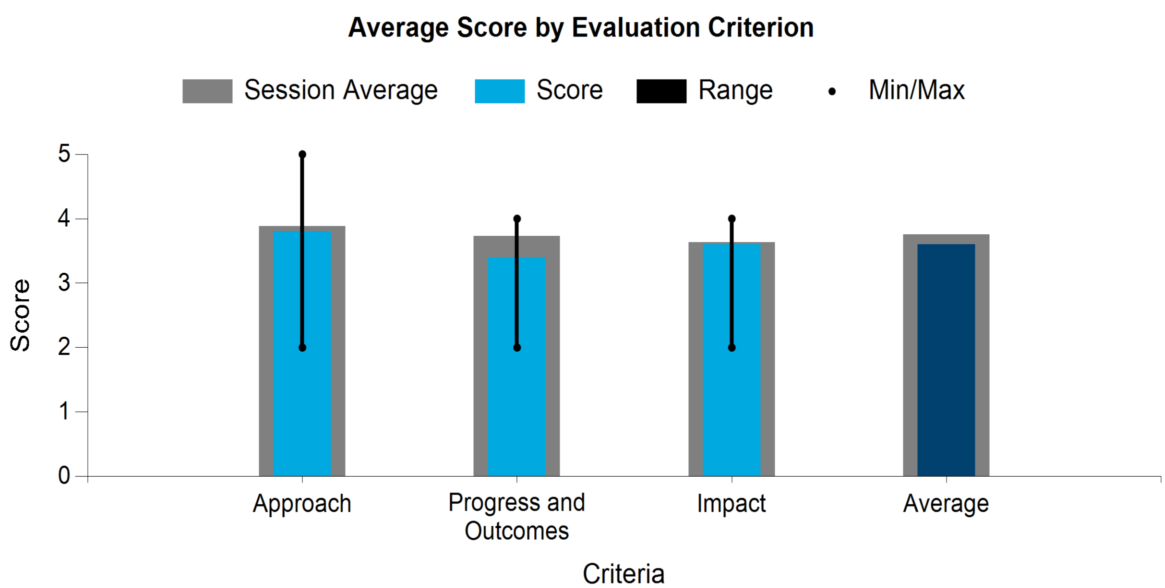
FUNDING AND PARTNERING MECHANISMS

Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	ABF12
Presenter(s):	James Gardner
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

Since its inception, the ABF has partnered directly with industry and academia to accelerate biologically produced fuels and chemicals toward commercialization and to develop new tools and capabilities that increase the ABF's ability to better support the synthetic biology and biomanufacturing communities, in its effort to support the SAF and decarbonization mission of BETO. The ABF's partnering mechanisms have since grown, matured, and diversified, and they continue to do so. With 37 partnerships either complete, in active R&D, or in contracting, the ABF's support of its external partners is strong, as are the relationships the ABF has developed with its external reviewers and partnering organizations, including the NSF. The ABF's ongoing partnering work with minority-serving institutions will continue its support of important DOE objectives in DEI in science. The positive impacts that the ABF has made through its partnerships, as well as the resulting tools and knowledge that the ABF can reapply, are lowering barriers to entry for small organizations and startups and offering rare expertise and capabilities to larger organizations as well. This presentation outlines these activities and achievements.



COMMENTS

- The ABF utilized multiple presentations to document their journey in developing a new strategic plan for the next funding cycle. These presentations grew off each other, and as a result, it is difficult to separate them as required in this review process. Instead, I have used the "Strategic Plan" presentation to provide feedback on this presentation as well. Please look there for my comments.
- Strengths:
  - DFOs provide a unique funding mechanism for industry to directly collaborate with the ABF and utilize the ABF's capabilities. This funding mechanism effectively motivates both industry and

ABF personnel to be deeply involved in the projects. Most projects are also highly aligned with BETO's goals for producing bio-based chemicals.

- A large number of industry partners have been involved with and directly benefited from the DFO funding mechanism. Excellent feedback was received from these industrial partners.
- The DFO projects also utilize a wide range of ABF technologies and showed a balanced distribution among different technical areas in DBTL, hosts, process, TEA/LCA, and software.

- Weaknesses/areas for improvement:
  - It is surprising that no DFO team worked on SAF projects, which is a central mission for BETO.
  - Although great overall progress has been made from DFO projects, some individual DFO teams have unsatisfactory performance. They either failed to deliver the proposed milestones or created little impact to industrial biomanufacturing or BETO's goal in producing sustainable bio-based chemicals/GHG reduction. Some monitoring mechanism is needed to ensure the funded teams perform their proposed tasks.

- The goals of the funding for the new strategic plan are overall very good. As mentioned many times in previous reviews, there is a high risk to being able to hit a high level of industry funding, mostly due to the long contracting period and complicated IP approval process. The ABF needs to redo its approach to IP and how it contracts projects to de-risk bringing in more industry partners and money. BOTTLE has worked out a very clear IP management plan that allows different levels of industry access to any IP developed. There is an option for industry to keep all the IP (and the national labs then get a higher percent royalty fee). The ABPDU also has worked out smooth contracting and IP understandings that allow them to contract in a few weeks, and industry does not have to share IP if it does not want to. The ABF should have developed something like this years ago. Again, this is another example of the ABF management not being focused, with a single person responsible for making the ABF as successful as possible.

- Overall, the ABF has demonstrated productive partnerships with impact to industry. Strengths: Projects have largely been successful and achieved relevant milestones. There are a few "return customers" such as Lygos, indicating that the work the ABF provided was seen as valuable. The new partnership strategies with NSF and minority-serving institutions will increase the impact of the ABF to advance research and technologies led by minority researchers. Weaknesses: Long contracting timelines are such that there is even risk of the original project scope becoming out of date/irrelevant. The ABF's projects with partners are quite wide and diverse; while this is in some ways a strength, I also see that it may limit the ability of the ABF to leverage industry projects as a way to advance the bioeconomy forward in a more strategic/coherent manner. Having projects with more related end goals may facilitate advances in the difficult sectors more easily.

- The greatest strength of the funding and partnering approaches has been the ability to evolve and improve based on prior experience, feedback, etc. Evolution of partnering mechanisms will be critical to implementation of the revised ABF strategy. The greatest weakness and most significant risk to ABF partnering is delays in formalizing agreements to get projects underway. If the ABF wants to increase funds-in partnering mechanisms, 12-month delays to complete agreements will be unacceptable to organizations working with performance milestones and timelines. In essence, there will always be organizations willing to accept 12-month delays prior to project initiation, but those are not the organizations capable of moving the needle on bioeconomy growth. Additional strengths include continued expansion of partnership funding organizations (now to include DOE, NSF, and BioMADE) and a DEI plan that includes funding opportunities specific for minority-serving institutions. During the competition for a limited number of partnerships (DFOs and FOAs), minimal attention is given to commercialization potential. Evaluation of partnerships to date reveals a very wide range of commercial potential, from high to vanishingly low. Low-commercial-potential projects may still be worthy of funding, but the benefit to the ABF and bioeconomy should be made explicitly clear in all applications. Benefits to the partner (e.g., company, academic institution), the ABF, and the bioeconomy should be provided in all future Peer Review materials. If the ABF wants to secure more funds-in agreements and improve oversubscription levels of DFOs and FOAs, improving both the quantity and quality of data provided on the ABF website is imperative. The ABF should look to the ABPDU as a model for elevating its information dissemination. Inclusion of case studies that provide information such as tools used, fold improvement in product, etc. would be very valuable. At the very least, these case studies provide specific examples of ABF capabilities.

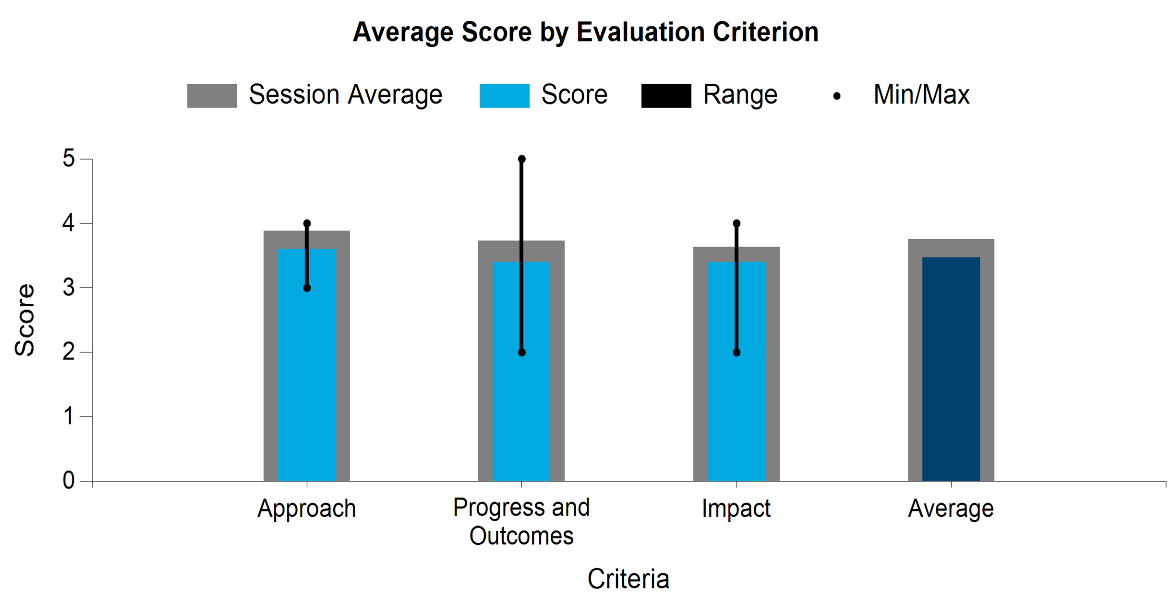
ABF PAST ACCOMPLISHMENTS – DBTL INFRASTRUCTURE, DEMONSTRATION PROJECTS, AND BEACHHEADS

Lawrence Berkeley National Laboratory, National Renewable Energy Laboratory, Sandia National Laboratories, and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	ABF2
Presenter(s):	Gregg Beckham; John Gladden; Jon Magnuson; Katy Christiansen; Nathan Hillson; Di Liu
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

Since 2016, DBTL infrastructure and demonstration projects have been core ABF activities. In 2020, beachheads were added along with the demonstrations as a strategic activity, to make more of the biochemical and bioprocess space accessible. The relevance of these tasks are that they (DBTL infrastructure) support the ABF and other BETO projects and can be leveraged by industry; and (demonstration projects and beachheads) assess BETO investments in ABF capabilities and are key drivers toward industry collaboration projects. Top challenges for the ABF have been leveraging past collaboration learnings with future collaborators, predictive scale-up and method transferability, and the intellectual framing of strategic beachheads (metabolic intermediates). Outcomes and technical accomplishments are highlighted in this presentation and span DBTL infrastructure, demonstration projects, and beachheads across bacteria, fungal, and yeast organisms.



COMMENTS

- The overall goals of the DBTL project are sound: enable a 10× improvement in DBTL cycles. Accelerating the development of strains and technologies for new target products and molecules is an important goal that is aligned with the ABF's mission. It allows a focus on building the tools and capabilities to enable these DBTL improvements. The approach, however, relies on "demonstrating projects," primarily through a focus on measuring the unmeasurable: It is not clear how the ABF can demonstrate a 10× improvement in DBTL, the baseline is not well defined, and it's unclear what technical metric would demonstrate that the ABF is succeeding. This lack of clarity undermines a focus on impactful tools and capabilities, as it's difficult to determine which tools and capabilities have impact.

- Progress is therefore difficult to measure and quantify. The ABF has surely built a capable suite of tools and performed sound science. Commercial applicability, however, is much less certain. The ABF's toolkit, from its analytical capabilities to ML integrations, should present an impactful narrative. Unfortunately, the ABF has not been able to tell that narrative cohesively. There are only anecdotal examples of the DBTL cycle performing, and the applicability of the "learn" portion of the DBTL cycle is particularly unproven. A focus shift toward industry feedback as an indicator of success and impact is recommended. If the ABF is truly accelerating the DBTL cycle beyond the state of the art, industry will seek out ABF support in further projects. Industry interest in only a portion of the ABF toolkit will provide evidence of which ABF innovations are commercially applicable. Follow-on funds and product commercializations after ABF collaboration will cement the impact of the ABF on the field.

- Current impact is therefore hard to quantify as well. The toolkit that the ABF has built, the hosts onboarded, and the learnings from multiple projects employing DBTL cycles appear to have value, but the lack of commercial success points is apparent. The ABF is not able to point to any one commercially mature product or molecule that they were instrumental in creating or accelerating, a troublesome sign for the applicability of the capabilities built at the ABF. A narrow focus on publications as the primary outcome of projects is misguided; publications may show scientific development, but they are a poor proxy for commercial applicability and overall impact. Further commercial validation, as noted above, will provide considerably more evidence of ABF impact.

- Strengths:

    - Excellent technical achievements have been made on the bacteria, yeast, and fungi projects. Transfer of the malonyl-CoA beachhead between multiple strains for 3-HP production was successfully demonstrated. Satisfactory TRY metrics have been obtained.

    - The presented work involved several research teams from multiple national labs and a large number of researchers. Coordinating and managing such a large team is a big challenge, but the ABF was able to demonstrate high efficiency managing such a large team and delivered good results.

    - The multi-omics analytical tools were proven to be useful, and have helped multiple industrial partners generate large data sets.

- Weakness/area for improvement: Challenges in quantifying the DBTL cycles were discussed. These challenges are well received by the review panel. However, as the major project goal, the ABF is still expected to provide some quantitative measures on the time and resources reduced when industry adopts ABF technologies.

- This review is focused more specifically on DBTL infrastructure, demonstration projects, and beachheads. A general review of the past goals and accomplishments of the ABF was given in the "ABF Introduction and Overview" session. I will reiterate one point that is highly relevant here. I think it's a mistake to abandon all DBTL metrics going forward. Revise the DBTL goals to be more realistic and relevant. Still, have a goal to reduce the DBTL cycle or even parts of DBTL that make the most sense, are the most commonly used, or the biggest bottleneck. It doesn't have to be every capability and every tool. The metric could be time needed to finish one complete experiment and learn from it (per tool or per instrument), and focus on making those individual unit ops more efficient. Drop wall time versus clock time. What matters is how long it takes you to learn from an experiment. If there is some large downtime (let's say you need to ship samples from one site to another, and that takes weeks), then that is part of your cycle time and something to target to be more efficient. Focus on gaining efficiencies and improving the infrastructure already in place.

- Most scores were moderate or low for judging impact on previous goals because there was a balance of very low scores and some high scores. Low scores because (1) nearly all DBTL goals were not met and (2) management structure was not sufficient to lead the ABF to success. High scores for overall a lot of solid work advancing synthetic biology and delivering on several projects that advance U.S. capabilities and advance industry to be impactful. Also good plans for addressing DEI.

- Good:

  - Overall, so many amazing tools and capabilities have been built in the ABF (Slides 15–19). The ABF really is a fantastic resource to advance BETO's goals and support industry to be a leader in synbio in the United States.

  - I don't remember hearing about the semiautomated combinatorial media pipeline in 2021. This seems like something really useful to industry, academics, and national labs. This is a good service that should be aggressively marketed, and this slide needs to be on the ABF website. See comments below on how to improve the website.

  - Better tools for tracking DBTL, and showed DBTL cycle data for results of transferring one molecule pathway to a different host. Hit the Q4 2021 milestone: "2X efficiency improvement in automated DBTL engineering cycle unit operations compared to FY22Q2_DBTLI_R1 non-automated baseline efficiencies demonstrated."

  - Impact and metrics slides show that a lot of good progress was made in last 3 years developing the tools and infrastructure to advance synthetic biology in the United States and help BETO's goals to decarbonize the chemical industry. Slide 28 is especially impressive, with muconic acid and 3-HP especially standing out as good examples of beachhead and exemplar to advance decarbonization of the chemical industry.

- Better, and could still use improvement:

  - A lot of these slides are very clear and show all the tools and capabilities of the ABF and what they have to offer (Slides 15, 16, 18, and 19). Why are these slides and images not being used on the ABF website? Slide 15 does a much better job at communicating all the amazing technical capabilities the ABF has to help partners than all the words currently on the ABF page. I would not worry if some of these activities are not being actively supported in the new strategic plan. The ABF said if a company wanted to use some of that infrastructure, then those capabilities would be used and further developed, so there should be no issue with advertising them. It's good that the beachhead slide is finally up on the website, but it's really buried, hard to find, and not at all obvious to industry or someone looking at the site to know the ABF has developed these beachheads. I only found it by clicking through the host onboarding capability. Is the semiautomated combinatorial media pipeline even mentioned on the ABF website anywhere? I tried clicking around and couldn't find it.

  - It's good that the beachheads got some traction, and the demonstration of muconic acid and 3-HP as exemplars is excellent work to further decarbonization of the chemical industry. However, overall it seems to have either not been of interest to much of industry, or it was not advertised to industry well. It's good the ABF is not pursuing beachhead strategy anymore.

- Bad: Overall, DBTL cycles were not met, and for reasons that are still not clear, were said to be hard to measure/quantify. It really isn't that hard to quantify how long it takes to go from one step to another, or from the start of an experiment to when data are returned.
- It is clear that the ABF has done a lot of really fascinating and novel work. The beachhead molecules were a hard task, and the ABF demonstrated significant progress toward those molecules. Past and future work on 3-HP is likely to have substantial impact across various industries. One of the other strengths of the ABF has been their improvements to the learn part of the cycle. The national labs have a dramatic advantage when it comes to access to computing power. It would be wonderful to see the ABF fully leverage that access to develop and support software that can accelerate synbio design. One drawback on that end, given the national lab structure, is that developing the software would need to be an ongoing project to enable the software to be updated, supported, and evolved according to industry needs. The current focus of the national labs on publications and more academia-like dissemination methods actually hurts the potential impact of the software and models that the ABF has the ability to create.
- This summary provides an assessment of progress/outcomes and impact. Approach was assessed in a previous review. The DBTL infrastructure goal was to design, operationalize, and maintain DBTL infrastructure as a core component of the ABF to support other ABF tasks. Substantial progress has been made in high-throughput screening and multi-omic analysis, resulting in multiple publications. Whether these advances obtain the 5–10× improvement in cycle efficiency is unclear because metrics were not provided. A semiautomated media optimization pipeline was also developed, and software was made more accessible to the visually impaired. The demonstration projects and beachheads goal was to develop bacteria, yeast, and fungi hosts to efficiently, cost-effectively, and sustainably produce beachhead and exemplar pairs to aid commercialization. As documented in the presentation slides, substantial progress was made in preparing organisms capable of producing high titers of multiple important molecules, although no indication was provided whether these processes are cost-effective. Tool development is expected to have a positive impact, as these can be applied to future research objectives. The impact of achieving milestones related to beachheads is difficult to assess. While certainly providing a demonstration of ABF competency and capabilities, whether a partner organization is interested in using these specific strains is not known at this time.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback, some of which was responded to above for the "ABF Introduction and Overview" presentation. Regarding the ABF not yet being able to point to a commercialized product that it has enabled, the early TRL nature of the ABF's value proposition does go hand in hand with significant lead times before a product may come to market. That said, Lygos saw a very significant leap toward a commercially viable process for producing isobutyric acid as a function of its collaboration with the ABF. Similarly, the strong collaborative relationship with ZymoChem has resulted in technology for producing polyglutamic acid that has garnered interest from large offtake partners and is nearing commercial viability. Further, Visolis has been able to raise very significant private funds by virtue of its technological advances, some of which arose from its successful ABF collaboration for mevalonate production. These are just a few examples of the impacts that ABF-enabled research is having in the community. With at least 20 distinct products and fuels to its credit, the breadth of biomanufacturing research to which the ABF has contributed is significant. However, relative to the length and vagaries of product development timelines, and the foundational role that ABF research plays for its collaborators, one could conclude that it is early days, yet. We acknowledge that the ABF team needs to do a better job of measuring and reporting the entirety of its impact. The recent expansion of the management and business development teams, along with the acquisition of grant management software, is affording us the time to more carefully monitor the ongoing impact that ABF R&D offers its partners and industry. Regarding the ABF website capabilities section, we agree that we can continue to make improvements to these pages. We will evaluate what graphics or images we can add to these pages to better communicate the ABF's capabilities.

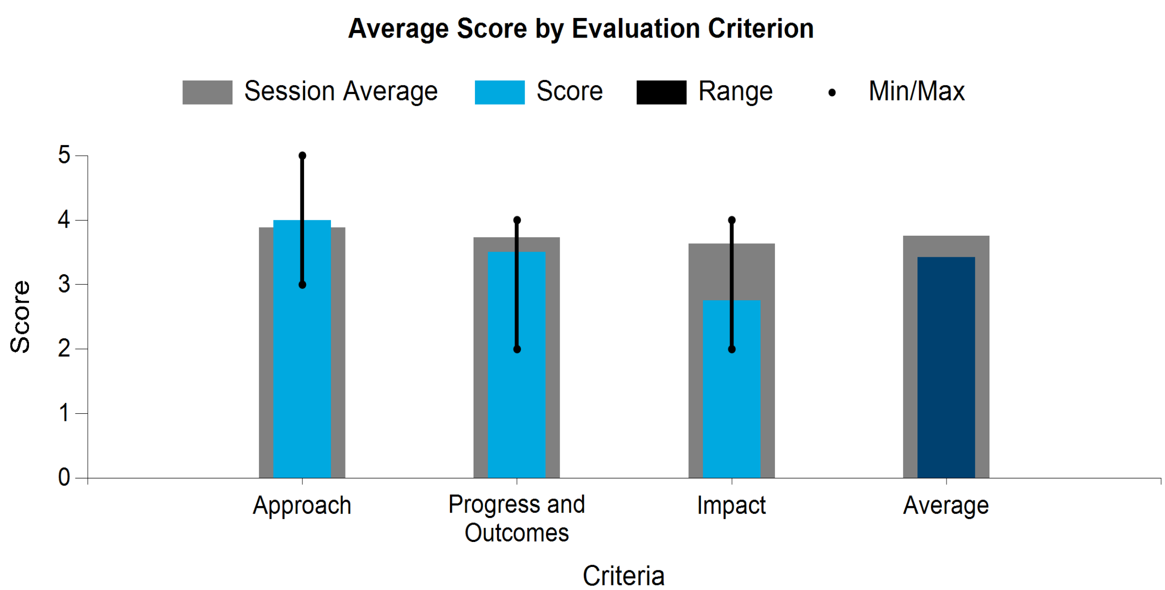
ABF PAST ACCOMPLISHMENTS – HOST ONBOARDING AND DEVELOPMENT

Oak Ridge National Laboratory and Los Alamos National Laboratory

PROJECT DESCRIPTION

WBS:	ABF3
Presenter(s):	Adam Guss; Katy Christiansen; Taraka Dale; Tim Theiss
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

Non-model microorganisms often have advantageous physiological traits that could be leveraged for advanced bioprocessing, such as the ability to thrive at low pH or to utilize uncommon feedstocks such as syngas or mixtures of oligomeric sugars. However, a lack of genetic tools and fundamental knowledge about these organisms hinders strain development. The role of the Host Onboarding & Development (HOD) team is fourfold: (1) evaluate and select hosts for use within the ABF, (2) develop genetic tools and data sets that allow new hosts to be used for DBTL cycles within the ABF and by outside stakeholders, (3) improve genetic tools for BETO “state of technology” organisms to increase DBTL cycle efficiency across the BETO portfolio, and (4) develop a web interface with information and data on each ABF organism for internal and external stakeholders. In this talk, the HOD team will discuss how we use our “tier system” framework for evaluating the readiness and guiding the development of an organism for DBTL cycles. We will discuss progress in host development, detailing advances in the development of genetic tools, synthetic biology parts, and biosensors for multiple organisms. Finally, we describe progress on the web portal, named HObT, for sharing host-specific information (e.g., development status, strain attributes, protocols/parts) within the ABF and with the community at large.



COMMENTS

- Building up the strain library at the ABF is a key activity that separates ABF capabilities from others in industry. By serving a potentially wide range of companies across a diverse host set, the ABF can maximize its applicability to industry and ensure its continued relevance. The goals and approach of the ABF in this space are therefore built on a sound theory, and this activity in particular demonstrates the need for governmental support to build the infrastructure and capabilities that industry is unlikely to develop alone and on its own. The knowledge built at the ABF on multiple strains, the benefits and trade-offs of each, and the process of working with each is unique knowledge that can separate the ABF from competitors.

- It is less clear, however, that the particular strains that the ABF has onboarded, or the decisions about which hosts to focus on, are the most important commercially. The ABF has fallen short in disseminating to industry their capabilities around hosts. HObT was presented as a solution to provide a standardized way of comparing hosts; however, the website is broken, information is missing, and its development and maintenance appears to be a low priority for the ABF. It is further unclear if HObT was designed with industry input to ensure that the parameters and information shown are of interest and use. This lack of focus on HObT is unfortunate and also indicative of the problems surrounding host onboarding at the ABF: the host library is a key differentiator for the ABF, and the ABF needs market feedback to both validate the importance of the strains that have been onboarded and help prioritize the next strains to bring on. The ability of the ABF to onboard strains and work with new hosts is not in doubt, although the velocity of these activities is uncertain. It is the commercial applicability of the hosts that is in question. Measuring impact based on publication count is a poor proxy for impact, especially as many journals are not open access, limiting the knowledge transfer to industry. More direct industry outreach is needed to better demonstrate the impact of the ABF's library and the particular strains with the most commercial potential. The strains that are utilized the most in industry engagement will help the ABF better understand which hosts to invest further resources into and what parameters are most important to industry, guiding the onboarding of new hosts that better meet industry needs.
- Strengths:
    - The use of the tier system to categorize hosts allowed the HOD team to better focus on a smaller group of strains with higher depth.
    - The HOD team has made the efforts to develop the HObT website that summarizes the most important information about microbial hosts and their tools.
    - The HOD team continued to make excellent progress on onboarding more strains, improving their tier levels, and developing genetic and sensor tools.
- Weakness/area for improvement: It is disappointing that the HObT website is not available to the public. As a result, it is also not possible to review the value of the website and the impact of their work.
- I think the HOD work is one of the best assets of the ABF. Slide 21 sums up the benefits and impact to industry very well. The team took feedback from 2021 very well and adjusted its approach to have a clear plan for how to balance breadth versus depth by developing the appraisal framework (Slide 14). This is a good process to evaluate how to use resources for greatest impact in HOD. The technical advances are significant, and it's clear this part of the ABF has brought real value to industry and work being done at the national labs. It's wrong to defund this work in the new strategic plan. The potential benefits of this work toward making a strong U.S. bioeconomy are huge. I can't stress enough that this work should continue. It might not be possible to continue the work at the same scope, but some work in HOD should continue. Below I offer ideas and comments on where to find the money and what to focus on.
- Before that, though, there is one large problem with the HOD, which is access and documentation of the HObT website. If it wasn't for the lack of public access to the information on the HObT website, I would have given the HOD work 5s in every category. However, the lack of public access to the data and advances in the HOD program have to be taken into account. The presentation makes it sound like the

HObT website is available to the public, but it is not. First, there is no link anywhere to HObT on the ABF website (if there is, it's so buried as to be practically not available). Due to reviewer access, I was able to find the website. However, there is no discussion of what the different tiers are, and I was not able to see anything expect the publications. None of the protocols or parts or any other aspect of the HOD work was accessible. From Slide 13 it looks like more data is there, but not available to the public. I tried registering but couldn't. It's imperative that the HObT website be made accessible to the public, to encourage industry to understand what the ABF has to offer. It's a big barrier to have to contact the team to inquire. That drives away interest. Also, as mentioned in pretty much every other review on the ABF, the website overall needs a massive overhaul and updating. There are so many great images and visualizations that explain the ABF, and in this case the HOD work, that should be on the website but are not—for example, Slides 10, 12, 15, and 16 (although the tier system needs a bit more explanation on Slide 10). These images should all be on the website to engage industry. At the very least (and I strongly recommend more than just this), funds need to be allocated to bring the HObT website to the general public and make it functional. When asked about this at the review, the answer was that "the website wasn't ready yet" for the public. I don't understand this, because the HObT website existed in 2021, and it doesn't look like much has changed since then. The website should have been made available to the public back in 2021. It's basically a waste of all the great work and success in HOD not to have the HObT website available to the public.

- It was said at the review that at the last minute, to balance the budget, the HOD work was being defunded going forward. That is a wrong overcorrection in response to the call for an updated strategic plan from BETO. As I said to BETO, and elsewhere in my reviews, I think the emphasis on SAF work in the ABF is misguided and an overcorrection. That SAF work should be reduced or eliminated and the funds allocated elsewhere. My first recommendation was to refund HOD. Here is what I said to BETO: The host onboarding is one area that the ABF and BETO funds can really make a difference to advance new technologies and develop new strains to enable new chemicals and pathways at better costs. This is expensive and time-consuming, and often industry is reluctant to take it on. If they do develop a unique microbe, they will keep it strictly proprietary. Host onboarding should pick a small number of microbes that have very different properties, would access very different feedstocks or fermentation abilities, and are likely to be tractable genetically. Then develop them to a high TRL rating to make them really useful. The apparent lack of progress on the HObT website since 2021 and the lack of helpful information to the U.S. research community from HOD is a problem that must be addressed. Regardless, if further work on host onboarding is done, there must be funds allocated to bring the website up to date and make the tools developed useful to the public, or BETO can consider a lot of that work and money wasted.

- The HOD team has done a superb job of developing new tools for numerous nontraditional organisms. I view the decision to focus on improving the utility of a smaller number of strains (raise tier classification) at the expense of expanding the list of organisms as a positive. Unfortunately, dissemination of information related to these developments has been abysmal. Publications are a useful mechanism to disseminate knowledge and new capabilities; however, the ever-increasing number of journals and limited availability to private-sector scientists demands the ABF website be the principal means by which all ABF capabilities are advertised. The HOB team indicated that 15 hosts have been successfully onboarded, but the ABF website provides a list of 11 strains. The team presented the HObT database as a public-facing tool, indicating that the major Version 3.5.0 was recently released. This reviewer was unable to find a link to HObT on the ABF website. After an extended internet search that was only justified because I was aware it existed and was intent on finding it, I was not able to register to log into HObT. During the Peer Review, ABF management acknowledged that HObT was not released for public availability but would be made available soon. (As of May 6, 2023, registration to the site remains unavailable.) The lack of communication between ABF management and a task lead is disappointing. A low score for impact reflects the lack of availability of this tool.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback, some of which was responded to above for the "ABF Introduction and Overview"; "ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads"; "ABF Past Accomplishments – Industry Engagement, Outreach, and Management"; and "ABF Past Accomplishments – TEA/LCA" presentations. To clarify, the HOD team is not completely sunsetting work, but rather moving to an externally facing activity, where collaborative funding opportunities will be used as needed to onboard and develop hosts that are specifically needed for industrial or other partners. This will help to ensure that ABF resources are put toward the direct requests and needs of industry. The point is well taken that continued host development is important, and we will also strongly consider reinitiating internally driven host development to supplement the HOD efforts that are collaborative with industry.

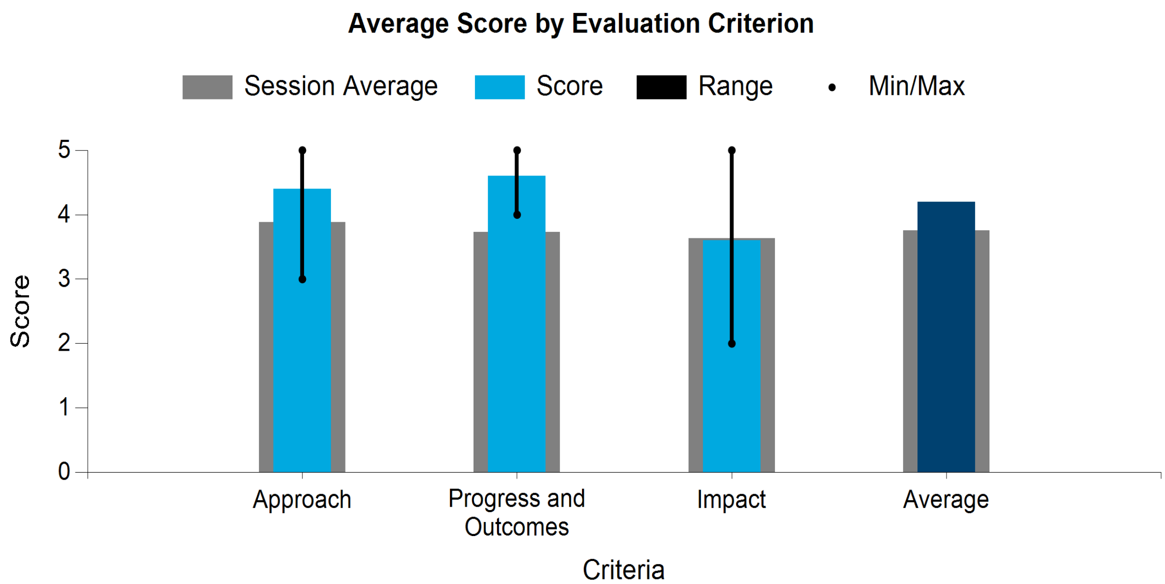
ABF PAST ACCOMPLISHMENTS – TEA/LCA

National Renewable Energy Laboratory and Argonne National Laboratory

PROJECT DESCRIPTION

WBS:	ABF4
Presenter(s):	Bruno Klein; Megan Krysiak; Thathiana Benavides
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

The Integrated Analysis task in the ABF conducts TEA and LCA to quantify the economics and environmental impacts of bioprocesses under development. The team from ANL and NREL develops TEA and LCA models of selected compound targets and hosts of interest to the ABF in an effort to provide an analysis-based foundation to the R&D. To date, the Integrated Analysis task has performed process modeling and analyses on multiple pairings of bioproducts and hosts, centered around major metabolic "beachheads" and "exemplar" molecules chosen for each of the metabolic pathways of interest. This presentation provides an overview of the approach used for TEA and LCA in the ABF and of the progress, outcomes, and impacts of TEA and LCA to support ABF goals, with a focus toward developing bio-based products that are both environmentally and economically viable.



COMMENTS

- TEA and LCA modeling is a core strength of the national labs and is of critical importance to the growth of the bioeconomy. There is a lack of information and data in the space that enables companies, from startups to Fortune 100s, to understand the likely costs of production for disparate products at a variety of production scales. As such, the ABF has a key role to play in sharing its expertise in LCA and TEA work to the industry to enable better research and commercialization decisions based on fundamental unit economics at scale. Unfortunately, the approach the ABF has taken with the TEA and LCA work limits its overall impact and undercuts its ability to be a driver for ABF outreach and success.

- The approach used by the ABF appears to champion model complexity and rigor over broader impact and applicability. Given the limited resources available at the ABF to support TEA and LCA work, it is logical to ask whether a more simplistic modeling paradigm that is nevertheless applicable to a wider set of molecules, and therefore impactful to a broader set of companies, would better serve industry. It appears that the current modeling approach suffers from false precision, wherein considerable model complexity provides a false belief in model accuracy and precision. In actuality, the TEA and LCA results have large uncertainty bounds. This is not a criticism of the results; TEA and LCA at TRL 2 to 4 require a broad set of assumptions, each with its own uncertainty, and results are always going to be approximate. The results presented appear to back this up: The contour plots for productivity and yield versus GHG emissions and cost are relatively simplistic, appearing as essentially a 1D reciprocal in the case of the GHG and a 2D reciprocal in the case of costs. This implies that a few key parameters govern the results, opening the door to simplifications. The question should thus be whether a significantly simpler model would provide similar precision in results, allowing for more output and impact with the same funding support. The use of AspenTech, for example, may not be necessary to calculate process variables and conditions when a simpler fundamentals-based technical model would suffice. If model simplifications and parameter stripping would have minimal impact on result quality, that would open the door to the ABF providing significantly more TEA and LCA for a variety of molecules and technologies with similar staffing and spend as today. This simplification may then allow further activities to demonstrate the validity of the model, including baselining off known and scaled production processes to determine model accuracy and precision in a more meaningful way.

- The TEA and LCA work would be more valuable if available to more companies, particularly in a stand-alone fashion. The ability to engage the ABF on a small-dollar, funds-in basis to perform a rapid LCA and TEA for a customer (with appropriate understanding of model uncertainties and potential errors) could provide the ABF with a beachhead market to approach industry, rapidly build credibility, establish relationships and trust, and enable follow-on projects to develop molecules and products when TEA results indicate a likely commercially viable product.
- Strengths:
    - Carrying out TEA/LCA for common beachhead/exemplar molecules is useful. The Integrated Analysis team reduced the scale of analyses by downselecting one exemplar per beachhead due to similarity between exemplars derived from the same beachhead. The approach has merits in covering a large number of molecules.
    - The Integrated Analysis team has made substantial progress on TEA/LCA. A total of eight different pathways were analyzed.
    - Analyzing the bioproduction from alternative pathways or in different microbial hosts can help industry choose the best bioprocess. These results are impactful.
- Weakness: It is not clear whether any TEA/LCA result from the Integrated Analysis team has been actually used by industry when developing their bioprocesses.
- Overall, the TEA and LCA work in the ABF, and offering these capabilities to the public and partners, is incredibly impactful. Most smaller companies or academic labs don’t have access or experience in these models, and it’s crucial to understand if a project is likely to succeed or fail (TEA), as well as the value to BETO and their goals for decarbonization (LCA). Beyond BETO, most companies in the synbio space are driven by a desire to improve their plant via some benefit like reduced energy or resource usage or less CO_2 emitted. The ability to partner with ABF to gain access to TEA and LCA capabilities is a powerful incentive. In addition, it’s important for more projects to have these analyses done to help inform BETO of projects more likely to succeed in advancing their goals.

- Often the trade-offs between yield and productivity are not understood and sometimes surprising. Having this information for the development teams to use is crucial to a successful project.
- Why the beachheads were not more adopted by industry partners is not clear, and could be due to a number of reasons (discussed elsewhere). However, the beachhead strategy in the old ABF model was well thought out from a TEA and LCA standpoint, and the targets made sense.
- The work in the presentation is well thought out, and it appears the TEA and LCA teams are well integrated into supporting the work of the ABF.
- LCAs/TEAs are a great way for the ABF to help advance the synbio industry. The national labs can conduct more thorough, well-informed, and robust analyses than many industry organizations have the bandwidth or in-house expertise to do. Examining the beachhead molecules in this manner was an insightful and productive endeavor. I think, however, that the impact of the TEA/LCA work by the ABF could be greatly increased if these models, instead of being put into an academic publication, were disseminated as an interactive web app that could be used by industry. This would allow users to change parameters based on their own supply chain costs and better understand when it may make sense to pursue biological alternatives for exemplar molecules that may be in their products. I think it also makes a lot of sense for the ABF to offer TEAs/LCAs as part of the work/services available for industry FOAs/DFOs.
- The TEA/LCA team provides strong support to ABF activities. Utilization of sensitivity analysis is a plus for situations where experimental data are not available. Is it possible for TEA/LCA to be proactively marketed to bioeconomy startups to provide critical economic assessment information for project planning, fundraising, etc.? After clicking through the Capabilities portion of the ABF website, I was never directed to a page that described TEA/LCA capabilities under Design, Build, Test, or Learn. When I searched "life cycle assessment," I found that if I scrolled down further on the Capabilities page, there was a link for Analysis Capabilities. It wasn't easy to find. Is it possible for the team to partner with IAB member organizations to refine and validate the ABF's TEA/LCA methodologies?

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback, some of which was responded to above for the "ABF Introduction and Overview"; "ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads"; "ABF Past Accomplishments – Industry Engagement, Outreach, and Management"; and "ABF Past Accomplishments – TEA/LCA" presentations. We agree there could be opportunities to apply a more broad-based approach toward process simulation in the future, while also recognizing the need of starting the effort with robust and well-informed models based on technical depth and rigor to establish a self-consistent foundation in the framework. In general, we have received feedback from the IAB and from other external stakeholders that reports and models/tools published by our teams have been well received and found good traction in guiding their own decisions and directions, particularly for longer-established projects that have had more opportunity for dissemination by length of time in the public domain (from which key pieces of model frameworks have been leveraged for Integrated Analysis activities in the ABF). One example is the Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET) model (a publicly available LCA tool that is used to provide a transparent and harmonized framework across feedstocks, pretreatment options, and conversion technologies to products), which has been leveraged in the consortium to provide environmental impacts of the bioconversion routes of interest.
- The rigorous approach toward TEA/LCA by the Integrated Analysis task has been acknowledged by the board of reviewers, as well as the fact that this approach has been successfully applied to set the stage in covering a broad space across eight different biomolecules. This feedback will be taken into

consideration in working to create reduced and more flexible models leveraging the work we have conducted in prior years. These models can allow for an in-depth probing of more process-relevant metrics for the downselected fuels and products of interest to the consortium, as they will focus on the aerobic production of different molecules and their respective downstream processes (although preliminary assessments point to the main economic and environmental drivers of the process being the same in either reduced or larger models). In the upcoming project cycle, the aspect of using TEA/LCA results as guidelines will be intensified, as the consortium will aim at transferring ABF technologies to the industry. The TEA/LCA team plans to further engage with partners and adapt our analysis to the needs of each technology/pathway, aiming at both providing recommendations toward goals for emissions reductions and cost viability and validating process simulation results.

- Regarding the visibility of TEA/LCA on the website, we will evaluate how we can rearrange our menus to make this information easier to find and accessible from multiple locations on the website. ABF's TEA and LCA capabilities have not been widely called upon by the DOE-funded projects that have moved forward in DFOs. While multiple groups have referenced TEA and LCA as part of the proposal's activities, they have more often than not chosen to perform these assessments internally, as part of their cost share, rather than including related tasks in the CRADA scope of work. One successful DFO proposal is utilizing TEA/LCA capabilities as part of the ABF's scope. But perhaps the reviewer is pointing to a need for the ABF to develop a broader and more thorough understanding of how ABF collaborative research is informing its partners' decision-making processes, both in the near term and long term. Be it through formal assessments like TEA and LCA or through other types of analyses, the ABF is keen to work with its partners and its advisory board to collect and use informative, impact-related data, and based on those data, augment the ABF's value proposition.

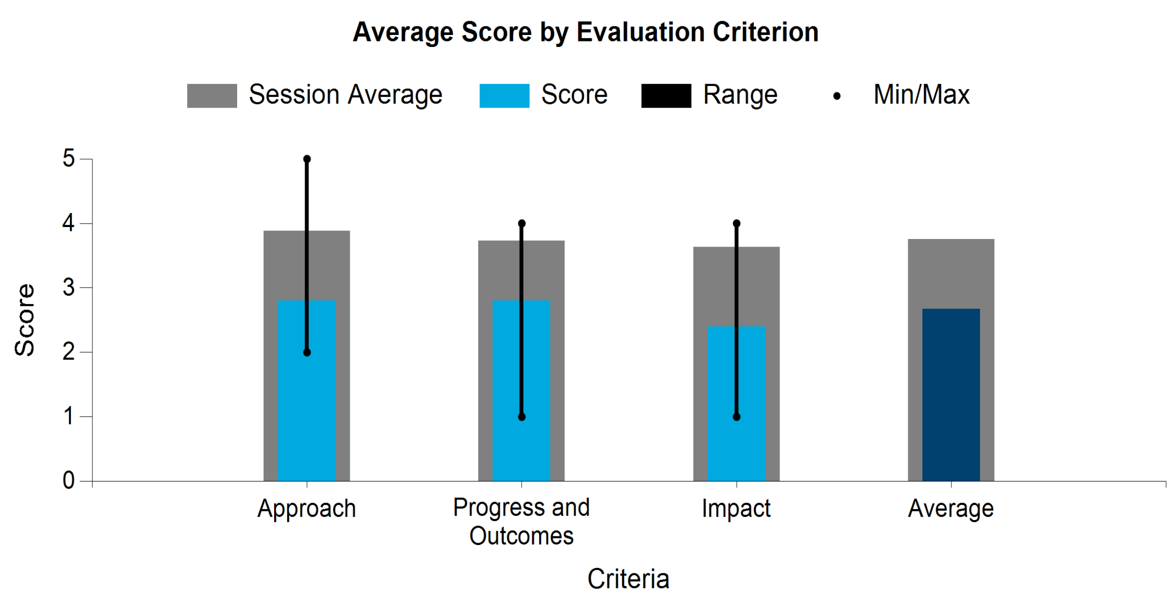
ABF PAST ACCOMPLISHMENTS – INDUSTRY ENGAGEMENT, OUTREACH, AND MANAGEMENT

National Renewable Energy Laboratory, Argonne National Laboratory, and Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	ABF5
Presenter(s):	Christopher Johnson; Emily Nelson; Megan Krysiak; Phil Laible
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

To develop infrastructure to support industrial biotechnology, an understanding of the needs of the industry is critical. As such, the ABF Industry Engagement and Outreach (IEO) team organizes and facilitates interactions with industry, providing feedback from the stakeholders that supports decision-making and project planning. Their activities also aim to increase the visibility of the ABF and attract collaborators from academic and industrial communities. These goals are accomplished through the workings of three highly interwoven, strategic focus areas: Assessment, Outreach, and Interactions. Overall, the IEO task contributes to the alignment of ABF activities with BETO's milestones and facilitates communication of the ABF value proposition to key stakeholders in industry, R&D organizations, and the public. The ABF management team's objective is to organize project management and project management infrastructure, develop internal and external communications, and provide deliverables to BETO. These activities apply to both the core project, with specific scopes of work described for each lab, and the collaboration projects, for which scopes of work are agreed with successful applicants to the ABF funding opportunity program. Management will coordinate with BETO leadership (to the extent possible) on new opportunities (e.g., DFOs, FOAs) and interactions with other federal agencies (e.g., NSF) to access ABF capabilities.



COMMENTS

- Though the overview and goals related to industry outreach that were articulated by the ABF have resonance, including facilitating tech transfer to industry, educating partners on ABF capabilities, and generating data on industry needs and shortcomings, the approach that the ABF has taken to achieving these goals is lacking. ABF's work in industry engagement and outreach appears poorly organized and lacking in coordination. An IAB meets irregularly, with poor meeting planning and goal setting for the group. The "Annual Industry Days" do not appear to provide the ABF with significant inbound funds-in project interest or useful feedback on the direction of the ABF, capability needs, or strategy. The ABF could not document successful examples of tech transfer out of the ABF to industry that resulted in commercial success.

- The root of the failures in industrial outreach may stem from a lack of interest on the part of the ABF to truly engage with industry, learn their needs, and adopt programs and tools for industry use. This is evidenced by the fact that many of the touted ABF outreach "successes" of the last funding cycle are nonfunctional: Its HObT host database is not open to outside users and isn't listed on the ABF website, the website itself lacks detailed information on capabilities, the ABF only appears to track social media "follows" instead of more useful indicators such as interactions or clickthroughs, etc. The ABF was unable to articulate a clear definition for what "industry" means and did not appear to have any organized industry segments. The needs of startups and Fortune 100s are different and likely need different outreach strategies. Another approach still is needed for peripheral industry participants, such as feedstock suppliers or consumer packaged goods companies. At Year 8 of the program, it is disappointing that there are not well-defined outreach strategies for each group. The overall impression is that the ABF appears more focused on developing its capabilities based on the research interests and specialties of the various PIs that make up the ABF consortium. While it's possible that these interests may in fact align with industry needs, the lack of a functional feedback loop with industry leaves the ABF at considerable risk of drifting from core industry needs, undermining its stated mission.

- The future hire of a dedicated business development manager is a welcome sign that the ABF understands many of these shortcomings; however, this hire alone will be insufficient to improve industrial outreach activities without buy-in from the various PIs at the ABF. To achieve success, the ABF needs to fully define its role; as of now, the ABF talks of serving industry but primarily functions as a science-doing enterprise. The ABF, however, is not just another FOA recipient, and therefore needs to reimagine itself as an enabling platform for industry. As such, its industry outreach activities should be driving decisions on budgets, capability development, and which tools to be retired due to lack of interest. Outreach should be occurring in some form on a daily basis, with regular contact and readouts with key decision makers at the ABF. IAB(s) should be engaged and involved in setting goals and strategy.

- I am sympathetic to the challenge of creating an industry-centric organization within the confines of the national labs. Difficulties in aligning the IP goals of the various national labs with industry requirements and streamlining contracting processes hamper industry engagements and will continue to act as headwinds on the ABF in the future without change and reform. Happily, the success of BOTTLE and the ABPDU to engage industrial parties with pre-negotiated IP arrangements provides a workable template for the ABF to emulate.

- Strengths:

    - The IEO team has made multiple efforts to improve the awareness of ABF technologies to industry and the broader society.

    - There are rapid increases in the report of ABF activities in social media that promote ABF's presence and technology.

    - Having the IAB is beneficial to the ABF.

  - The team has been updating the ABF's website with its newest technologies and capabilities.

- Weakness/area for improvement: The assessments from one-to-one interactions have provided valuable information from industry's perspective. It is not clear how the ABF used the assessment results to improve their activities.

- This review is focused specifically on "Industry Engagement, Outreach, and Management." A general review of the past goals and accomplishments of the ABF was given in the "ABF Introduction and Overview" session. This part of the ABF acknowledged that "efforts delocalized in early years of the foundry" and "activities refocused and expanded with increased budget in rescoping exercise." It's good to see the honest reflection at the start. Despite renewed focus and money midway through, it's clear the strategy to really connect with industry can still be much improved. Beachheads were not widely adopted by industry. Overall it seems to have either not been of interest to much of industry, or it was not advertised to industry well, or both. It's not clear which is the case.

- The new plan to adopt a professional business outreach person for the ABF is an excellent idea, based on the BOTTLE consortium model. Also, the website for the ABF needs significant upgrading. This will help attract industry awareness and help them understand what capabilities are offered. Many of the slides in various presentations have really clear graphics and easy-to-understand visualizations of the tools and capabilities offered by the ABF. These slides are way better at communicating what the ABF has to offer than all the text on the ABF website. I would not worry if some of these activities are not being actively supported in the new strategic plan. The ABF said that if a company wanted to use some of that infrastructure, then those capabilities would be used and further developed, so there should be no issue with advertising them. It's good that the beachhead slide is finally up on the website, but it's really buried, hard to find, and not at all obvious to industry or someone looking at the site to know that the ABF has developed these beachheads. I only found it by clicking through host onboarding capability. Is the semiautomated combinatorial media pipeline even mentioned on the ABF website anywhere? I tried clicking around and couldn't find it.

- There was a lot of discussion during the review days and internally among the reviewers about the structure of IP and how the way IP, CRADAs, and contracting is a barrier to industry engagement. The ABPDU said they can contract in a few weeks. The BOTTLE consortium has worked out streamlined IP for faster contracting (not needing every national lab to review and sign off on it) and clear IP levels for different amounts of industry funding versus exclusive rights. Clearly these are things the ABF can learn from and copy. For the current plan, it's going to be very challenging to achieve a significant increase in industry money into the ABF in the near future, especially if contracting takes a year. It will take time to get to >50% of the ABF's budget committed to external partnerships and reach an average of more than fivefold oversubscription for the ABF's funding opportunities.

- The management structure of the ABF probably significantly contributed to the lack of a cohesive IP plan. It lacked a single point of accountability (someone full time in charge) who would take on streamlining IP, or making sure it got done. One of my recommendations to BETO (shared by the review panel) is to change the proposed management structure to have a lead PI be solely accountable and responsible for running the ABF. There should not be any decision by committee. The current plan has a lead PI and executive committee in the same box. That is still a committee. The ABF needs a 100% dedicated full-time employee running it. This person should be an "outsider" with no emotional connection to the past 6 years of the ABF. The executive committee reports to and advises the ABF PI, but does not make decisions. It's clear that the ABF has really suffered from decision by committee and a lack of someone whose job is 100% running the ABF.

- Most scores were moderate or low for judging impact because there was a balance of very low scores and some high scores. Low scores because (1) industry outreach and engagement could be significantly better for the ABF and (2) management structure was not sufficient to lead the ABF to success. High scores for overall a lot of solid work advancing synthetic biology and delivering on several projects that advance U.S. capabilities and advancing industry to be impactful. Also good plans for addressing DEI.
- The industry engagement component of the ABF overall appears ad hoc and infrequent. The IAB does not appear to be well engaged (several of the listed companies do not have active members in the IAB currently). There was no summary provided of the kind of interactions that the ABF has with the IAB, what support have they provided, the lessons learned, and how the ABF has incorporated feedback. I also find it odd that the ABF does not share or consolidate the information from industry interviews and engagements into some kind of road map that outlines the challenges, pain points, gaps, etc. in the synthetic biology space. That kind of product could actually be quite helpful for the industry and would also help the ABF guide its effort in a more strategic manner. A gaps analysis is mentioned in the milestone table, but there were no details on this in the slide decks or during Peer Review. Going forward, I do agree that the IAB should be diversified quite a bit to include industries that may not use synbio much currently but that could benefit from transitioning toward biological solutions. The ABF could play a key role in understanding and addressing the needs and wants of those companies and helping to move them toward biological alternatives.
- The management of the ABF seems okay. However, given that the management structure is changing, I would and did recommend that the ABF have a full-time or nearly full-time lead to coordinate ABF efforts and ensure that changes are implemented efficiently and that industry is routinely engaged.
- IEO efforts are falling short of what is needed for the ABF to thrive in the role of sought-after partner to industry. A lead individual is assigned to each goal. Outreach, interaction, assessment, and an appropriate list of activities for each are provided. Lack of business development and marketing experience is recognized as a risk, but management should be more aggressive about remedying the situation quickly if ABF partnership goals are to be achieved. Outreach materials do not provide the level of information and detail needed to attract the number or quality of partnerships that are the goal. For example, the website categories of “Capabilities” and “News” should provide information and examples so that bioeconomy organizations immediately recognize the ways in which the ABF can assist them in solving their own challenges. Direct feedback from current and former IAB members to peer reviewers would be beneficial for future reviews. Two risks related to management inefficiencies caused by the distributed model and slow execution resulting from consensus-style management are not given the appropriate level of attention. These risks are not being managed effectively. Regarding the distributed model, the question is not “Is all the work getting done?” but “Could all the work be completed with fewer resources to make some available for additional activities?” Consensus-style management adds a second layer of inefficiency to the current ABF model. The executive committee consists of a group of talented, creative, and effective scientists. The goal should be a management team of effective, decisive managers.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback, some of which was responded to above for the “ABF Introduction and Overview” and “ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads” presentations. Regarding ABF contracting timelines and IP licensing and how these activities compare across the ABF, ABPDU, and BOTTLE: First, there are multiple strategies and process improvements we are pursuing to improve the ABF’s contracting timeline. Among them are automated document production, designated workflow ownership for document processing, possible elimination of CRADA usage requirements for non-practicing institutions, greater oversight from ABF management as a function of expansion of management full-time employees, and perhaps more effective relationships with the DOE site offices at each of the ABF labs. However, the reviewer offers both a false comparison between ABF and ABPDU contracting mechanisms and a slightly incorrect timeline for ABPDU contracting. Many of the ABPDU's external collaborations with industry utilize the funds-in (self-paid), strategic partnership project mechanism for contracting, which takes about 3 months to complete. The ABPDU can often turn to the strategic partnership project because there is less expectation of new IP to arise from the research. This stands in contrast to the ABF's research, where companies and institutions are relying on federal dollars to fuel new innovations. The funding source and scope of work usually results in the requirement for a multi-lab CRADA. The BOTTLE model is also quite different and is serving as an example for the ABF moving forward, as the ABF seeks to adopt more activities similar to BOTTLE, such as moving to the all-funds-in, large-company focus, as well as the nature of the materials, technologies, and objectives of the consortium. All that said, however, the ABF does acknowledge that there is likely much that can be learned from both the ABPDU and BOTTLE. As the ABF's business development activities continue to expand and diversify, the group is evaluating all of the available contracting models and all of the ways in which to collapse the contracting timeline. IP licensing outcomes and increased contracting speed will be key performance indicators for these processes. Due to time constraints, we were unable to present many details that might have been helpful to the reviewers related to how industry engagement, outreach, and management interact to respond to feedback received in one-on-one interviews, industry days, meetings with the IAB, and forums for industry interaction.

- We agree that the ABF needs to be more responsive to industrial needs in order to have impact and are working toward strategies to address this need. As such, and as mentioned in this presentation and elsewhere, the ABF plans to hire a dedicated business development co-lead, who we envision will work closely with the IEO and management teams to increase and improve our ability to identify and respond to industrial needs and partnering opportunities. We believe this could represent a step change with respect to the ABF's industrial impact and overall direction. Another important pivot on the horizon is a movement toward 50% of the ABF's funding being allocated for industrial partnerships in the form of funding opportunity projects and other partnerships. Industrial responsiveness is intrinsic to the projects, and an increase in their funding should promote greater industrial impact.

- Regarding the ABF website, we have continued to update the website each year and agree that more work can be done to improve it, particularly to make it more relevant to industry in ways the ABF can help them and to provide more detailed information on the ABF's capabilities. We will continue to evaluate how the website can be improved and to make sure all relevant information and capabilities are represented. The IEO team does track detailed analytics on social media interactions, impressions, link clicks, comments, shares, and more on a monthly basis. However, given the time constraint, we were unfortunately unable to present this level of detailed information. In response to comments and concerns about using the IAB of the ABF as effectively as possible, a prominent component of the restructuring exercise and ongoing discussions between industry engagement efforts and BETO management (and, in the future, ABF business development) is to better define the roles and goals of having an advisory board for the ABF and tailoring interactions and utilization efforts of the board for these outcomes. We welcome these changes and improved interactions, as they will be needed as industrial collaborations and new types of partnerships intensify. As discussed above, moving forward, the ABF PI will have more authority (backed by BETO) and decision-making ability. While this change will be beneficial in many ways, even an omnipotent ABF dictator would not singly be capable of addressing the contracting challenges faced by the ABF, an issue much larger than the consortium itself. The ABF disagrees that the PI should be an "outsider" with no past connection to the ABF. The ABF, including its PI, is prepared for and supportive of making substantial changes, as illustrated by the strategic re-envisioning of the ABF and its implementation thereof.

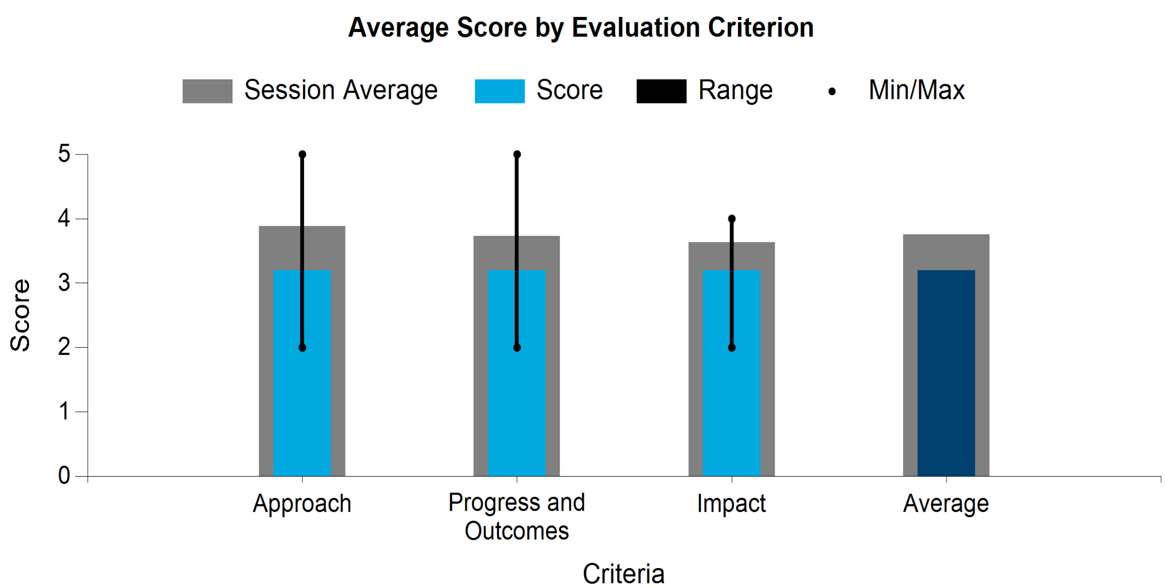
ABF – LESSONS LEARNED AND INTRODUCTION TO FUTURE PLANS

Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	ABF6
Presenter(s):	Katy Christiansen; Nathan Hillson
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

In June 2022, the ABF presented to BETO its concept for operations in FY 2023–2025. This presentation included a section dedicated to "Lessons Learned from Past Years." In September 2022, BETO instructed the ABF to do strategic planning, including directives to create a "Reviewing History" working group to assess what worked well and what did not work well historically. The relevance of this activity is that it ensures that the ABF's future plans are made wisely. Top potential challenges include applying lessons learned in a nuanced fashion, overcoming the temptation to maintain the status quo, and applying consensus-driven lessons learned equitably. The outcomes of this activity include the gathering of lessons learned over the past 7 years of ABF operations, along with the outcomes of the "Reviewing History" working group, which for example includes ranked lists of what did and what did not work well historically for the ABF. These lessons learned have been applied to the ABF's strategic and implementation planning processes. At the end of the presentation, a brief introduction to the ABF's future plans is provided.



COMMENTS

- The ABF utilized multiple presentations to document their journey in developing a new strategic plan for the next funding cycle. These presentations grew off each other, and as a result, it is difficult to separate them as required in this review process. Instead, I will use this space to specifically speak to the "lessons learned" portion of the presentation and the process through which the ABF conducted its strategic planning process. A review of the new strategic plan can be found in the review of later presentation materials.

- The ABF has found itself after its initial 8 years facing an identity crisis, stuck between an apparent desire on the part of the ABF to essentially maintain status quo activities and the desires of BETO to drive to activities that more clearly demonstrate impact and results. This is not to say that ABF personnel do not understand or recognize the failures of the organization in the past or the difficulties with which impact can be measured based on its prior goals and strategies. However, the implicit message throughout the lessons learned presentation was that BETO was imposing a new strategic direction upon the ABF, and that the ABF did not wholly agree with the new approach. This is unfortunate. Whether the ABF is at fault for past activities failing to align with BETO priorities or whether BETO has changed its priorities on the ABF and unfairly moved goalposts is not particularly relevant at this stage; what matters is that the success of the ABF and the ABF's position in BETO's success is undermined when trust between the organizations is damaged by a misalignment between the goals and ideas of leadership. The apparent breakdown of trust that has occurred in this instance is concerning and appears to have negatively impacted the ability of ABF leadership and BETO to collectively work together to find a strategic direction of interest to BETO and ABF PIs.

- The level of engagement between the ABF and BETO during the strategic review process is not clear; however, the indications from the presentation provided paint a picture wherein the ABF circled the wagons during their strategic review process, to the detriment of that process and the resulting plan. It is clear from the materials BETO prepared that their goal was to ensure that the funds spent through the ABF were impactful and could be readily connected back to commercial deployments and successes. The ABF's approach through the strategic review therefore should have been to focus on the components of its portfolio most likely to achieve such impact. Instead, the ABF appears to have taken a narrower approach, focusing on strategies to respond to the details of the criticisms (measurability of goals and demonstration of commercially relevant molecules) instead of engaging in a more thorough examination of the activities likely to drive impact. There are certainly important questions that the ABF sought to work through during their strategic planning exercise: How to protect the "core" that has been built over 6 years from atrophying? How to demonstrate the value of their tools? How best to demonstrate commercial interest and traction? The problem is that the ABF seems to have failed to recognize that industry is a key partner in answering those questions and ensuring the resulting plan was most likely to achieve impact; their voice should have been instrumental in guiding strategy for a future ABF more responsive to industry needs.

- The way the ABF is managed and run is part of the issue. The ABF is primarily governed by a set of national lab PIs, and no one PI appears to have the buy-in of the others to make critical decisions on behalf of the whole. None of these PIs spends a majority of their work hours on the ABF, resulting in a distracted and misaligned governing group that makes a focused strategic planning process that much more difficult. The ABF would benefit from a senior leader who spends a large majority of their time on the ABF specifically and who has the trust of BETO and the other PIs to make key strategic decisions on behalf of the whole. Similar to a CEO acting on behalf of a board, this person should oversee the day-to-day operations of the ABF and set strategy and goals, for eventual approval by the governing body (PIs, BETO, or some combination thereof) at regular intervals. A streamlined governance structure could do much to help the ABF overcome some of the institutional inertias and blind spots that seem to have tripped up the ABF in this most recent strategic planning cycle.

- Strengths:

    - The ABF's past lessons learned is an effective approach that has allowed the ABF to learn from multiple issues associated with previous technical goals, methods, and management. Changes were proposed to address these issues.

  - The shift of metrics from TRY improvements to focus on TEA and GHG emissions makes sense. TRY metrics alone cannot inform industrial success and societal impact. Using TEA and GHG emissions as metrics will allow the ABF to better focus their efforts on promoting the biomanufacturing industry and better align them with BETO's missions.

- Weakness/area for improvement: Accurately tracking DBTL cycles and comparing DBTL times with and without ABF technologies is indeed challenging. For the past 7 years, the ABF has been proposing to use these metrics to evaluate their success. It is unfortunate that such a challenge was only realized after 7 years of ABF activities. So far, the new metric makes sense. This also serves as a warning to the ABF to constantly practice the "past lessons learned" activity to evaluate the new metrics.

- The numbers reflect a review of the past ABF goals, metrics, accomplishments, and impacts. Same as given in the ABF introduction and overview.

- Some specific comments on the slide deck in this presentation are below.

- It's clear that the DBTL cycle time metrics were not going to be met and were not being captured in the ABF in order for them to meet their milestone goals. On Slide 10, the team lays out the arguments for why DBTL was hard to capture and why it was not as relevant to tracking progress. The latter argument has merit, and focusing on impact factors such as TEA and GHG reduction are more aligned with BETO's mission. That being said, it really should not have been impossible to come up with a way to track DBTL. Slide 10 says DBTL failed to capture other useful metrics showing progress like sample throughput, resource intensity, and number of cycles needed [to learn]. That is all part of DBTL, and improvements on those metrics should lead to a reduction in DBTL cycle time. Moving forward, the metrics in the new strategic plan are mostly easier to quantify, and the ABF should be able to track progress toward them.

- Moving away from beachheads to only molecules "directly of interest to industry via industry partnerships" [except the molecules being developed in the core activities] is a good idea. The beachheads were not engaging industry, and the TEA/LCA for them was difficult to assess.

- The new appraisal framework for host selection and prioritization is a good compromise to breadth and depth and should continue in the next 3 years (we were told in the meetings that all HOD work had been cut in the final budget).

- Bioprocess round robins: Tech transfer is difficult, and "everything matters" when trying to reproduce a fermentation or manufacturing campaign at a different site. The process of doing the tech transfer is often very helpful to understand the baseline system. Seems like the ABF is learning that. This will be helpful when transferring processes from a national lab back to an industrial partner. However, I also caution the ABF to do the minimal piloting and scale-up work required to meet their goals or partner goals, and to work with BioMADE to do more work on scale-up.

- Slides from the ABF seem to indicate good engagement with the IAB. Feedback from the advisory board is that they feel like an afterthought and the ABF does not come fully prepared to discuss matters, and the fact that the industry board was only asked to participate in the new strategic plan at the very end to review once all the decisions had been made shows the ABF does not engage effectively with the IAB. This needs to be addressed in the next 3 years.

- Ideas on how to improve the IP and CRADA negotiations are mentioned many times in other places in this review.

- Some of the lessons/analyses they presented seemed poorly suited for having learned the “right lessons.” For instance, their lessons learned regarding IAB use largely focused on meeting format as opposed to actually requesting feedback from the IAB on the work that the ABF had done and how to do it better. I think better engaging with the IAB is important, but I’m concerned that this is the lesson that was shared here, especially when it was also clear that the IAB was not engaged in the strategic replanning that occurred. Listing a future function of the IAB to give postdoc industry panels is also a poor use of the IAB. The slide on host onboarding decisions is not at all clear. What was actually learned about which host should be elevated, as well as which should not be? Are there any clear signals from industry on promising hosts that could unlock new frontiers if upgraded to Tier 4? Or completely novel hosts that should be onboarded, at least at Tier 1 or 2, because then industry could take it from there? There is not any “lesson” presented on how to prioritize organism onboarding in a strategic manner. Shifting from purely TRY metrics to parameters that are informed by TEAs/LCAs is a good lesson learned in my opinion. It was also great to see that they were able to improve their CRADA processing time, though it is still very long. The purpose and selection criteria behind the Miro poll results presented were not at all clear. Were votes limited by person? Where things that rated low in the “didn't work well” category deemed successes or failures? Why were none of the “things that worked well” deemed worthy of discussion? The approach here is quite messy and lacks actionability.

- Scores for this presentation were not meaningful, resulting in a selection of 3 on all counts. The ABF’s willingness to undertake a strategic re-envisioning process reflects positively on the organization’s desire to be a forward-moving, relevant participant in the growth of the bioeconomy. There is no doubt significant progress on all scientific fronts has been made over the history of the ABF. Two acknowledged challenges will be highlighted. Regarding the temptation to maintain the status quo, I fear the ABF may fall prey to avoiding meaningful, though perhaps painful, decisions. Second, applying consensus-driven lessons learned equitably highlights the danger of consensus-driven management. Whether a strategy/activity/tool is effective should not be subject to agreement of all parties. The strategy/activity/tool is effective if it provides value. Did it result in meaningful improvements in ABF research (rate of discovery, TRY improvements, etc.)? Were partners enthusiastic to use it? Did it draw potential partners to the ABF? I also find the following comment troublesome: “without disproportionately adversely affecting a small demographic.” Nobody has an established right to participate in the ABF. If some demographic big or small is not contributing to the ABF mission, then the unfortunate reality is that piece must be removed for the good of the organization. The Miro-assisted self-assessment provided some curious information. When asked “What is working well?” top performers (tool development, multi-omic capabilities, multiscale processes, and pathway development) received 8 or 9 votes, but organizational culture (3), teamwork (0), and strong collaborative relationships within the ABF (0) scored very low. When questioned, lab leaders expressed their fealty to the distributed model. Is it possible that lab leaders, with more time available for inter-lab communication, feel a strong sense of collaboration and teamwork, but that task-oriented scientists/engineers/administrative staff lack a similar sense of teamwork?

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback, some of which was responded to above for the “ABF Introduction and Overview”; “ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads”; “ABF Past Accomplishments – Industry Engagement, Outreach, and Management”; “ABF Past Accomplishments – TEA/LCA”; “ABF Past Accomplishments – Host Onboarding and Development”; and “ABF Past Accomplishments – Process Integration and Scale-Up” presentations. The ABF and BETO had extensive and intensive interactions during the ABF’s recent strategic planning and implementation planning activities. The ABF team is committed to its new direction, which will support BETO in achieving its ambitious 2030 decarbonization goals. We agree that industry, as a key stakeholder and beneficiary, should inform how the ABF evolves and prioritizes its activities. We did provide our strategic plan to our IAB for their feedback, and we did receive some responses. Our choices of SAF and biochemical targets will be informed by industry feedback (as part of go/no-go milestones at the end of FY 2023).

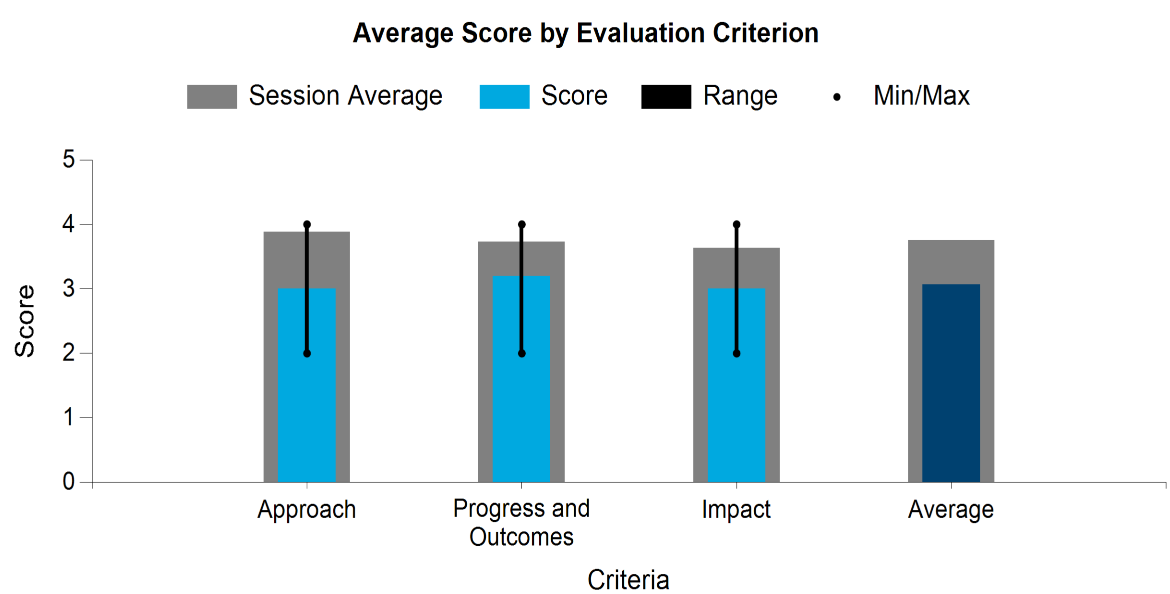
ABF FUTURE STRATEGY – STRATEGIC PLAN

Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	ABF8
Presenter(s):	Katy Christiansen; Nathan Hillson
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

In September 2022, BETO instructed the ABF to do strategic planning, including guidance regarding the process. In December 2022, the ABF completed its strategic plan. The relevance of this activity is that it ensures that the new ABF strategic plan is timely and well aligned with BETO's goals. The impacts of this activity include the genesis of a reimagined DOE ABF and the progression into the ABF implementation planning process. Top challenges included contrasting planning process preferences across the ABF national labs, overcoming the temptation to maintain the status quo, and that any reorganization can jeopardize an individual or team's sense of belonging. The outcome is that the ABF developed a strategic plan, using an inclusive and transparent process, that follows BETO's guidance and provides a compelling and implementable path forward. This presentation focuses on the new vision and mission statements, identified strategies, and updated organization chart. The next presentation will focus on the selected goals and FY 2025 deliverables for each strategy.



COMMENTS

- The ABF has found itself after its initial 8 years facing an identity crisis, stuck between an apparent desire on the part of the ABF to essentially maintain status quo activities and the desires of BETO to drive to activities that more clearly demonstrate impact and results. This is not to say that ABF personnel do not understand or recognize the failures of the organization in the past or the difficulties with which impact can be measured based on its prior goals and strategies. However, the implicit message throughout the strategic planning presentations was that BETO was imposing a new strategic direction upon the ABF, and that the ABF did not wholly agree in the new approach. This is unfortunate. Whether the ABF is at fault for past activities failing to align with BETO priorities or whether BETO has changed its priorities on the ABF and unfairly moved goalposts is not particularly relevant at this stage. What matters is that the success of the ABF and the ABF's position in BETO's success is undermined when trust between the organizations is damaged by a misalignment between the goals and ideas of leadership. The apparent breakdown of trust that has occurred in this instance is concerning and appears to have negatively impacted the ability of ABF leadership and BETO to collectively work together to find a strategic direction of interest to BETO and ABF PIs.

- The ABF's updated strategic plan suffers as a result. The plan falls short in identifying relevant goals and measurable targets to demonstrate achievement of its mission. The ABF appears to be inhibited by an unworkable governance structure that lacks empowered leadership or individual accountability. As presently constructed, the ABF appears to operate as a consensus coalition of PIs at national labs, each with individual research interests and budgetary needs. Prior to the most recent budgetary cycle, no one PI within the ABF had visibility into the actual spend at the other partner labs, a worrying indicator that no one person is empowered to ensure the success of the ABF's mission. Further, the PIs that drive ABF work at each lab are only able to allocate a minority subset of their time to ABF activities. Although this is standard practice within the national labs, the result is that no one person wakes up every morning and goes to sleep every night thinking about the ABF. At best, this seems to have resulted in a sort of institutional inertia where no one individual is fully empowered to take responsibility for the organization as a whole. At worst, the sometimes competing research interests and budgetary needs of each lab have led to a lack of institutional direction. ABF leadership seems to have an understanding of this dynamic; the continued references during the review that BETO oversight was driving changes to strategy implied that the changes were unwanted and that self-reflection at the ABF was not possible without an external forcing function. In developing this new strategic plan, the ABF betrayed a lack of ownership of their future direction by at times seeking to shift responsibility for potential future shortcomings to BETO.

- The ABF is filled with considerable potential, has done and continues to do good science, and has built unique capabilities. At issue is the tension between a view that the ABF should be primarily a research organization driving science in response to the research interests of the various scientists who work and interact with the ABF, and a view that the ABF is meant to be a platform upon which government funds can be best leveraged to enable industry to innovate faster and better. This tension is apparent in both ABF talking points and BETO talking points as well, and the identity crisis resulting from the inconsistent messaging is holding the ABF back. To best achieve the impact that BETO seems to be driving toward, the ABF needs to reimagine its role in the ecosystem as one of service provider, talking in the language of clients and customers. Validation and proof of impact will come from the level of interest received by industry in ABF services, as well as the level of cash-in support that the ABF can achieve. Focusing on tool benchmarking or internal research projects risks missing the market. In order to successfully pivot to a customer-centric role, the ABF will likely require a change in organizational structure to one that revolves around a single PI who is aligned in vision with BETO, empowered to make decisions, and lacks distractions: They should spend a majority of their time on ABF activities. This will free the ABF to better confront its operational challenges and engage in self-reflection based on industry feedback. Perhaps seven labs aren't needed to drive the ABF's vision, or perhaps some labs don't have tools and capabilities valued by the market. The ABF must be in a position to engage in this difficult self-reflection and make hard choices around the use of its limited funds.

- A key first task for the ABF should be seeking a reset in industry engagement. It is unclear to this reviewer whether the goals and approaches articulated by the ABF for this new strategic plan have any connection with the needs of industry, or are tethered to capabilities that are in need within the market. The ABF has a difficult task as an organization that focuses on TRL 2–4; in general, such early-stage work is often too risky and commercially disconnected for industry to pay major attention, and yet the needs and wants of industry are critical in deciding which platform technologies and capabilities to develop to support the technologies that will have industrial applications in a few years' time. In response to this tension, the ABF currently engages in internal need-finding to make decisions around which areas to focus funding, but without industrial feedback and engagement, there is significant risk that these choices are academic in nature and lack commercial viability or interest. Tools to pull in industry feedback are currently unused or underused. The ABF has an IAB that it engages with on an irregular basis and does not seek material input from on key decisions or strategies, including this latest strategic plan. The support of large industrials, such as Boeing, was championed at points; however, that outreach did not appear to be part of any coordinated, deliberate outreach strategy to engage industrial players, gather feedback, and respond to the industry needs. A dramatic rethinking of the ABF's engagement with industry will set the stage for further changes and realignments that will best position the ABF for impact.

- A rethinking of the budget mix in the latest strategic plan should go hand in hand with this new focus on industrial engagement. It made sense for the ABF to spend 75% of its budget on AOP activities while it grew its toolbox and capabilities. At this point in its life cycle, that split no longer makes sense, and a majority of funds should be directed toward industry through DFOs to ensure that the tools developed by the ABF are of use to industry. Some internal capabilities may not garner industrial interest; that may be a sign that they are not industrially relevant or competitive against alternatives. This engagement will help drive further decisions on where to focus limited AOP cash, which capabilities to support and which to discard, and which innovations to invest in. The ABPDU provides a guide for the type of industry outreach and service that the ABF can achieve.
- Similarly, it is reasonable for the ABF to try to identify likely molecular targets of commercial interest, including SAF and the specific biochemicals of interest (muconate and 3-HP). However, the goal of driving significant progress on four targets should be built around commercial engagement. A key refrain heard during the presentation was that "industry engagement is based on capabilities, not products," a statement that does not match with the "four core products" focus of the new strategic plan. Although it appears the idea is to use the four products as a mechanism to show the value of the ABF, the described goals in the "go/no-go" reviews are qualitative at best and risk becoming a confirmation of the PIs' priors. Industry engagement can once again help ensure the best utilization of resources and avoid confirmation biases within the team. By pushing for four targets developed through DFOs instead of using AOP funds, the ABF can seek industrial partners for its four target molecules and further solicit proposals for other products and pathways. Through a competitive process with industry, the ABF will be better positioned to identify the four targets with the highest probability of commercial applicability and likelihood of success, multiplying impact. SAF may prove to be a poor target for ABF activities given the long history of failures utilizing synbio techniques for fuels production. Four might not even be the right number. If four targets are desired, it is highly unlikely that the ABF will see success in all targets chosen, and other potential molecules of interest should be considered to provide for attrition of targets and eventual downselect at a later time as progress is made.
- Benchmarking, which was brought up through the strategic plan as a mechanism to prove impact, should be deprioritized or removed altogether, as it likely does not represent a good use of resources. Other metrics, primarily commercial interest and funds-in support, will implicitly demonstrate the value of the ABF vis-à-vis alternatives. The tool capabilities doesn't mention TEA; however, it was noted that TEA drove decisions presented elsewhere in the presentations, a core disconnect. TEA and LCA work is something the ABF has and can continue to build a strong capability in, one that is readily applicable to industry and can be rapidly deployed through funds-in contracts on a small-dollars basis to gain initial traction with industrial partners and establish working relationships. IP issues related to contracting and speeding time for CRADA approvals and contract reviews was mentioned as a challenge, but no serious proposal was presented to move contracting time frames to a commercially relevant time scale (as BOTTLE and ABPDU have done).

- As noted above, the issues with the current strategic plan do not appear to be caused by any single person or problem, but rather result from a collection of issues that limit the flexibility and creativity of the ABF as presently constructed. The ability for the ABF to maximize impact will require structural changes to overcome these challenges and enable the organization moving forward.
- Strengths:
    - The new strategic plans are better aligned with BETO missions on promoting GHG reduction, SAF, and renewable bulk chemicals.
    - The new goals and metrics are adjusted to focus more on transfer of ABF technologies to industry. These adjustments are appropriate. Higher impacts to industrial biomanufacturing can be expected.
    - The strategic implementation unit has substantial merits. To avoid issues as learned from the past (e.g., realizing challenges in measuring DBTL cycles after 7 years of efforts), having the strategic implementation unit constantly monitor and provide feedback to the executive committee of the ABF would be beneficial.
    - The business development and partnering agreements unit will also be helpful. The review meeting discussed multiple cases where collaborations with industry were delayed by establishing a CRADA. The business development and partnering agreements unit may help to shorten this process.
- Weaknesses/areas for improvement:
    - Building industrial partnerships was listed as one of the four strategies to pursue, and a milestone of achieving at least two funds-in projects was described. This can be a risky strategy because a successful industry partnership relies on appealing technology/success from the other strategies. Considering the current large gap in economically viable SAF manufacturing, it is extremely challenging to have funds-in projects on SAF within the next 2 years. Similarly, having funds-in projects on tools can be challenging because most companies (particularly small companies) focus on developing products rather than tools. Thus, most likely the funds-in projects will come from industrial interests in commercializing one of the two proposed chemicals, muconic acid and 3-HP. Both of these chemicals are good targets; however, there are only two of them. So it might be challenging to attract two funds-in projects in 2 years.
- These comments are the same for the ABF Future Strategy (1) Strategic Plan; (2) Goals, Milestones, and Deliverables; and (3) Implementation Plans:
    - The ABF and BETO have both struggled for years with how the ABF fits in with BETO's mission. This struggle is still ongoing. While it's clear the ABF needs new direction, management, and goals, at the same time, BETO needs to decide whether or not it's going to support an outwardly facing biofoundry focused on supporting synthetic biology. BETO was absolutely correct in calling out the ABF's failures to deliver on previous goals, and to force a reorganization of the ABF. That being said, the ABF was founded with a vision to support and advance synthetic biology in the United States, both for industry and at the national labs. This has frankly never seemed to fit well with BETO's overall mission statement in the past. However, with the Biden administration's call to decarbonize the chemical industry, the ABF finds itself more aligned with BETO than in its previous history. My recommendation is for BETO to support the ABF consortium as it was intended—namely, to be outwardly facing, heavily engaged with industry, and provide services to all U.S. research efforts (industry and academia) to advance synbio goals and develop America as a leader in bioproduction of molecules our world needs. This means changing the current focus of

the ABF away from some of their core work and putting funds back to supporting external partners and ABF infrastructure.

- I recommend the ABF revise their goals in the current strategic plan. This is not going to be something the ABF (and maybe BETO) wants to do. However, the current strategic plan is not well thought out in some areas, and seems to overcorrect and try to appease perceived BETO unhappiness. It's much better to spend another few months rethinking and replanning than waste $45–$60 million over the next 3 years.

- Specifically, the core SAF targets seem out of scope with the ABF's mission and put in to appease BETO. First, the economics of SAF from lignocellulosic sugars is never going to work. Not unless BETO is OK relying on massive government subsidies for SAF, far more than the current subsidies. It's not possible to be economically viable to make SAF currently from cheap sugar cane, using a terpene strain that has near-maximum theoretical yield and a very simple and cheap purification process. The extra costs of lignocellulosic sugars only make the economics worse. The ABF should get clarity from BETO on what level of subsidy is OK to assume if they are going to pursue this path. Second, instead of the ABF trying to guess what would be the best SAF molecule for them to develop, they should be engaging with the big industry players to understand what they want, if there is any overlap between what is needed/wanted, and what the ABF/synbio can help develop. The ABF and BETO need to be brutally honest here, and if the economics of hydrocarbon production from cellulosic sugars is not going to be the most economically viable route to SAF, then don't work on this in the ABF. With regard to the CBP work proposed by the ABF, the CBP is very high risk and high reward. I don't know enough about the challenges of CBP to know if the ABF is adequately addressing the risks, and therefore the probability of success. I do think the CBP work overall is aligned with BETO and is in the national interest to fund at the national labs. It is this kind of "blue sky" visionary work that industry won't do because of the risk, cost, and timelines involved. This is where government funding of basic science can push development of new technologies. That being said, should this work be done in the ABF? Again, I cannot judge that because little detail was given on why the ABF thinks they are best suited to do this work.

- Assuming some or all of the proposed SAF work is dropped from the ABF strategic plan, what should they do with the money? Some recommendations (in rank order): (1) Continue to host onboarding work, which we learned was cut completely. This is my number 1 recommendation for the money. The host onboarding is one area that ABF and BETO funds can really make a difference to advance new technologies and develop new strains to enable new chemicals and pathways at better costs. This is expensive and time-consuming, and often industry is reluctant to take it on. If they do develop a unique microbe, they will keep it strictly proprietary. Host onboarding should pick a small number of microbes that have very different properties, would access very different feedstocks or fermentation abilities, and are likely to be tractable genetically. Then develop them to a high TRL rating to make them really useful. I have a lot to say about the apparent lack of progress on the HObT website since 2021 and the lack of helpful information to the U.S. research community from this work when reviewing this part of the ABF presentation. Regardless, if further work on host onboarding is done, there must be funds allocated to bring the website up to date and make the tools developed useful to the public, or BETO can consider a lot of that work and money wasted. (2) Develop another chemical target, if there is another one as developed and with clear TEA and CO_2e reduction benefits. (3) Put more money to partner-facing projects (FOAs) that support BETO's goals and will also support industry and commercial realization of BETO's goals.

- Several aspects of the technical targets had not yet been worked out by the time of the BETO review in April. Given that the ABF had 4–5 months already to replan, this is surprising and disappointing. The tools section of the strategic plan is not well thought out at all. They have not come up with criteria to even choose which tools to benchmark, or how to conduct benchmarking. It seems like no one wanted to give up their pet project, and with no one really in charge, they are having a hard time figuring out what to pursue further. It is good to not spend time and effort trying to build a capability that is already publicly available that people can access. DOE/BETO/national labs should focus on offering capabilities or research tools that are not available or that industry is not going to do. However, I caution that the ABF should not throw out a capability or tool even if it is measured to be not as good as something already out there. It might be that the ABF provides a different benefit that makes the tool/capability useful to researchers and industry. For example, an ABF capability might be almost as good as something already commercially available, but ABF's might be cheaper, more accessible, or offer more capacity to a limited service. The ABF needs to figure out their criteria and how they are going to benchmark tools immediately and complete the assessments as soon as possible. In the current plan, it looks like this will not be done until the end of 2025.

- Lastly, I think it's a mistake to abandon all DBTL metrics going forward. Revise DBTL to be more realistic, but still have a goal to reduce the DBTL cycle (or even parts of DBTL that make the most sense, are the most commonly used, or the biggest bottleneck). It doesn't have to be every capability and every tool. A metric could be time needed to finish one complete experiment and learn from it (per tool or per instrument) and focus on making those individual unit ops more efficient. Drop wall time versus clock time. What matters is how long it takes you to learn from an experiment. If there is some large downtime (let's say you need to ship samples from one site to another, and that takes weeks), then that is part of your cycle time and something to target to be more efficient. Focus on gaining efficiencies and improving the infrastructure already in place. There is some acknowledgement of this in the strategic plan; under tool milestones it says, "Operational performance gains of significant impact demonstrated for at least 2 ABF benchmarked technologies."

- The ABF said there was large interest from chemical companies for the proposed 3-HP and muconic acid targets. (I know from my own company that industry is very interested in muconic acid to make nylon.) These two core projects are much more aligned with the capabilities the ABF has built, have a high chance of success, and align with BETO's goals. These two projects should definitely continue and are a good change from the beachhead approach, which for whatever reason did not appear to get much industry traction.

- The shift in emphasis to bring in more external money (FOA and DFO) and have >50% of the ABF's budget committed to external partnerships by 2025 is a good change of direction and furthers the goals of the ABF to support industry and other research to translate lab work to real-world changes in decarbonization and reducing CO_2. It's going to be very challenging to achieve a significant increase in industry money into the ABF in the near future, especially if contracting takes a year. It will take time to get to >50% of the ABF's budget committed to external partnerships and reach an average of more than fivefold oversubscription for the ABF's funding opportunities. The 2024 milestone to have two funds-in projects means the ABF needs to land those partnerships in a few months if contracting is going to take a year. Also, the length of time to contract must be improved. The ABF needs to redo its approach to IP and how it contracts projects to de-risk bringing in more industry partners and money. BOTTLE has worked out a very clear IP management plan that allows different levels of industry access to any IP developed. There is an option for industry to keep all the IP (and the national labs then get a higher percent royalty fee). ABPDU also has worked out smooth contracting and IP understandings that allow them to contract in a few weeks, and industry does not have to share IP if it does not want to. The ABF should have developed something like this years ago.

  - There was no mention of how the ABF will measure reduction of CO_2e in their partner projects. Given the ABF's track record regarding an inability to quantify metrics, this does raise concern.
  - The ABF revised management plan is significantly better than the old management structure. The one area that still needs to be changed is the lead PI being solely accountable and responsible for running the ABF. There should not be any decision by committee. The ABF needs a 100% dedicated full-time employee running it. This person should be an "outsider" with no emotional connection to the past 6 years of the ABF. The executive committee reports to and advises the ABF PI, but does not make decisions. It's clear that the ABF has really suffered from decision by committee and a lack of someone whose job is 100% running the ABF.

- Approach: Given the focus on industry partnerships and funds-in projects under the new strategic plan, I cannot reconcile the lack of industry stakeholder outreach. At minimum, current and past industry partners should have been engaged to provide feedback in an iterative fashion. The lack of industry feedback on the new strategic plan makes me worry that the goals and structure they created may not be well received by industry. Though they mentioned during Peer Review that they will engage with industry to validate the choice of those molecules in the coming months, I again question why this was not already done as part of the strategic planning.

- Progress and outcomes: Given that the core activities will now only focus on four molecules, it may be worthwhile to reduce the number of labs that receive core funding to ensure that progress can be made to achieve the desired benchmarks. Additional labs can receive funding for industry-directed projects. However, I do understand and appreciate the need to balance maintaining consistent staffing and having dedicated funding to support researchers across the ABF. While I see the new org chart as better suited to address the ABF's new goals, it may also be helpful to increase the full-time employee allocation of the ABF lead PI, given that past organizational structure has been slow or unable to address the recommendations of prior Peer Review reports.

- Impact: While the new metrics that the ABF has set forth are relevant to BETO initiatives, some of them are not explained in sufficient context to evaluate appropriately. For instance, is the 500-kiloton reduction for each project? Over all the projects that the ABF does? Over what time frame? Is the metric achieved when the CO_2 reduction occurs (e.g., when the product replaces a fossil fuel alternative)? Or is this based on the theoretical, predicted CO_2 reduction measured in initial TEAs? In aiming to increase the proportion of funds-in work as part of their portfolio, there are several operational constraints, discussed during the Peer Review, such as long contracting times and IP models that will likely limit their ability to meet those targets. Though the ABF and BETO can attempt to alleviate some of the bureaucratic hurdles, much of the power to change those systems lies outside ABF and BETO control (e.g., DOE side offices, IP standards of federally funded research and development centers).

- Progress/Outcomes and Impact were given scores of 3, but these are not meaningful for a forward-looking plan. Approach was also given a score of 3, but in this case reflects shortcomings in the approach to developing a new strategic plan and the plan itself. The revised ABF vision and mission aligns with the BETO mission and research priorities. Four strategies will be pursued: partnerships, tools, SAF, and biochemicals. Focusing on SAF and biochemicals is directly relevant to BETO research priorities. Continued focus on tools development is anticipated to advance the field of synthetic biology, which, when applied to SAF and biochemical projects, will advance commercial potential. Partnerships enable public utilization of ABF tools and expertise, which was the original motivation for establishing the ABF. Going forward, the quantity and quality of funds-in partnerships will provide a measure of the ABF's role in growing the bioeconomy. A lack of outside organizations eager to partner with the ABF will be indicative of challenges (e.g., inadequate marketing/self-promotion of ABF capabilities, slow contracting process, unmanageable IP scenarios, or identical tools available at same/lower cost from other providers). This will provide an incentive for the ABF to remediate deficiencies identified in the current review process. Deficiency remediation is expected to improve the oversubscription and quality of partnerships (commercial potential) resulting from DFO and FOA mechanisms. If the ABF wants to increase partnerships with private organizations, a stronger emphasis must be placed on identifying and remediating challenges in establishing partnerships. Direct, specific feedback from current and former IAB members should have been integrated at the initiation of strategic planning rather than after the strategic plan was in place, as indicated in the presentation. Different ABF national labs and teams having contrasting planning process preferences was presented as a challenge to arriving at a new strategic plan. This is an acknowledgement that the distributed model adds a significant level of complexity and inefficiency to the ABF structure. Reorganization jeopardizing an individual or team's sense of belonging was also presented as a challenge, which indicates a mindset whereby labs and research programs have higher priority than the ABF. That is not correct. ABF structure, operations, and achievement of milestones have priority over any individual or team. Regarding the new organization chart, the lead PI resides in the same box as the executive committee, and this unit interacts directly with the ABF advisory board and provides oversight to strategic implementation. Based on this structure, the lead PI has no additional decision-making or responsibility. The ABF's consensus-driven decision-making in the past has proven to be inefficient. Creation of a new strategic plan provides an opportunity to change this model. Engagement/outreach and business development/partnering agreements are shown as not reporting to anyone. If engagement/outreach and business development/partnering are not performing, who has the responsibility to provide that feedback and force changes to be made? A different approach might be to have the lead PI answerable to the BETO technology manager, and engagement/outreach, business development/partnering, and strategic implementation answerable to the lead PI. The executive committee could be on the same level as the lead PI to provide advice, but no component answers directly to the executive committee. This model would improve efficiency, provide decision-making authority to the lead PI, and make the lead PI answerable to the BETO technology manager.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback, some of which was responded to above for the "ABF Introduction and Overview"; "ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads"; "ABF Past Accomplishments – Industry Engagement, Outreach, and Management"; "ABF Past Accomplishments – TEA/LCA"; "ABF Past Accomplishments – Host Onboarding and Development"; "ABF Past Accomplishments – Process Integration and Scale-Up"; and "ABF – Lessons Learned and Introduction to Future Plans" presentations. The ABF and BETO have set a goal that by the end of FY 2025, 50% of ABF resources should be associated with collaboration projects, and in that sense, the ABF is on a path toward more of a "customer"-facing entity. While industry (or other collaborator) proposals (whether funds-in or funding opportunity) are clearly directed by the "customer," core industry projects—in which internally devised ABF projects receive industry cost share (demonstrating their interest)—can also be influenced by and benefit from collaborator partner interactions. Should the ABF not receive sufficient interest in core industry project opportunities, the ABF has contingency plans (e.g., redirecting resources from internal projects to funding opportunities) to achieve the target 50% resource allocation target. Benchmarking is very related to the ABF becoming more of a "customer"-facing entity as well, as it helps the ABF prioritize its tool development activities and demonstrate the value of ABF capabilities to prospective customers.

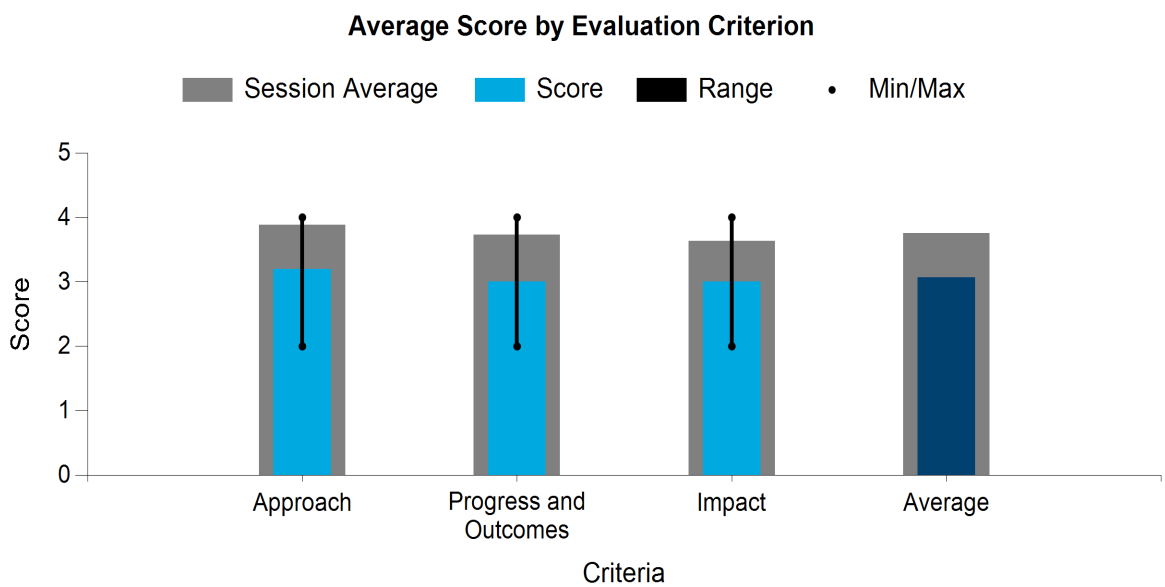
ABF FUTURE STRATEGY – GOALS, MILESTONES, AND DELIVERABLES

Lawrence Berkeley National Laboratory, National Renewable Energy Laboratory, Sandia National Laboratories, and Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	ABF9
Presenter(s):	Gregg Beckham; John Gladden; Jon Magnuson; Katy Christiansen; Nathan Hillson
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2022

In December 2022, the ABF completed its strategic plan, which included goals and deliverables for FY 2023–2025. The relevance of setting these goals and deliverables is that they ensure that they are timely and well aligned with BETO's goals. Top challenges include developing goals that serve the ABF and BETO beyond FY 2025, developing deliverables that do not dictate their implementation, and developing deliverables that are likely accomplishable (even without knowing precise budget constraints or implementation details). The outcomes of these activities are a set of goals for the ABF, including partnerships, tools, SAF, and biochemicals, along with FY 2025 deliverables for each goal. This presentation covers in detail the deliverables for each goal. Milestones will be covered in the subsequent Implementation Plans presentation.



COMMENTS

- The ABF utilized multiple presentations to document their journey in developing a new strategic plan for the next funding cycle. These presentations grew off each other, and as a result, it is difficult to separate them as required in this review process. Instead, I have used the "Strategic Plan" presentation to provide feedback on this presentation as well. Please look there for my comments.

- Strengths:

- The overall goals and milestones for the four targeted areas are appropriate. Achieving these proposed milestones will bring substantial impacts to industrial biomanufacturing.
- Muconic acid and 3-HP are reasonable biochemical targets given the ABF's previous achievements and experience in producing these chemicals. Previous TEAs/LCAs also showed potential for economically viable biomanufacturing, and highlighted areas for further technology development.

- Weaknesses/areas for improvement:
  - A quantitative milestone is needed to describe the gains of significant impact for two ABF tools. It is not clear how much impact is significant and how to quantitatively measure the impact by FY 2025.
  - The rationale to select CBP of ethanol as a SAF target is unclear. Commercial benefits of CBP are well received. However, it is not clear whether ethanol is a right choice for SAF, given its low energy density and low heating value. Innovations for CBP ethanol production are also limited.
  - The 500-kiloton CO_2e reduction should not only be a deliverable for the partnerships team. It should be the target of the entire ABF team. Failure to achieve this milestone can be caused by insufficient technology transfer to industry, or by ABF technologies not being of interest to industry.
- These comments are the same for the ABF Future Strategy (1) Strategic Plan; (2) Goals, Milestones, and Deliverables; and (3) Implementation Plans:
  - The ABF and BETO have both struggled for years with how the ABF fits in with BETO's mission. This struggle is still ongoing. While it's clear the ABF needs new direction, management, and goals, at the same time, BETO needs to decide whether or not it's going to support an outwardly facing biofoundry focused on supporting synthetic biology. BETO was absolutely correct in calling out the ABF's failures to deliver on previous goals, and to force a reorganization of the ABF. That being said, the ABF was founded with a vision to support and advance synthetic biology in the United States, both for industry and at the national labs. This has frankly never seemed to fit well with BETO's overall mission statement in the past. However, with the Biden administration's call to decarbonize the chemical industry, the ABF finds itself more aligned with BETO than in its previous history. My recommendation is for BETO to support the ABF consortium as it was intended; namely, to be outwardly facing, heavily engaged with industry, and provide services to all U.S. research efforts (industry and academia) to advance synbio goals and develop America as a leader in bioproduction of molecules our world needs. This means changing the current focus of the ABF away from some of their core work and putting funds back to supporting external partners and ABF infrastructure.
  - I recommend the ABF revise their goals in the current strategic plan. This is not going to be something the ABF (and maybe BETO) wants to do. However, the current strategic plan is not well thought out in some areas, and seems to overcorrect and try to appease perceived BETO unhappiness. It's much better to spend another few months rethinking and replanning than waste $45–$60 million over the next 3 years.
  - Specifically, the core SAF targets seem out of scope with the ABF's mission and put in to appease BETO. First, the economics of SAF from lignocellulosic sugars is never going to work. Not unless BETO is OK relying on massive government subsidies for SAF, far more than the current subsidies. It's not possible to be economically viable to make SAF currently from cheap sugar cane, using a terpene strain that has near-maximum theoretical yield and a very simple and cheap

purification process. The extra costs of lignocellulosic sugars only make the economics worse. The ABF should get clarity from BETO on what level of subsidy is OK to assume if they are going to pursue this path. Second, instead of the ABF trying to guess what would be the best SAF molecule for them to develop, they should be engaging with the big industry players to understand what they want, if there is any overlap between what is needed/wanted, and what the ABF/synbio can help develop. The ABF and BETO need to be brutally honest here, and if the economics of hydrocarbon production from cellulosic sugars is not going to be the most economically viable route to SAF, then don't work on this in the ABF. With regard to the CBP work proposed by the ABF, the CBP is very high risk and high reward. I don't know enough about the challenges of CBP to know if the ABF is adequately addressing the risks, and therefore the probability of success. I do think the CBP work overall is aligned with BETO and is in the national interest to fund at the national labs. It is this kind of "blue sky" visionary work that industry won't do because of the risk, cost, and timelines involved. This is where government funding of basic science can push development of new technologies. That being said, should this work be done in the ABF? Again, I cannot judge that because little detail was given on why the ABF thinks they are best suited to do this work.

- Assuming some or all of the proposed SAF work is dropped from the ABF strategic plan, what should they do with the money? Some recommendations (in rank order): (1) Continue to host onboarding work, which we learned was cut completely. This is my number 1 recommendation for the money. The host onboarding is one area that ABF and BETO funds can really make a difference to advance new technologies and develop new strains to enable new chemicals and pathways at better costs. This is expensive and time-consuming, and often industry is reluctant to take it on. If they do develop a unique microbe, they will keep it strictly proprietary. Host onboarding should pick a small number of microbes that have very different properties, would access very different feedstocks or fermentation abilities, and are likely to be tractable genetically. Then, develop them to a high TRL rating to make them really useful. I have a lot to say about the apparent lack of progress on the HObT website since 2021 and the lack of helpful information to the U.S. research community from this work when reviewing this part of the ABF presentation. Regardless, if further work on host onboarding is done, there must be funds allocated to bring the website up to date and make the tools developed useful to the public, or BETO can consider a lot of that work and money wasted. (2) Develop another chemical target, if there is another one as developed and with clear TEA and CO_2e reduction benefits. (3) Put more money to partner-facing projects (FOAs) that support BETO's goals and will also support industry and commercial realization of BETO's goals.

- Several aspects of the technical targets had not yet been worked out by the time of the BETO review in April. Given that the ABF had 4–5 months already to replan, this is surprising and disappointing. The tools section of the strategic plan is not well thought out at all. They have not come up with criteria to even choose which tools to benchmark, or how to conduct benchmarking. It seems like no one wanted to give up their pet project, and with no one really in charge, they are having a hard time figuring out what to pursue further. It is good to not spend time and effort trying to build a capability that is already publicly available that people can access. DOE/BETO/national labs should focus on offering capabilities or research tools that are not available or that industry is not going to do. However, I caution that the ABF should not throw out a capability or tool even if it is measured to be not as good as something already out there. It might be that the ABF provides a different benefit that makes the tool/capability useful to researchers and industry. For example, an ABF capability might be almost as good as something already commercially available, but ABF's might be cheaper, more accessible, or offer more capacity to a limited service. The ABF needs to figure out their criteria and how they are going to benchmark tools immediately and complete the assessments as soon as possible. In the current plan, it looks like this will not be done until the end of 2025.

  - Lastly, I think it's a mistake to abandon all DBTL metrics going forward. Revise DBTL to be more realistic, but still have a goal to reduce the DBTL cycle (or even parts of DBTL that make the most sense, are the most commonly used, or the biggest bottleneck). It doesn't have to be every capability and every tool. A metric could be time needed to finish one complete experiment and learn from it (per tool or per instrument) and focus on making those individual unit ops more efficient. Drop wall time versus clock time. What matters is how long it takes you to learn from an experiment. If there is some large downtime (let's say you need to ship samples from one site to another, and that takes weeks), then that is part of your cycle time and something to target to be more efficient. Focus on gaining efficiencies and improving the infrastructure already in place. There is some acknowledgement of this in the strategic plan; under tool milestones it says, "Operational performance gains of significant impact demonstrated for at least 2 ABF benchmarked technologies."
  - The ABF said there was large interest from chemical companies for the proposed 3-HP and muconic acid targets. (I know from my own company that industry is very interested in muconic acid to make nylon.) These two core projects are much more aligned with the capabilities the ABF has built, have a high chance of success, and align with BETO's goals. These two projects should definitely continue and are a good change from the beachhead approach, which for whatever reason did not appear to get much industry traction.
  - The shift in emphasis to bring in more external money (FOAs and DFOs) and have >50% of ABF's budget committed to external partnerships by 2025 is a good change of direction and furthers the goals of the ABF to support industry and other research to translate lab work to real-world changes in decarbonization and reducing CO_2. It's going to be very challenging to achieve a significant increase in industry money into the ABF in the near future, especially if contracting takes a year. It will take time to get to >50% of the ABF's budget committed to external partnerships and reach an average of more than fivefold oversubscription for the ABF's funding opportunities. The 2024 milestone to have two funds-in projects means the ABF needs to land those partnerships in a few months if contracting is going to take a year. Also, the length of time to contract must be improved. The ABF needs to redo its approach to IP and how it contracts projects to de-risk bringing in more industry partners and money. BOTTLE has worked out a very clear IP management plan that allows different levels of industry access to any IP developed. There is an option for industry to keep all the IP (and the national labs then get a higher percent royalty fee). The ABPDU also has worked out smooth contracting and IP understandings that allow them to contract in a few weeks, and industry does not have to share IP if it does not want to. The ABF should have developed something like this years ago.
  - There was no mention of how the ABF will measure reduction of CO_2e in their partner projects. Given the ABF's track record regarding an inability to quantify metrics, this does raise concern.
  - The ABF revised management plan is significantly better than the old management structure. The one area that still needs to be changed is the lead PI being solely accountable and responsible for running the ABF. There should not be any decision by committee. The ABF needs a 100% dedicated full-time employee running it. This person should be an "outsider" with no emotional connection to the past 6 years of the ABF. The executive committee reports to and advises the ABF PI, but does not make decisions. It's clear that the ABF has really suffered from decision by committee and a lack of someone whose job is 100% running the ABF.
- Approach: My comments on the approach to strategic planning have already been covered in responses to other presentations.

- Progress and outcomes: Regarding benchmarking ABF processes to the equivalent industry-accessible state-of-the-art baselines, when asked to further clarify this during the Peer Review, they stated that any proprietary industry methods would not be appropriate comparisons. As such, it is unclear what these benchmarks will be or what purpose they will truly serve if the goals are not specified beforehand. For instance, is this benchmarking metric for the development of tools? If so, which tools? What parts of the process are important to measure? Time, scale of project, output, etc.? For projects that don't have direct TRY outputs (e.g., modeling approaches), what is the benchmark? I also see a discrepancy with the goal to develop at least six new tools while reducing the core function to develop only the four stated molecules. There is also some tension in the goal to increase oversubscription while also increasing the number of funds-in projects, as having more cost share or 100% funds-in will make it less appealing to industry.
- Impact: The planned increase in industry-funded work will require the labs to safeguard more of the work that they do and keep it from public knowledge (e.g., through exclusive licenses). With the four-molecule focus of the core work, the new plan may limit the ABF's eventual public impact. It also bifurcates the identity of the ABF in two; one side as a research entity advancing government priorities and the other as a contract research organization for industry.
- Scores for Progress/Outcomes and Impact are not relevant for project planning; hence, neutral scores of 3 were given. Approach was given a score of 4 because there is substantial merit to the approach developed. Goals and deliverables have been set that align with the revised strategic plan.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback. We responded above for the "ABF Introduction and Overview"; "ABF Past Accomplishments – DBTL Infrastructure, Demonstration Projects, and Beachheads"; "ABF Past Accomplishments – Industry Engagement, Outreach, and Management"; "ABF Past Accomplishments – TEA/LCA"; "ABF Past Accomplishments – Host Onboarding and Development"; "ABF Past Accomplishments – Process Integration and Scale-Up"; "ABF – Lessons Learned and Introduction to Future Plans"; and "ABF Future Strategy – Strategic Plan" presentations.

BIOCHEMICAL CONVERSION AND LIGNIN UTILIZATION

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Biochemical Conversion and Lignin Utilization Technology Area is one of 11 technology areas that were reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 18 presentations were reviewed in the Biochemical Conversion and Lignin Utilization session by five external experts from industry, academia, and nonprofit sectors. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks (https://www.energy.gov/eere/bioenergy/biochemical-conversion-and-lignin-utilization).

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $42,369,587.00, which represents approximately 8% of the BETO portfolio reviewed during the 2023 Project Peer Review. During the Project Peer Review meeting, the presenter for each project was given 20 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including the scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Beau Hoffman and Lisa Guay as the Biochemical Conversion and Lignin Utilization Technology Area review leads, with contractor support from Ryan Lawrence (Boston Government Services). In this capacity, Beau Hoffman and Lisa Guay were responsible for all aspects of review planning and implementation.

BIOCHEMICAL CONVERSION AND LIGNIN UTILIZATION REVIEW PANEL

Name	Affiliation
Lisette Akers*	LignoBio LLC
Xianglan Bai	Iowa State University
Genevieve Croft	Schmidt Futures
Jeffrey Dietrich	Rarebird
Christopher Rao	University of Illinois Urbana-Champaign

* Lead Reviewer

BIOCHEMICAL CONVERSION AND LIGNIN UTILIZATION REVIEW PANEL SUMMARY REPORT

Prepared by the Biochemical Conversion and Lignin Utilization Review Panel

INTRODUCTION

BETO focuses on developing technologies that convert domestic lignocellulosic biomass (e.g., agricultural residues, forestry residues, dedicated energy crops) and waste resources (e.g., municipal solid wastes, animal manure, biosolids) into affordable low-carbon biofuels and bioproducts that significantly reduce carbon emissions on a life cycle basis compared to equivalent petroleum-based products. These bioenergy technologies can enable a transition to a clean energy economy, create high-quality jobs, support rural economies, and spur innovation in renewable energy and chemicals production—the bioeconomy.

The program supports diverse projects under two primary focus areas: low-cost sustainable aviation fuel (SAF) and lignin valorization. The biochemical track supports projects for biomass pretreatment, sugar production, and the fermentation of sugar and syngas to fuel chemicals and polymer precursors. The lignin valorization track supports projects that utilize lignin for chemicals, fuels, and polymer synthesis. Scale-up and demonstration projects focus on identifying and addressing commercial-scale challenges and reducing production costs. Novel technology-based projects focus on developing the knowledge base and overcoming barriers early in technology development. Industry engagement is strong in most of these projects. Several projects show great commercial potential and hit their milestones. To gauge whether these metrics are meaningful, it would have helped to see more failure to gauge how much risk BETO is taking. It was unclear whether only successful projects were presented or whether every project was successful, which seems somewhat questionable, or, at very least, that the program is too conservative.

The program is funding fantastic science and technology projects that are well aligned with BETO's near-term (2030) goals of supporting the development of SAF and renewable chemicals and recyclable plastics with low-carbon emissions. The reviewed projects demonstrate alignment with the strategic goals for this technology area. The new (2023) Multi-Year Strategic Plan presents a valuable opportunity to consider place-based and regional approaches to this technology area (as well as others), which is for the most part absent in the existing suite of funded projects. It appears that BETO is appropriately managing project progress, as evidenced by "go/no-go" decisions that have curtailed unproductive lines of inquiry as well as the redirection of certain research focus during the course of the merit review process. Several principal investigators (PIs) noted constructive communications with BETO staff in providing active guidance on research projects and direction.

Overall, the general strategy makes sense with multiple complementary projects, and most projects are on track. The focus on techno-economic analysis (TEA) and scale-up are key strengths of this program. Overall, the technology area is successful. It has a defined strategy, including goals and technical targets that complement BETO's overall mission.

STRATEGY

The program focuses on developing new approaches and technologies to support the BETO 2030 goals of low-cost biofuels and lignin valorization. The program's goal is well reflected in the diverse projects it supports. From biomass fractionation, sugar production, and sugar/syngas fermentation to thermochemical and biological conversion of lignin and lignocellulose-derived sugars, all projects' goals directly or indirectly support low-cost SAF. The portfolio is weighted toward projects linked to the development or utilization of lignin and lignin-derived sugars resulting from deacetylation and mechanical refining (DMR) pretreated biomass.

The program supports technology development and demonstration at multiple scales. BETO has also funded a range of commercial projects, thus diversifying the portfolio to incorporate projects at higher technology readiness levels (TRLs). Due to the proprietary nature of work and the lack of technical details, it is more difficult to accurately evaluate these projects, and it is recommended that steps be taken to increase visibility into technology development status and the associated performance metrics. While developing commercially viable technology is the program's strong focus, the portfolio also supports fundamental studies at multiple scales.

In addition to supporting mature technologies in their scale-up and commercially relevant process development, the portfolio explores novel technologies and innovative concepts. The addition of cell-free systems seems appropriate, but the focus on products rather than technical de-risking and scale-up appears to be a missed opportunity. The expansion of the BETO product portfolio to include more biochemicals and bio-based material projects is viewed as a strength. These products are typically of greater value than fuels, and thus, generally speaking, have a higher probability of commercial success.

As the field of biofuels and biochemicals continues to evolve, we can anticipate that artificial intelligence and machine learning technologies are expected to play increasingly important roles in bioprocess development. Proactive investment in developing competencies in these areas may help ensure that BETO projects can enhance their ability to analyze large datasets, optimize processes, and guide decision making, ultimately leading to more efficient and effective research and development (R&D) efforts.

The strength of the portfolio is the use of TEA as a guiding principle to direct the science. While this is easy to propose, it is often difficult to implement in practice. The BETO projects, specifically at the National Renewable Energy Laboratory (NREL), have done an outstanding job of using TEA to guide scientific decisions. In addition, the various support activities in analytics, modeling, etc., provide real utility not only to the BETO portfolio but also the field at large. BETO has made good progress toward developing a range of foundational technologies (e.g., TEA and life cycle analysis [LCA], modeling, analytical services) that can help support projects across the BETO portfolio. An expansion of effort and/or investment in these areas is recommended because these technologies appear to be contributing to increased R&D efficiency, shorter R&D timelines, and good project management. For example, TEA and LCA are crucial tools in evaluating the economic feasibility and sustainability of biofuel and biochemical production processes, and every project should undergo frequent and in-depth TEAs/LCAs to ensure that R&D are being efficiently directed toward achieving BETO programmatic goals.

Additionally, investing in analytical support, including advanced analytical techniques and instrumentation, can greatly aid in the characterization and analysis of complex biomass feedstocks, intermediates, and final products. Accurate and comprehensive analytical data are critical for understanding the chemical and physical properties of biomass components, evaluating process performance, and ensuring product quality. Thus, increased investment in analytical and computational support would enable BETO to obtain more robust and reliable data, leading to better-informed research outcomes.

The program portfolio stimulates multidisciplinary collaborations among academics, national labs, and industries to leverage diverse expertise, which is highly beneficial in developing commercially viable technologies backed by strong science; however, there seems to be a tension in funding projects at national labs via lab calls versus projects led by industry and academic researchers via funding opportunity announcements. Of the 18 projects we reviewed, a university researcher was the lead on only one (and the presentation was made by an industry partner). National labs serve DOE goals, cultivate extraordinary expertise, and can provide continuity over time. Overall, the quality of the research delivered is high; however, BETO may consider whether it is missing opportunities to diversify lead and supporting PIs through emphasis on lab calls. It is appropriate to fund crosscutting and analytical projects via lab calls. These projects are providing important services to ongoing research at NREL and—to an extent—other national labs and groups.

These projects have developed and made publicly available several useful tools, protocols, and analyses. To what extent can BETO expand these services to provide broader reach beyond NREL?

It is laudable that BETO began to include a requirement for diversity, equity, and inclusion (DEI) goals in proposals and funded projects as of 2021. The inconsistency of implementing this requirement for some (more recently funded) and not all funded projects in the portfolio is a challenge. While some projects funded prior to the DEI requirement acknowledged DEI goals, others did not. Many of the projects that did include DEI goals focused on intentions to develop partnerships with minority-serving institutions (MSIs) or intentions to recruit interns and graduate students from underrepresented minorities. It may be constructive for BETO to provide more guidance, case studies, or support services to advance meaningful DEI engagements in funding proposals and funded projects.

STRATEGY IMPLEMENTATION AND PROGRESS

We commend the BETO teams for exploring different technologies, often orthogonal to the dominant approaches in the field. We need new ideas and technologies, and the work on DMR and lignin are big steps in this direction. The diversity of technical approaches being explored—particularly around lignin usage and valorization—is, at this point in time, a strength because it increases the overall impact and probability of the approach to realizing BETO's environmental (i.e., greenhouse gas [GHG] emissions reduction) and product (i.e., sugar, biofuel, and biochemical) cost targets. In short, this approach helps maximize the likelihood that the funded projects will contribute toward achieving the program's long-term biofuel and biochemical targets. Another strength is a mix of projects de-risking more established technologies while simultaneously pursuing more risky ones, like cell-free systems. The suite of funded projects represents leading-edge research as well as research that can develop solid progress or refine the state of the art (SOA). The funded projects span the process chain and are well divided between upstream processing (pretreatment and deconstruction) and downstream bioconversions (lignin valorization and fermentative biochemical production).

The use and application of TEA for guiding technology development is a key strength. This is a unique aspect of the program and one that could be a model for other biofuel-related research and technology development. Key project milestones should be, across the board, TEA and/or LCA informed, whenever possible. The program has made large strides in the development of TEA and LCA and increasing the analyses into technology development plans and tracking; however, an area where the program may fall short is in the consistent application of TEA and LCA in project milestone setting across all projects. More consistent application will help ensure that all portfolio projects are pointed toward high TRLs, improved commercial metrics, and/or environmental benefits. Many projects had go/no-go and end-of-project milestones based on process outputs that are technically relevant but not the most TEA- or LCA-relevant metrics. For example, many bioconversion processes use titer as the goal, when yield and productivity are typically more relevant for determining commercial potential. Shifting focus toward these primary performance parameters would help ensure that the technologies being developed are driving toward beneficial outcomes for the performer, the government, and, more broadly, the biofuels and biochemicals field.

DMR process: The program is funding projects that are at the leading edge of work in the field. Following the scale-up challenges associated with dilute acid biomass pretreatment, the program responded by heavily investing in DMR. BETO, via NREL, has put the focus on this process versus the conventional dilute acid process, which has a track record at the commercial scale, with the valid argument that the lignin from the DMR or chemical-recovery-free DMR (CRF-DMR) process is less condensed that than of the dilute acid process, and therefore offers a wide range of applications compared to the sulfur lignin. As the readiness level of DMR has advanced, the program is doing a good job layering in downstream projects that aim to address downstream technical challenges. BETO, via NREL, is also pursuing continuous enzymatic hydrolysis (CEH) in conjunction with the DMR processes, but it is not clear if either DMR process (DMR or CRF-DMR) is scalable.

Cell-free system: The program supports three cell-free system projects where terpenes, isobutanol, butanol, and hexanol are the target products. The program's investment in cell-free technologies is a strength; this field is inherently risky (i.e., TRLs are low), but the approach has the potential to both expand the range of accessible products and realize large step changes in process rates compared to microbial bioconversion technologies. The advantages of a cell-free system in overcoming cell toxicity, enabling diverse products, and achieving high titer and production rates are well justified in these projects. Most of these projects have made great progress by meeting or exceeding the project milestones. Robust computation-aided identification of pathways, enzyme engineering, and low-cost cofactor synthesis demonstrated in these projects greatly improves the current SOA in cell-free technologies and advances science; however, it should be noted that the barrier due to the extremely high production costs is unlikely to be overcome in the short term. For example, TEA estimates the cell-free-based isobutanol cost to be \$3.57/kg even after reducing the cofactor cost by 98% (from \$9,000 to \$200), which is significantly higher than its current market price (\$440/metric tonne). While the current projects produce fuel molecules, targeting higher-value products (e.g., bio-based pharmaceutical chemicals) will help accelerate cell-free system technology adoption and commercialization. Although higher-value products have niche markets, they are commercially more viable than cost-competitive fuels, and delivering early "wins" will help de-risk the deployment of the technology toward lower-value product targets (e.g., fuels and commodity chemicals).

Lignin valorization: The program supports several projects that produce lignin-based chemicals and SAF molecules. The approaches taken in these projects, such as obtaining reactive lignin based on lignin-first reductive catalytic fractionation (RCF), catalytic oxidation for bioavailable monomers, and biological funneling to single molecules, are scientifically meritorious and novel. These projects led by NREL nicely complement each other in their project efforts. Although the advantages of a lignin-first biorefinery in producing higher-quality lignin products are well demonstrated in the current projects, carbohydrate streams derived from the RCF process and their fermentability should also be evaluated in future projects to better justify the viability of lignin-first biorefineries. It is also noted that in all lignin valorization projects, lignin is depolymerized first and then upgraded to chemicals or for polymer synthesis. Although the projects made great progress, the challenges of this valorization pathway should not be overlooked and must be clarified. For example, the dependency of the conversion and product on lignin source, the challenges in product separation and purification, and the high capital and operating costs for catalytically converting lignin should be better informed in future projects. Other lignin valorization pathways that do not require depolymerizing lignin should also be supported. For example, utilizing lignin's high carbon content and aromatic structures to develop property-advanced materials is attractive in this context.

RECOMMENDATIONS

Recommendation 1: Cell-free projects should focus more on technology de-risking and scale-up and less on producing new chemicals.

Because scale-up is the key question concerning the potential of cell-free systems, the panel recommends directly investigating this issue.

Recommendation 2: The viability of most of the commercial projects is questionable, unlike NREL's projects.

The panel suggests that the NREL team performs TEAs for these projects in order to provide a consistent baseline for evaluating feasibility.

Recommendation 3: There appears to be an unmet opportunity to expand into single-cell protein.

Feedstock to food/feed is a gap in the BETO portfolio because alternative proteins fall into the scope of decarbonization, where there is a growing consumer demand/interest and where there is opportunity to provide substantial GHG and environmental benefits relative to the status quo. The panel recommends that BETO incorporates this opportunity into its downstream bioconversion strategy using TEA and LCA to gauge impact relative to incumbent technologies.

Recommendation 4: Academic researchers are less well represented in leading projects.

The program may benefit from an increased variety of research approaches, and the research community may benefit from an expanded network of BETO-funded research. The panel encourages BETO to expand its outreach and program emphasis to reach new potential PIs and participating entities (be they industry or academic institutions). The panel also encourages BETO to expand these services and/or increase accessibility to provide broader reach to diverse potential customers. The increased academic representation could take the form of independent projects but also increased collaboration/partnering with academic labs.

Recommendation 5: The program has invested in supporting analytical and modeling technologies; however, this may be an area where additional investment is warranted since these tools have the ability to accelerate timelines and improve overall R&D efficiency.

One specific area that may warrant increased investment is the development of LCA tools as well as the application of LCA alongside TEA so that a complete picture of both financial and environmental benefits can be assessed, which is of particular note given programmatic emphasis on reducing GHG emissions.

Recommendation 6: BETO began to include a requirement for DEI goals in proposals and funded projects as of 2021.

The inconsistency of implementing this requirement for some (more recently funded) and not all funded projects in the portfolio is a challenge. The panel encourages BETO to provide more guidance, case studies, and support services to advance meaningful DEI engagements in funding proposals and funded projects.

BIOCHEMICAL CONVERSION AND LIGNIN UTILIZATION PROGRAMMATIC RESPONSE

INTRODUCTION

The Biochemical Conversion and Lignin Utilization Program is grateful to the reviewers for their contributions, recommendations, questions, and feedback during the 2023 Biochemical Conversion and Lignin Utilization Project Peer Review session. The program recognizes that this is a significant investment of time to review the projects, travel, and prepare the reviews following the in-person meeting. The program appreciates that each reviewer was willing to contribute their time and expertise to this meeting.

The program is proud of the research that was showcased and appreciates that the reviewers see merit and have optimism about the commercial potential/impact for the projects. Numerous technologies funded by the Biochemical Conversion and Lignin Utilization Program have been commercialized in recent years and/or raised significant amounts of private equity funding toward scale-up and commercialization. Additionally, several of the technologies originally funded by this program have been funded at the pilot and demonstration scales by the Systems Development and Integration Program.

Reviewers noted that they were unsure if there were projects in the portfolio that have failed that would allow them to understand the amount of risk the program is taking. BETO does discontinue and has discontinued projects for lack of technical progress in the past, and the projects presented in this session represented all the actively funded projects by BETO in the space. As discussed here, the program has utilized third-party technical verifications for more than 10 years now with these projects to assess process. The use of these experts identifies both red flags warranting discontinuation and, more frequently, ways that projects' progress can be enhanced. Projects that have been discontinued are exempt from presenting. Given the nature of R&D, BETO does not expect every project to succeed but employs rigorous merit review and project management practices to improve the likelihood of success.

The program appreciates that TEA and LCA are recognized as "guiding principles" of the program and decisions about research investments and promise. The TEA and LCA efforts at the national laboratories and that are associated with many of these projects have long been recognized for publicizing their design reports, process models, and economic assumptions. In recent years, and as decarbonization has grown in priority, BETO has encouraged projects to move away from firm goals in terms of "dollars per gasoline gallon equivalent (GGE)" and focus on the current economic viability of the processes/technologies. Some of these firm cost targets were quite ingrained as metrics by the program and researchers, and work remains to make this philosophical change from "What does it take to achieve $3/GGE?" to "What is the current cost and state of technology?" The move away from hard costs has also been influenced by non-R&D factors, such as policies and tax credits, that will have major impacts on feasibility.

New to this Project Peer Review cycle was the inclusion of a DEI criteria as part of the review. BETO recognizes that this is a new component to the program and that this can be challenging for the reviewers to assess, particularly when only some projects have specific DEI or environmental justice components. In addition to being a new focus area for the research being funded, BETO and other DOE offices are striving to provide more meaningful guidance for reviewers about how to incorporate these elements into lower-TRL projects.

Once more, the program would like to thank the reviewers for their service to the office and for their suggestions on how to continue to improve.

Recommendation 1: Cell-free projects should focus on de-risking as opposed to the production of new chemicals.

The cell-free portfolio is relatively limited within the program; however, significant strides have been made to date, including demonstrating full cofactor recycling, the potential for biomimetics, immobilization and scaffolding, and other technologies that benefit any cell-free molecule. Many of these initial "deal-breaking" barriers were identified in a prior workshop held by BETO, and some of the current challenges being discussed were either not practical to address at that time or not yet identified. The program recognizes that there are many remaining challenges, and these include those of scale-up. BETO's approach toward cell-free R&D has been to ensure that the barriers are addressed sequentially for this technology to be viable. In the case of the initial cell-free work at NREL, 2,3-butanediol (2,3-BDO) was chosen as an exemplary molecule to demonstrate proof of principle. Since then, BETO has shifted to molecules that are much more likely to be made via cell-free pathways, including butanol and isoprenoids. BETO sees cell-free as a mid- and long-term technology and will continue to invest in this as appropriate.

Recommendation 2: Ensure consistent TEA for industrially led projects.

The program recognizes this point and has heard this concern before. In part, this is a consequence of the meeting format (a public presentation). BETO instructs projects to *not* include any information that would be considered proprietary or confidential. The willingness of certain projects to share TEA or other commercialization data can vary depending on the entity. BETO recognizes that this can be frustrating to the reviewers and can make these projects difficult to review. National lab projects often are willing to divulge their TEA assumptions, but often industrially led projects do not include this information.

As part of the verification process, BETO does contract with subject matter experts from NREL and elsewhere to evaluate the TEA, LCA, and associated assumptions for the industrially led projects. These results are confidential and business sensitive and thus protected under nondisclosure agreements. BETO uses the recommendations of these verifications to inform project management decisions to ensure that TEAs and LCAs have credibility.

Recommendation 3: Study the relative impact/value of single-cell protein.

BETO concurs with the recommendation that single-cell protein and alternative proteins present significant potential for decarbonization. BETO is exploring the market and LCA analysis of single-cell protein. BETO recently ran a Small Business Innovation Research solicitation specifically targeted at sustainable protein. BETO will collaborate with other agencies, namely the U.S. Department of Agriculture (USDA), to ensure that efforts in this space are complementary. At present, BETO defers much of the focus in this area to the USDA but will continue to collaborate and explore ways that its work can enable this industry.

Recommendations 4 and 6: Academic researchers are largely unrepresented, and overall guidance on DEI is lacking.

As noted, BETO recognizes that DEI and environmental justice elements were only included as elements of projects in 2021 and later. Since the time of the Project Peer Review, BETO has distributed updated DEI guidance to the DOE national laboratories. The guidance includes considerations and examples that researchers could consider across multiple areas: integrating into existing DEI program participation, opportunities for the research team, and considerations for the research process and outcomes. In addition, the DOE Office of Energy Efficiency and Renewable Energy as a whole has updated its funding opportunity announcement template to include more specifics and expectations on the community benefit plans for future solicitations. With that said, BETO also has considerable work to do to incorporate these principles into its culture and associated funded projects.

With regard to the inclusion of academic researchers in BETO-funded work, the program notes that more than half of the projects that presented in this session have one or more funded university partners. As recent solicitations have targeted higher-TRL approaches and higher quantities of product (such as the clean cellulosic sugars funding opportunity announcement), this has naturally resulted in more industry partnerships; however, even in the case of that solicitation, university partners play key roles in those projects.

Recommendation 5: Increase investment in economic/environmental modeling efforts.

Funding resources for these projects have been limited in recent years, and this is reflected in a shift away from the end-to-end design cases that can take significant time from the economic analysts. To ensure that the various R&D projects in the portfolio still have access to these analysis capabilities, we have encouraged the creation of TEAs and LCAs that might explore smaller system boundaries—for example, the cost and carbon intensity of producing a clean sugar intermediate as opposed to going to a final finished fuel or product. Additionally, many of BETO's economic and environmental models, such as the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model, are funded under the Data Modeling and Analysis Program. That program has been working to improve the collaboration and frequency of handoffs between the experimental, process/economic modeling, and supply chain and sustainability analysis teams.

BIOCHEMICAL PLATFORM ANALYSIS

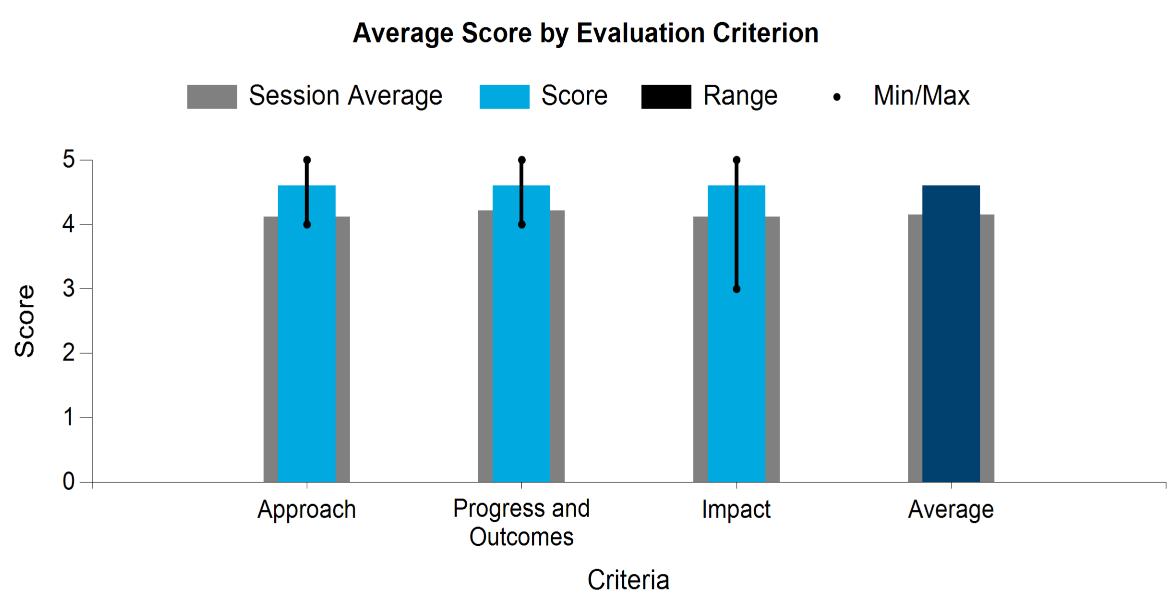
National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.1.0.100
Presenter(s):	Ryan Davis
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,500,000

The Biochemical Platform Analysis project conducts process modeling, TEA, and support for LCA spanning a range of biomass conversion pathways based on biochemical processing concepts making use of sugars, lignin, and other biomass components. This is a high-impact project providing both direct support to DOE-BETO in establishing TEA/LCA metrics for integrated conceptual processes (which are utilized by BETO to guide program goals and planning documents) as well as support to other NREL and partner projects by evaluating specific steps within such an integrated model framework to identify key technology barriers that must be addressed through research prioritization.

This is a well-established project with a long history of delivering value to researchers and BETO management. The analysis conducted in this project serves an important function to provide a process context for the R&D activities funded by the program (i.e., to provide the “so what” answers to key questions on economics and the sustainability of conversion technology concepts), in support of ultimately meeting the latest program goals to maximize decarbonization potential at 70% or more GHG reduction from conventional fuel benchmarks while maintaining economic viability. Key achievements since the 2021 Project Peer Review include demonstrating continued improvements to state-of-technology cost benchmarks while expanding analysis to additional promising pathway options.



COMMENTS

- The goal of this project is to provide process design and economic analysis for the BETO program. Detailed TEA is a critical aspect of the BETO program and one of its overall strengths, especially how it is used to guide the overlying science and engineering. The key applications are 2,3-BDO and butyric acid. Both targets are well motivated based on TEA, as is the motivation for a lignin-first biorefinery concept. The project also provides some key costs for valorizing lignin, which, in turn, provides targets for the technical projects. The team is making excellent progress, providing key targets for other projects.

- This project is central to the BETO portfolio in lignin utilization and biochemical conversion. It is what makes the BETO program unique among the various federal initiatives supporting biofuel development. The impact is clearly articulated, benefiting not only the BETO program but also the entire biofuels community as it provides a clear benchmark and framework for analysis.
- This project is central to BETO's portfolio and should continue to receive support.
- The project serves a valuable purpose within BETO's biochemical conversion portfolio: providing process design and analytical support to guide research toward achieving economic and sustainability goals. It maintains consistent focus on BETO GHG and cost reduction goals. The overarching approach is reasonably aligned with the needs of the impressive number of research efforts it interfaces with, predominantly research conducted at NREL. The team seems nimble in responding to challenges and in periodically reassessing and resetting its course forward. The project's findings are available to and well received by the broader community.
- DEI goals are relatively new to BETO. The project has an interest in pursuing DEI goals, and it has initiated outreach to an MSI. Additional guidance or resourcing from BETO or NREL could strengthen these efforts.
- Considering future directions, I applaud the project's plans to expand research from a focus on traditional biomass feedstocks to include waste feedstocks. These alternative sources of biomass will be increasingly important to achieving sustainability goals.
- The project has made significant progress toward integrating TEA across the BETO portfolio, particularly at NREL. The team has effectively used TEA to support decision making in early-stage R&D planning, ensuring that biorefinery economics are considered from the outset of the projects. Further, the use of sensitivity analyses to reassess priorities based on new R&D results reflects a proactive approach to project management. In short, this project provides invaluable support for other BETO projects that may lack TEA/LCA expertise and budget and helps improve overall partner project research efficiency and direction.
- Historically, coordination between TEA and LCA has been limited; however, the project is taking steps to better align these activities and incorporate aspects of LCA, such as leveraging the GREET model to estimate carbon intensity. Given the growing importance of reducing GHG emissions as a project success criterion, this coordination between TEA and LCA is critical for robust decision making, and it is recommended that this objective is even further emphasized.
- TEA has been effectively used to support diverse technologies across the BETO portfolio. One notable example is the successful switch from adipic acid to beta-ketoadipic acid for lignin valorization, resulting in a four-times increase in productivity and addressing a key cost driver. The project has also demonstrated the value of TEA in optimizing process parameters, improving yield and productivity in projects such as the dioxolane-based technology and optimizing C5 sugar utilization.
- The project has made the TEA models and tools available to the public, with significant downloads of the TEA models in the past 3 years; however, it is noted that the tools are still perceived as black-boxed, and efforts to increase their accessibility, such as through publications or simplified tool sets (e.g., an expansion of the Excel-sheet-based models that were recently published), would further accelerate

adoption and align with the project's stated objectives of increasing industry engagement, especially among small businesses.

- Regarding DEI, the project has worked to build out TEA/LCA capabilities at MSIs, providing students with training and working toward a joint manuscript.
- It is not clear what mechanisms have been put in place to accurately screen processes knowing that TEA from a lower TRL does not usually translate into the target economic viability at higher TRL. Could the PI clarify what has been put in place?
- This project is one of the most important projects in the BETO portfolio. The project works closely with other BETO-relevant projects to bridge lab research and commercial realization of the technologies. The risk identification and mitigation strategies are adequate. The project analyzed various BETO-relevant research, such as 2,3-BDO or organic acids to fuel pathways and lignin coproduct inclusion. It is great to see how this project has updated its model to reflect the technological advances in its TEA. The most important contribution of TEA/LCA to most of the BETO projects is perhaps to inform them of the critical factors affecting product costs and GHG emissions while technology is still under development. This information will help researchers adjust the processes and identify promising pathways to move forward, de-risking technology at the early stage of technology development. The 2,3-BDO pathway optimization performed in this project is an excellent example. The high impact of this project is quantifiable, evidenced by the high downloads of TEA reports, high-impact papers the team published, and the project results that affected the industry decision. The team's approach to improving the credibility of the modeling is commendable. The team works closely with external consultants and stakeholders to receive input and feedback. A DEI plan is in place. Overall, this is an important project, and the team did a great job.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive comments and recognition of the importance of this project. We agree it will be critical to further increase coordination between TEA and LCA efforts moving forward in light of the increased priorities around decarbonization, and we plan to continue working with BETO and other laboratory partners to proactively identify ways to structure modeling efforts to co-optimize cost and sustainability metrics in concert. On the question about screening low-TRL processes, we often begin our TEA considerations for early-TRL concepts based on fundamental questions such as defining maximum theoretical yields or minimum-severity operating conditions. This can help quickly screen out concepts that cannot meet minimum thresholds for economic viability as constrained by untenably low yields and/or high processing costs compared to other established process benchmarks. From that point, concepts that pass this initial screen may be evaluated through "feasibility-level" TEA (not necessarily warranting the rigor of more comprehensive "design case" pathways) with an emphasis on sensitivity scans to highlight key drivers or uncertainties that must be addressed as the concept moves toward higher TRLs, and accordingly more in-depth TEA modeling, also often soliciting engineering subcontractor assistance to validate economic viability for more mature technology concepts. Regarding the comment on increasing public accessibility to simplified TEA tools, we note that the models that we do publish (https://www.nrel.gov/extranet/biorefinery/aspen-models/) are not necessarily "black box" because they are complete Aspen Plus model files with accompanying TEA spreadsheets, although we acknowledge that being based in Aspen Plus, they are not readily accessible to a wide audience. Although many of the fully integrated biorefinery processes that we model require the thermodynamic rigor of a process simulation package such as Aspen Plus in order to provide reliable mass and energy balance information on which to base TEA/LCA calculations, moving forward, we will also seek to prioritize the publication of more simplified cases, such as the NREL sugar model, using user-friendly Excel tools for broader accessibility.

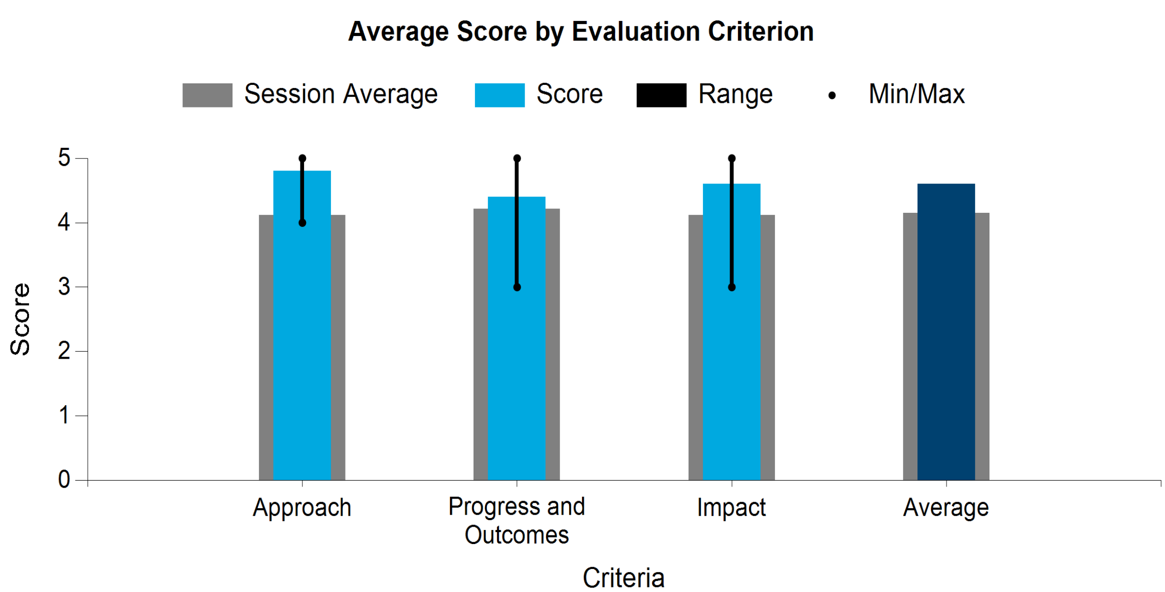
LIGNIN-FIRST BIOREFINERY DEVELOPMENT

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.2.3.106
Presenter(s):	Gregg Beckham; Laura Hollingsworth; Megan Krysiak
Project Start Date:	10/20/2017
Planned Project End Date:	09/30/2023
Total Funding:	$2,040,000

The Lignin-First Biorefinery Development project aims to develop a cost-effective and scalable biomass fractionation strategy based on RCF. The RCF process uses a protic solvent, hydrogen gas or a hydrogen donor, and a metal catalyst in the presence of intact biomass to produce a stable, depolymerized lignin oil and a polysaccharide pulp, which can both be converted to value-added products in parallel processes. RCF is a promising strategy to enable the use of woody feedstocks in biochemical conversion processes and is also promising as a means to valorize lignin with equal emphasis to biomass carbohydrates. Guided by TEA and LCA and in collaboration with industry partners, we are actively developing RCF methods to (1) avoid the need for exogenous hydrogen gas, (2) substantially reduce reactor pressure via the use of low-vapor-pressure solvents, (3) separate the lignin solvolysis and catalytic processes through reaction engineering solutions, (4) reduce solvent loading below what can be achieved in typical batch reactors, and (5) avoid or minimize the use of organic solvents. The project also collaborates closely with the Lignin Utilization and Lignin Conversion to SAF projects for critical substrate handoffs and analytics. Overall, the project is enabling new approaches that ultimately can enable RCF to be a feedstock-agnostic method to valorize both polysaccharides and lignin.



COMMENTS

- The goal of this project is to develop a bioprocess centered on valorizing lignin through reductive catalytic fractionization. The key strength of this approach is that it provides a unique solution to biofuel production and can handle woody biomass. In other words, the process is feedstock agnostic. On the technical side, the key strength is the development of analytical methods for resolving different linkages and structures. Another strength is the adaptation of an existing industrial process for cracking C–C lignin bonds. In particular, the team is focused on developing viable and practical solutions for depolymerizing lignin.

- Overall, this is an exciting project that is making excellent technical progress, especially with reducing the key drivers in cost. The project is well managed with a clear risk management plan. The technical work is impressive and impactful, as illustrated with multiple collaborations with companies.
- This project is one of a suite of lignin projects supported by BETO and led by NREL. This portfolio of projects fits together well in direct support of BETO's goals for lignin valorization. This project, early in the process of achieving lignin utilization, pushes the process of removing lignin from the plant cell wall in the directions of greater efficiency and increased sustainability. The project appropriately uses TEA and LCA to guide the research toward the greatest impact. The project has demonstrated the success of RCF in processing a variety of feedstocks. It would be interesting to see if these successes can be achieved with additional heterogeneous or blended feedstocks.
- The research addresses challenging problems. The project's industry collaborations validate the relevance of this work to real-world interests and objectives.
- A lignin-first biorefining strategy, which involves removing lignin from the plant cell wall, has shown promise in accessing stable lignin oil from woody feedstocks. This approach is aligned with BETO's lignin valorization goals for 2030 and has broad applicability because the outputs (i.e., sugars and lignin-derived phenolics) can serve as inputs for a range of downstream conversion processes.
- One key strength of this approach is the focus on process viability, development, and optimization, rather than complete process integration to end products. By leaving downstream conversion work to industry and national lab collaborators with specialized expertise, the team can concentrate on advancing the TRL of RCF and increasing its impact as a foundational technology that can be combined with diverse bioconversion technologies.
- The extensive use of TEAs and LCAs has provided actionable recommendations for process improvements and optimization targets, guiding R&D directives such as catalyst selection, solvent type and loading, and process optimization. The progress made in the approach is significant, as evidenced by advancements across nearly all major cost centers in the TEA model, such as reducing reactor pressure and solvent loading. This progress has laid a solid foundation for planned integrated process development. While an updated TEA has not been performed to estimate the net TEA and LCA benefits of process improvements to date, it is likely that these benefits are substantial. In summary, the RCF strategy shows tremendous promise and, with further development, is anticipated to make a significant contribution toward achieving SAF and lignin valorization goals.
- Regarding DEI, as presented, there remains room for additional effort and attention to be paid here.
- The project made some satisfactory progress while investigating various parameters (single versus mixed solvents, presence/absence of hydrogen, and solvent recycling loop).
- One recommendation moving forward would be to focus on exploring the potential observed with RCF water-based solvent and find ways to improve the process efficiency when water is used as the sole solvent. One key question that would need to be answered is the rate of condensation in the RCF water-based solvent.
- The project aims to develop economic RCF of biomass by performing an experimental study guided by TEA. This project is one of the lignin valorization projects led by NREL, and the lignin oil produced in this project has been upgraded by several other projects; thus, the success of this project also benefits

other relevant projects. The team has made excellent progress toward the project goal. The team has carefully assessed the project risks and developed mitigation plans. The project approach is commendable. The RCF process is studied in greater detail in this project. From biomass type, reactor configuration, scale, use (or not) of H_2, solvent selection, solvent loading, and catalyst type to product separation, the team considered both the economic aspect and scalability of the process. Industry engagement is also strong. TEA sensitivity analysis to inform factors affecting the minimum selling price (MSP) is a great way to optimize the technology. It shows that RCF capital cost, delignification, and reactor pressure are the top three factors affecting the MSP. Solvent recovery is another key factor. The project evaluates a water-only RCF to reduce reactor pressure and lower solvent costs. Overall, the project made great progress and the team conducted excellent research.

- A few recommendations to consider: (1) Although the lignin-first approach can improve extracted lignin, lignin is still a supplemental source, and cellulose pulp is the main driver of the biorefinery. It would be helpful if the correlations between different RCF approaches and the resulting pulp quality (for cellulose/xylan retention, lignin content, and inhibitory compounds) were also discussed. (2) Solvent consumption can significantly alter TEA results. It is recommended to carefully evaluate solvent consumption when alcohols are used in the system. (3) Was wastewater treatment considered when water is the solvent? (4) The results with different biomass types could be elaborated to evaluate if the different RCF processes are truly agnostic to the feedstock.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive feedback on the Lignin-First Biorefinery Development project. We agree with the reviewer's comment regarding the need to extend this work to blended or heterogeneous feedstocks. Another reviewer's comment remarked on the need to update the TEA and LCA models, which we are doing as the work progresses, and the reviewer is correct that all the process advancements obtained thus far have contributed substantially to reducing estimated costs, energy consumption, and GHG emissions. In terms of DEI activities, we agree with the comment that "there remains room for additional effort and attention to be paid here," and we plan on formally incorporating DEI milestones in the proposal for future project work (fiscal years [FY] 2024–2026); however, we have many DEI activities that were not mentioned on slide 5, including mentoring of interns for workforce development, allocating funds for early-career staff to present at conferences (promotes networking and scientific outreach), and emphasizing proper data citation in meetings to ensure recognition of all staff, specifically interns and technicians. In terms of the use of water as a cosolvent or a sole solvent, that is a major focus of the project going forward, and we have used our flow-through reactor system to estimate the kinetics of condensation, which will inform the at-scale reactor design work that we are conducting with industry partners, as briefly described during the presentation. Regarding questions of pulp quality, we have previously shown that RCF pulp is readily digestible by cellulase enzymes, and work in the Feedstock-Conversion Interface Consortium has shown that the resulting sugars from RCF pulp-derived hydrolysate can be converted microbially with little performance differences relative to clean sugars. We will follow up on this again in FY 2024–2026 if the project is renewed for another 3-year project cycle. In terms of solvent consumption, this is a long-standing question in the literature, and as discussed during the Q&A, we have intentions to conduct isotope labeling experiments to this end in the near future; the use of water would mitigate this concern. Wastewater treatment is modeled explicitly in our TEA. Regarding the feedstock-agnostic comment, we only had time to cover a single slide on this work, but this work is detailed in https://doi.org/10.1039/D2GC04464A. We very much appreciate the positive feedback from the reviewers, and we look forward to sharing our future progress on this exciting fractionation approach!

PRODUCTION OF LOW-COST AND HIGHLY FERMENTABLE SUGAR FROM CORN STOVER VIA THE CHEMICAL-RECOVERY-FREE DEACETYLATION AND MECHANICAL REFINING PROCESS

National Renewable Energy Laboratory

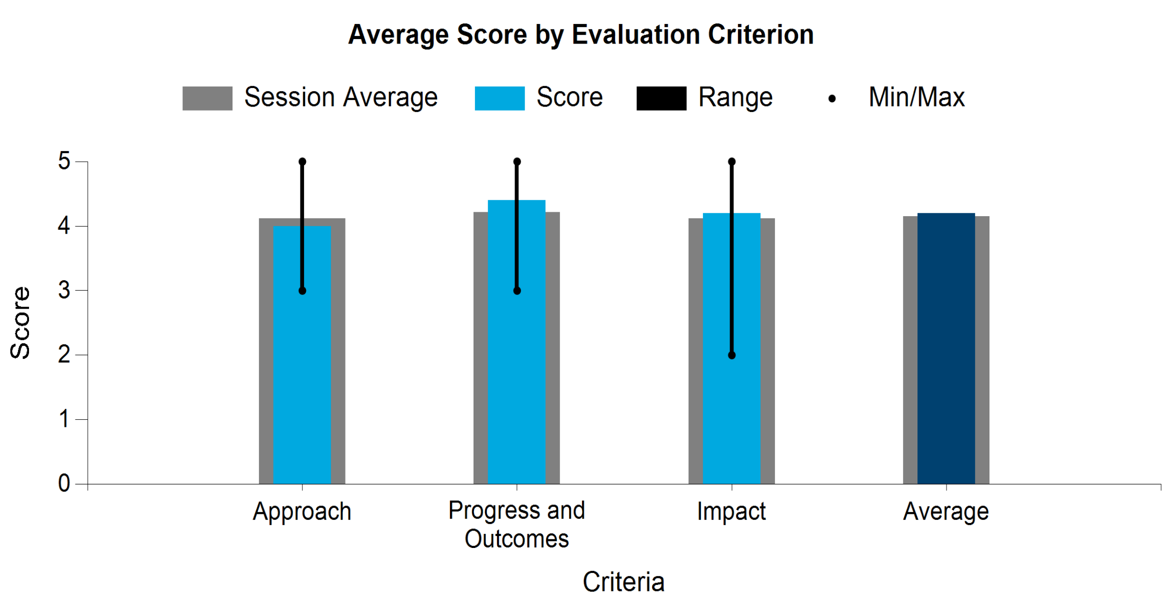
PROJECT DESCRIPTION

WBS:	2.2.3.701
Presenter(s):	Xiaowen Chen
Project Start Date:	10/01/2021
Planned Project End Date:	12/31/2025
Total Funding:	$3,500,000

Early second-generation cellulosic ethanol plants have faced challenges with low fermentability of the sugar hydrolysates produced by dilute acid pretreatment. To address this issue, NREL has developed a scalable atmospheric pressure and low-severity biomass deconstruction and fractionation process called DMR. This process demonstrates superior performance in converting corn stover to high-concentration, low-toxicity sugars at high yields; however, the recovery of NaOH is a complex and expensive process that requires a significant initial capital investment.

To further reduce the minimum sugar selling price (MSSP) of the DMR process, the goal of this project is to develop a CRF-DMR pretreatment technology. This technology should produce highly fermentable cellulosic sugars at an MSSP of $0.20/lb. Additionally, the project aims to enhance the deacetylation step by using chemicals that can also function as fertilizers. This approach can further lower the overall DMR sugar cost by avoiding the chemical recovery step.

The project is a collaboration between industry and academic partners, with the objective of de-risking the downstream sugar conversion process by increasing its availability and performance.



COMMENTS

- The project is focused on developing the DMR process for biomass pretreatment. A number of different pretreatment processes have been developed, all with different strengths and weaknesses. DMR is a promising one, assuming that NaOH can be recovered. It also nicely complements the work being funded by other programs within DOE focused on other approaches. Even though there has been significant prior work on developing the DMR process, this is a new project, so there are few results. That said, the project is exciting and appears to have a solid technical and management plan.
- This project is one of the jewels of the BETO program. Whether or not this technology becomes viable, it is very promising and worthy of investigation and investment. Deconstruction is still the major bottleneck, particularly at the pretreatment stage. DMR is a unique and promising technology, so it should be pursued.
- The technology approach involves considerable environmental and sustainability benefits over the predominant technologies in use.
- The presentation of this project was very clear and deliberate in explaining the context for and potential impact of the successful execution of this research. The project explicitly addresses circularity in the utilization of lignocellulosic feedstocks: It includes the proposal that byproducts of the CRF-DMR process may go back into the soil for fertilization and carbon sequestration benefits. The TEA and LCA may not adequately capture the potential opportunities and risks of this circular element of the technology. This fertilizer opportunity is an interesting proposed co-benefit of the CMF-DMR process. If successful, this use could increase carbon sequestration and reduce the GHG footprint of the CMF-DMR process; however, significant research would be required to ensure that this would not have unintended consequences, including potential introduction of toxins into soils. Few details on this research were provided because it is largely in the domain of USDA collaborators on the project. It is encouraging to see a potential interface between BETO- and USDA-funded research.
- The overarching goal of this project is to develop a cost-effective method with low GHG emissions to produce sugars and lignin from corn stover and other biomass feedstocks by improving the DMR process. This project has strong potential to add value across the BETO portfolio and support the programmatic goals of producing SAF, improving the economics of biofuels/biochemicals, and reducing GHG emissions associated with manufacturing these end products.
- From a project management perspective, a project strength is its leveraging of knowledge gained from scaling up dilute acid pretreatment processes, including challenges with continuous solids handling, and previous work developing on a DMR process. Insights from each of these areas are being used to guide the work plan, which is expected to contribute significantly to reducing both R&D and scale-up risks.
- The team has proposed a simple but innovative solution that involves a two-stage deacetylation process using ammonia and potassium-based salts during pretreatment, which eliminates the need for energy-intensive NaOH recycling. Although the project is still in its early stages, previous work on a two-stage deacetylation process using sodium carbonate supports the technical feasibility of the overall process. Using sodium carbonate in the first stage, the project has demonstrated over 90% glucose yields and achieved a modeled $1/GGE reduction in minimum fuel selling price (MFSP), as well as a modeled 23% reduction in GHG emissions. Further, the resulting sugars were of suitable quality for use in microbial fermentations. If successful, the proposed ammonia-/K-salt-based approach may further decrease the MSP by 25% and GHG emissions by a modeled 48%. Therefore, the economic and environmental advantages of the technology could be substantial and warrant investigation.

- A critical assumption in this project is that the waste stream comprising N/P/K will be an effective fertilizer. The LCA and TEA presented are hinged on this assumption. Toward that end, the reviewer suggests that the level of effort placed on fertilizer replacement testing be substantially increased—for example, through industry collaborations and additional academic partnerships. If the results are positive, it would significantly de-risk this aspect of the project and increase its impact; however, if the results are negative, addressing this challenge during the project lifetime would be critical.
- Efforts to support DEI were not presented, and attention should be paid to ensure that the project incorporates one or more mechanisms to support this program objective.
- A process yields comparison between DMR and CRF-DMR is needed. The PI interchanges process yields and conversion yields, and it is confusing.
- A TEA comparison between DMR and CRF-DMR side by side would be very helpful.
- No risks are outlined for the new CRF-DMR process.
- It is challenging to review the CRF-DMR process when, as of today, everything is just TEA based. Were assumptions used to generate the TEA? If so, on what basis were these assumptions selected in the absence of lab data?
- The black liquor has toxic components. The PI should look at the black liquor's toxicity from the CRF-DMR process before assuming it will be good to be added to the soil as is without testing for potential issues.
- At what scale has CRF-DMR been tested as of today? No data as of today. Everything is just TEA based. DMR is the process that has been mostly tested as of now.
- The project is just starting the initial verification, and thus there is no real project progress to evaluate; however, the presenter did an excellent job explaining the project background and the approaches. The disadvantages of dilute acid pretreatment and the problem with NaOH treatment are clearly explained. The success of the previous project with two-stage DMR is also presented. The use of ammonia and alkali salts for DMR and the use of the residues for fertilizer is well justified. Although the waste stream containing lignin and nutrition elements from the DMR treatment differs from the lignin-based fertilizers synthesized in previous studies, the overall concept is novel, and the approach is logical. The project management and the industry engagement are excellent. Collaborating with academia, national labs, and industries to evaluate the fermentability of DMR hydrolysate for multiple products and fertilizer applications is also commendable. The project risks and mitigations are not discussed in the presentation; thus, additional information will be helpful. The biggest concern is about directly applying the waste liquor in soils. Any foreseen challenges and mitigation strategies could be elaborated. A DEI plan should also be described.

PI RESPONSE TO REVIEWER COMMENTS

- We greatly appreciate and welcome the feedback from the reviewers regarding our CRF-DMR project. It has been noted that the project has the potential to contribute value to the BETO portfolio and support programmatic goals related to SAF, improved biofuel/biochemical economics, and reduced GHG emissions associated with end product manufacturing. Incorporating the suggestions and concerns of the reviewers is a priority for us as we move forward with the project. We recognize that the toxins produced during pretreatment and the direct application of waste liquor in soil could be a major concern. To address this issue, we plan to conduct a comprehensive compositional analysis of the liquor, including both organic and inorganic components, using inductively coupled plasma spectroscopy, X-ray fluorescence, gas chromatography–mass spectrometry, and other relevant methods. Further, we intend to collaborate closely with USDA, Washington State University, and the University of Connecticut to assess the impact of potential toxins on soils. Additionally, we will increase our efforts to test the replacement of fertilizer, as suggested by one of the reviewers. One reviewer has pointed out that there needs to be more elaboration on the risk and mitigation strategies of the project. One of the major risks associated with the project is the possibility of not achieving equivalent high sugar yields as the two-stage DMR process that uses Na_2CO_3 and NaOH. This could result in high MSSP and GHG emissions from the produced sugar and derived fuel/chemical products. To mitigate this issue, we propose using SO_2 or oxygen to oxidize the lignin after the ammonia and potassium hydroxide pretreatment to solubilize more lignin and increase sugar yields. Another risk is that toxins produced during pretreatment may reduce the value of waste liquor for fertilizer replacement. As mentioned, our mitigation strategy is to conduct a comprehensive compositional analysis of the liquor and collaborate closely with relevant experts to assess its impact on soils. Despite the promising preliminary results from the TEA and LCA, it is important to note that the project is still in the verification stage. This is because the TEA and LCA were based on several assumptions, particularly regarding the sugar yield obtained through the use of NaOH and Na_2CO_3. As the project progresses, we plan to update the TEA and LCA results accordingly.

SPERLU SELECTIVE PROCESS FOR EFFICIENT REMOVAL OF LIGNIN AND UPGRADING

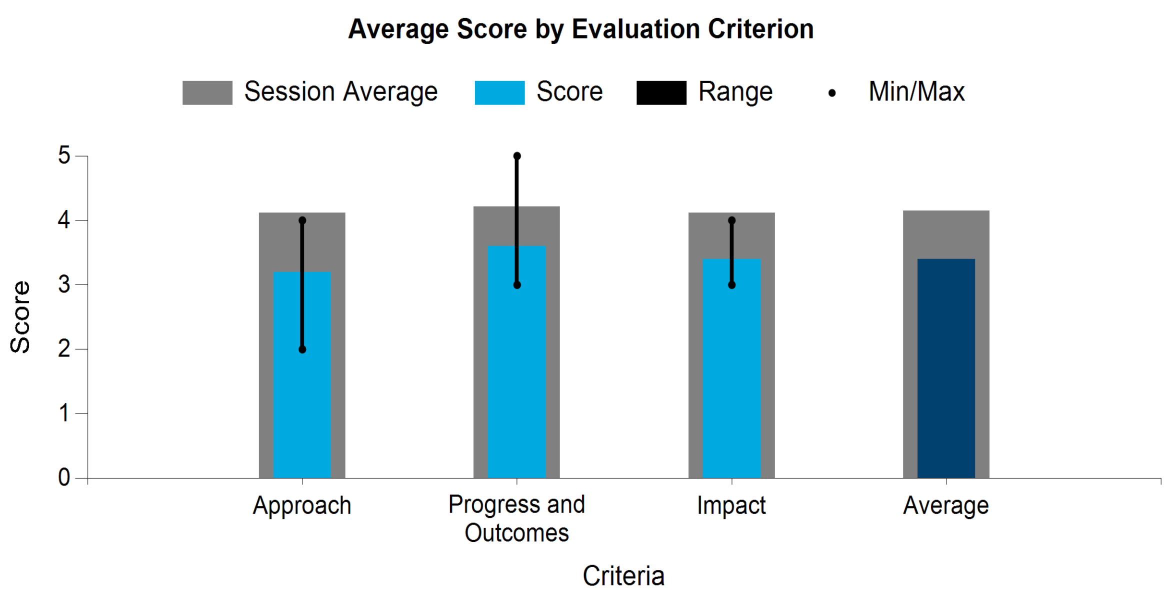
Spero Renewables, LLC

PROJECT DESCRIPTION

WBS:	2.3.1.212
Presenter(s):	Ian Klein
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2023
Total Funding:	$2,077,875

To meet the growing demand for bio-based chemicals and improve the profitability and efficiency of the emerging biorefinery industry, lignin is an abundant and attractive feedstock. Spero Renewables, LLC has developed a proprietary and patent-pending technology, the Selective Process for Efficient Removal of Lignin and Upgrading (SPERLU). The technology is a catalytic deconstruction and upgrading of lignin in lignocellulosic biomass or commercially available technical lignin to produce biophenol products. The SPERLU process has been demonstrated and vetted on a lab scale to convert commercially available technical lignin to biophenols in yields of 60%–90% (based on lignin). The biophenol products can be separated and further upgraded through catalytic or biological means.

Spero performed a detailed kinetic study of the SPERLU process and used the resulting kinetic data to design and construct a mini-pilot-scale reactor for the routine production of hundreds of grams of biophenol products. Spero's lignin-based biophenols have been demonstrated for use as a drop-in replacement for bisphenol A (BPA) in the synthesis of thermoset polymers. Spero's lignin-based thermoset polymers exhibit excellent mechanical properties and can be used in many applications. Additionally, a collaboration with NREL was used to evaluate the feasibility of upgrading SPERLU products through biological means into valuable chemicals. A comprehensive TEA and LCA have been completed and support the case for commercialization of the SPERLU technology. Through this project, Spero has significantly de-risked the SPERLU technology and is actively planning larger-scale pilot projects.



COMMENTS

- The goal of this project is to convert lignin into biophenols as potential replacements for BPA using a catalytic approach. The work looks interesting, but the project is difficult to evaluate due to the lack of technical details. The team appears to have achieved its milestones, but, again, progress is difficult to evaluate. In addition, it was unclear what assumptions went into the TEA/LCA. One suggestion would be to have the TEA at NREL provide this analysis because it would give an unbiased view of whether the SPERLU process will ever be economically viable. Another suggestion would be to have a closed session where the reviewers, having signed nondisclosure agreements, could better evaluate the technology and progress.

- Management seems to have worked, as adequate progress was made to achieve project goals on time; however, limited information was shared. Risk management steps were stated (monthly project meetings and TEA of process changes), but individual risks identified before experimentation began were not identified. Once experiments began, challenges were identified as they arose, and dealt with. In contrast to other presented projects, this project did not present diversity, equity, inclusion, and accessibility (DEIA) goals or activities. Limited information is available by which to understand the technical aspects of the SPERLU process. Evaluation would benefit from greater elaboration of risks and mitigation strategies.

- The pivot from biomass feedstocks to technical lignin shows dexterity in project management as well as the benefits of an initial project strategy that considered and evaluated multiple feedstock types. Few details are provided. It would be helpful to better understand the difference in financial, logistical, and other costs associated with sourcing technical lignin versus woody biomass.

- The PI asserts that the project has met its goals on time with the end date of the project. As such, appropriate progress has been made. The project met the goal of producing >200 g of biophenols/day as of February 2023.

- The approach seems expensive relative to the potential impact. It would be valuable to better understand existing and anticipated future demand for BPA, be it from petroleum or renewable feedstocks. The SPERLU process is proprietary and patent pending. Should this project succeed, to what extent would this technology be broadly available for use, and to what extent would it result in sustainability gains in the production of petrochemical replacement products?

- There are gaps in the information presented regarding the purity of the monomer and dimer biophenols resulting from the SPERLU process. High monomer purity is crucial for generating polymers of commercial quality. It is expected that some byproduct formation may occur during processing, which would need to be addressed during monomer purification.

- The data presented on the lignin-based polymer specs do not clearly indicate if these polymers are true drop-in replacements for epoxidized bisphenol A (DGEBA). While parameters such as glass transition temperature and storage modulus are important, they alone are insufficient to claim that these polymers meet downstream user requirements. Therefore, the project could benefit from additional collaborations with industry and national labs to explore different applications of the output polymers in order to better understand their potential.

- The calculated net present value of 12% for the plant sizes required indicates a significant degree of scale-up and commercialization risk. If assumptions are overly aggressive or process performance diminishes with increasing scale, the overall economics of the project may be jeopardized. For example, the relatively long process times (e.g., 6 hours reported with technical lignin) expose the project to increased risk if this metric fails to scale.

- Overall, the impact of the technology on BETO's overall portfolio and long-term goals may be diminished due to the technical difficulties encountered with using lignin from poplar and other biomass feedstocks. Although these challenges may be addressed to some extent through increased catalyst loading or solvent volume, the process economics may diminish while the environmental impact increases. Further research and collaborations may be necessary to overcome these challenges and fully realize the potential impact of the technology.

- By using technical lignin data, show that the lignin/solvent ratio is reduced to 5:1. That is achieved without a solvent recycling loop. One recommendation would be to investigate the effect of solvent recycling on further reducing the ratio to an acceptable number that is economically viable. Another recommendation would be to investigate if the recycled solvent could potentially be toxic to the microorganism.

- The global market size of BPA is over $20 billion and will continue to grow; thus, a low-cost, bio-based replacement of bisphenol for thermoset production will provide a sufficiently large market for lignin valorization. In this project, biophenols are obtained from lignin using a catalytic, solvent-based process. The bio-based epoxide developed in this project showed comparable Tg and storage modulus, proving their applicability. The TEA and LCA show positive net present value and GHG reduction. The project management and industry engagement are adequate. From the project title, it looks like the team originally targeted CRF lignin removal from biomass; however, it seems like the team's focus is shifted to technical lignin because they find that using whole biomass requires a significantly higher amount of solvent than lignin, hurting TEA. It was reported that technical lignin could yield much more biophenols than whole biomass and directly produce dimeric phenols. Surprisingly, nearly 80% of biophenols were produced from technical lignin. Because the presentation did not disclose their process, it is difficult to evaluate the scientific merit of the project. The biophenol purity and solvent requirement are identified as the risks. It would be helpful if the team commented on the purity requirement in polymer synthesis and the challenges in obtaining consistent polymer properties. Based on the gas chromatogram given in the presentation, considerable byproducts are presented. High-temperature vacuum distillation is mentioned as a purification method. It will be helpful if the team comments on its effectiveness. Lignin oils are thermally unstable, and constituent compounds have high boiling points. The purpose of Task 2 (biotransformation) is unclear. What are the input and output of this task? How is this task related to other tasks?

RECYCLABLE THERMOSET POLYMERS FROM LIGNIN-DERIVED PHENOLS

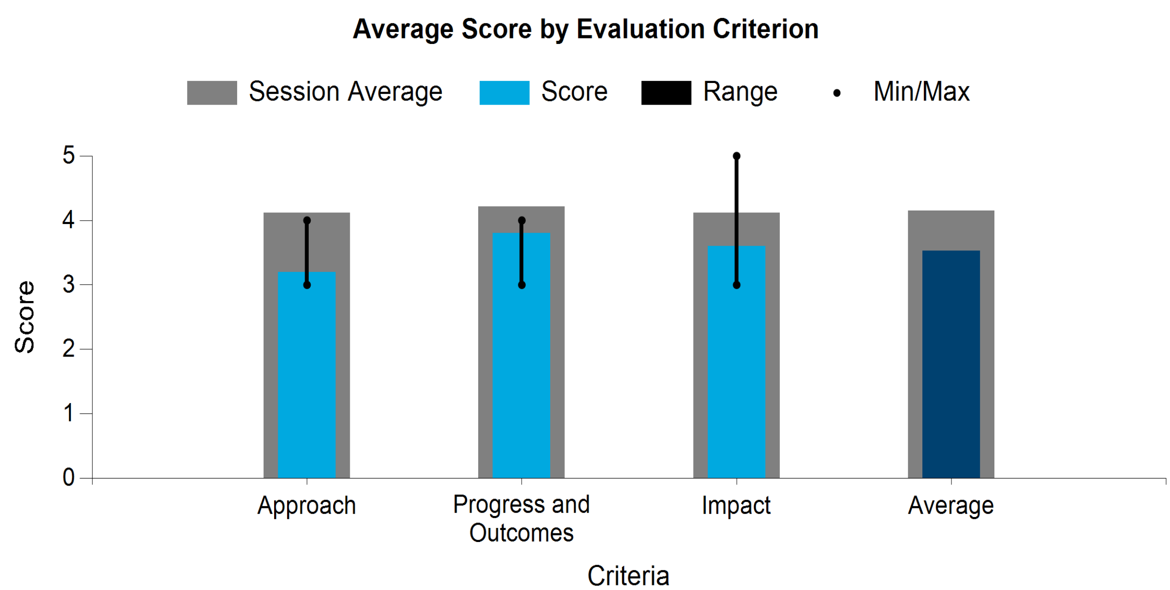
Spero Renewables, LLC

PROJECT DESCRIPTION

WBS:	2.3.1.416
Presenter(s):	Ian Klein
Project Start Date:	10/01/2019
Planned Project End Date:	07/31/2024
Total Funding:	$2,500,000

Recent innovations at Spero Renewables have resulted in a proprietary technology for producing decomposable and recyclable thermoset polymers. Thermosets are a class of polymers that are irreversibly cured from soft solids or liquid prepolymer, with the aid of heat or other action of energy. Because of the permanent cross-links, thermosets generally possess outstanding mechanical properties, chemical and thermal resistance, and excellent insulation. Thermosets are now commonly used as the plastic matrix in performance composites, also known as carbon-fiber-reinforced composites. Despite the outstanding material properties of carbon-fiber-reinforced composites, the non-decomposable and nonrecyclable nature of thermosets has limited the widespread application of thermoset composites. It is estimated that hundreds of millions of dollars are lost each year from the landfilling of thermoset composite wastes.

Spero Renewables' recyclable thermosets incorporate bio-based feedstocks derived from lignin, which can be incorporated at more than 50% of the mass of the polymer. Through this project, the technology is being refined to produce thermosets that can be decomposed under mild conditions yet possess comparable thermomechanical properties to conventional BPA-based thermosets. Spero's thermosets can be chemically recycled, with the thermomechanical properties of recycled thermosets comparable to virgin thermosets. Through collaboration with Argonne National Laboratory, a comprehensive LCA of the synthesis and recycling of Spero's thermosets and carbon-fiber-reinforced composites is underway. TEA is being used to validate the commercial potential of Spero's technology. At the conclusion of this project, Spero expects to have sufficient data to enter large-scale pilot production ahead of commercialization.



COMMENTS

- The goal of this project is to produce carbon fiber composites using lignin-derived phenolics. The key strength of this approach is that it replaces BPA and yields a recyclable material that can be depolymerized. Like many industrial projects, this one was difficult to evaluate due to the lack of technical details. While impressive results are shown, it is unclear what the benchmarks are. This project was also materials focused with not much discussion of lignin.
- Overall, this appears to be an interesting project, but the feasibility and impact are difficult to evaluate due to the lack of technical details.
- Limited information is available by which to understand the technical aspects of the project. The evaluation would benefit from greater elaboration of processes, risks and mitigation strategies, LCA, TEA, and results.
- Progress seems to be promising; Spero seems to be hitting its targets in terms of material qualities and recyclability.
- In principle, the research is interesting. It would be valuable to have recyclable thermoset composites; however, there are major unaddressed questions regarding whether and how, if technically possible, the recycling of these thermoset polymers would actually take place. Enabling the recycling of small consumer goods is identified as a more near-term goal, and the recycling of larger industrial composites would be expected to be a longer-term goal due to the safety testing that would be required.
- The project is still in its early stages, making it challenging to predict the commercial impact of the product resins and technology as well as their final alignment with BETO's programmatic goals; however, there are promising indications that the product resins possess properties that could be attractive across a wide range of commercial applications, including carbon fiber composites. The project has successfully developed resins with excellent recyclability, minimal change in storage modulus, "welding" or adhering capability, and high fatigue resistance compared to reference BPA. These favorable properties make the resins a promising candidate for various industrial uses, as demonstrated by the project's successful engagement with potential commercialization partners.
- The technical approach of using a chemically recyclable resin based on reversible bonds is novel and attractive, but the level of detail provided is insufficient to appropriately assess the feasibility and approach. For example, more information about the catalyst used is needed to provide substantive input on the technical risks and the overall feasibility of the approach. Additional details would enhance the understanding and evaluation of the project's overarching technical strategy.
- The TEA indicates that the process may be profitable even at production volumes as low as 1,000 metric tons per year, which is typically considered as demo scale for most plants. This suggests that the project's technology has the potential to be economically viable and commercially scalable, further enhancing its potential impact.
- There is a need for more comprehensive material properties analysis to further validate the potential for commercial adoption of the polymers. Currently, only a limited set of parameters, such as glass transition temperature and storage modulus, have been reported. To gain wider acceptance in the industry, it will be crucial to generate more data on various material and mechanical properties as well as to evaluate the compatibility of the developed materials with existing BPA processing equipment.
- Overall, the project seems to be on track with projected milestones. Satisfactory results have been achieved with tasks 4 and 6.

- A recommendation would be to test how many cycles can be achieved without losing efficiency. Data only show up to two generations.
- Although thermoset polymers with reversible bonds are reported by others, making them using lignin is attractive. Recyclable thermosets will potentially reduce the disposal of waste plastics; thus, the impact of this project is multifold. The project management and approach are appropriate. The project targets recyclable carbon fiber composites, which is highly commendable. Because carbon fiber has high production costs and its recycling has been ineffective, being able to recycle both carbon fibers and polymer resin is highly attractive. The bio-based thermoset developed in this project showed high material performance and good recyclability. The results of the solvent-dissolution recycling, the welding-repaired resin, the separation of intact carbon fibers, and the fatigue tests of the recycled composites all suggest the excellent properties of the products. The TEA looks promising too. The team is proactively marketing its polymer by working with international companies.
- The potential risks and mitigations are not mentioned in the project. Due to the limited information given in the presentation, it is difficult to fully evaluate the potential risks of this project. While it mentions that the product contains more than 50% lignin, polymer synthesis is not disclosed; thus, the potential risks in polymer synthesis are unknown. The recycling solvent is also not disclosed; thus, its relevance to LCA and potential environmental pollution cannot be determined. Polymer recycling has been demonstrated using virgin resin; however, the project should evaluate how environmental degradation and impurities in post-application resins affect the recycling chemistry.

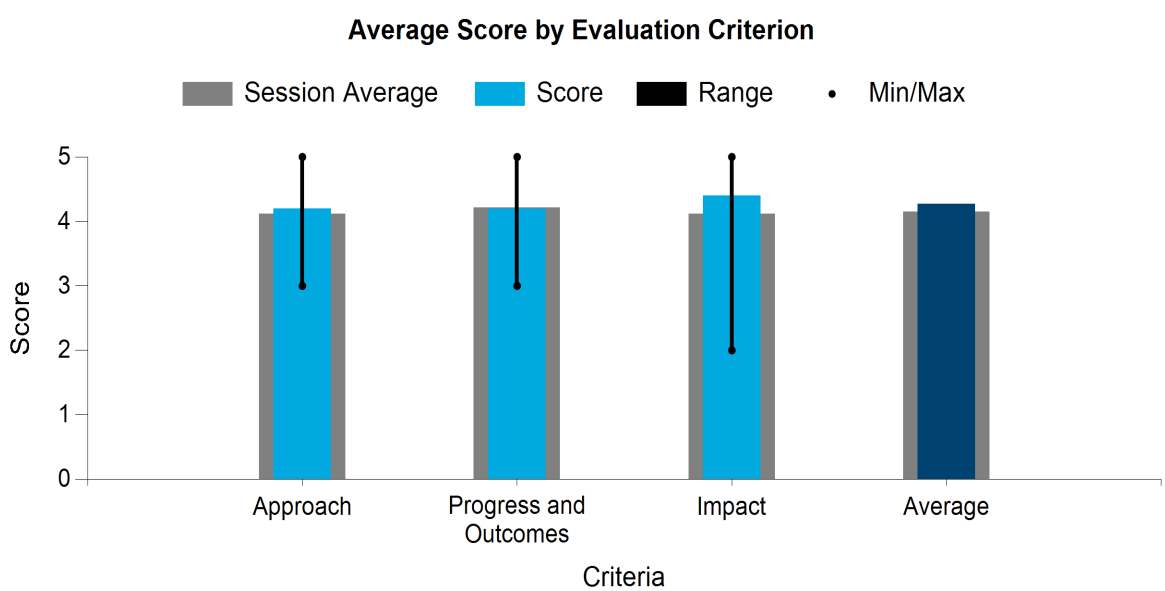
BIOLOGICAL LIGNIN VALORIZATION

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.2.100
Presenter(s):	Davinia Salvachua; Gregg Beckham; Laura Hollingsworth; Megan Krysiak
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$2,100,000

The Biological Lignin Valorization project develops microbial strains and associated bioprocesses to convert lignin-derived aromatic compounds into value-added bioproducts. Our main objective in the project is to achieve industrially relevant bioproduction metrics that can directly contribute to the economic viability and improved sustainability of the integrated lignocellulosic biorefinery in collaboration with complementary BETO-funded lignin valorization projects. Specifically, the project works closely with the BETO-funded Lignin Utilization project, which provides bioavailable aromatic compounds from chemo-catalytic lignin depolymerization. We use the robust soil bacterium *Pseudomonas putida* as our primary microbial host for the conversion of lignin-derived compounds to bioproducts. To date, we have focused on atom-efficient bioproducts that can be used as either direct replacement chemicals or performance-advantaged bioproducts, including cis,cis-muconic acid, beta-ketoadipic acid, and 2-pyrone-4,6-dicarboxylic acid. From model aromatic substrates, we have achieved titers of each of these compounds approaching 40 g/L and productivity values ranging from 0.5 to more than 1 g/L/h, all at 90% molar yield or higher. From real lignin streams, we have thus far achieved 24 g/L, 0.66 g/L/h and theoretical yield of beta-ketoadipic acid. A major pursuit now is to reach industrially relevant performance metrics on an expanded slate of lignin-derived streams.



COMMENTS

- The goal of this project is to develop strains of *P. putida* to convert lignin monomers into value-added chemicals such as adipic and muconic acid. The technical work is outstanding and provides a unique route for lignin valorization. The team are world leaders in the area. The basic strategy is to exploit *P. putida*'s ability to metabolize aromatic compounds by engineering strains unable to completely oxidize the substrates so that valuable intermediates are produced instead. This requires the addition of a second carbon source to provide the energy for lignin monomer bioconversion.

- The team is making good progress, and the project is well managed. The only criticism is that the details of the TEA were vague—it was unclear what the MSP was actually measuring.
- This project is one of a suite of lignin projects supported by BETO and led by NREL. This portfolio of projects fits together well in direct support of BETO's goals for lignin valorization. This project approaches lignin valorization via biology, developing strains and bioprocesses to produce single coproducts from lignin. Management and technical approaches are reasonable. The team has identified risks and appropriate mitigation strategies.
- These may have been identified in the project management strategy, but the presentation would have benefited from greater elaboration of risks and mitigation strategies, particularly around potential toxicity and other variables affecting strain performance.
- The integration of this project with other ongoing lignin projects at NREL is a strength, as are collaborations with industry partners.
- The project aims to develop *P. putida* strains and bioreactor processes to valorize diverse monomeric compounds derived from varied lignin deconstruction methods, including alkaline, lignin-first, and hydrodeoxygenation (HDO). This approach leverages the host microbe's native aromatic compound import, catabolism, and tolerance, lightening the biological engineering load and allowing the team to focus on strain and bioreactor process optimization. Toward that end, the team has already made good progress toward increasing acetate, aromatic byproduct, and salt tolerance.
- In addition to valorizing lignin, the project's impact stems from the development of a manufacturing technology that is environmentally advantaged and cost-competitive with nonrenewable adipic acid. As described, the conversion of lignin to muconate or beta-ketoadipate has the potential to deliver substantial decreases in GHG emissions (GGE) compared to petroleum-derived adipic acid (i.e., 40%–50% reduction, dependent on lignin conversion to adipic acid). Likewise, the modeled future production cost for lignin-derived beta-ketoadipate is on par with petro-based adipic acid and, in an integrated biorefinery context, can contribute substantially to lower fuel selling prices (i.e., MFSP reduction greater than $2/GGE).
- The performance metrics presented (titer, rate, and yield) are important indicators of process efficiency, and achieving high conversion yields and volumetric productivities are oft-cited challenges across most conversion technologies utilizing microbes. While achieving a 40-g/L titer is an important technical goal (FY 2023 goal), this metric alone provides limited insight into the actual commercial feasibility of the technology.
- Of note, the strain may be catabolizing a large fraction of glucose to CO_2 to generate adenosine triphosphate (ATP) to cope with substrate and/or production inhibition. At low pH—i.e., at or below the organic acid's (or acids') pKa—organic acid diffusion into the cell may necessitate ATP for re-export. Because the rate of diffusion will increase with concentration, a titer ceiling may be encountered. Data presented on the effect of glucose-to-aromatic compound ratio indicate this could be occurring.
- Last, the project could take additional, incremental steps to support programmatic DEI goals.
- Conversion yields (lignin to bioavailable monomers) seem to be solely driven by the monomers' bioavailability. It would be beneficial to have a sense of what the overall process yields are as well as the process viability.

- The heterogeneity of lignin and lignin-derived products is the most challenging problem with lignin valorization. In this context, the chemical deconstruction of lignin followed by biological funneling to single compounds is scientifically meritorious and highly attractive. In this project, the team works with other BETO-relevant projects to obtain bioavailable lignin compounds for bioprocessing. The risks are identified, and mitigation strategies are reasonable. The results are impressive—the team reports nearly 100% conversion based on model monomers and corn-stover-derived bioavailable monomers. Bioavailable monomer mixtures extracted from poplar are also converted in high selectivity. Acetate was also demonstrated as a carbon source to reduce or eliminate glucose costs. The industry collaboration is strong. Working with industry for strains, bioprocess development, upstream separations, and industrial lignin streams will facilitate a commercially viable technology. DEI focused on creating a healthy and safe research environment. Overall, the project team did a great job and is on track to success. The presented results are based on model compounds and high-purity extracted bioavailable monomers. Considering lignin-derived aromatics can be strong imitators, it would be helpful if the team could comment on the purity requirement in extracting bioavailable monomers and the toxicity of the non-bioavailable aromatics if they co-present.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the review team for the positive feedback! For MFSP (slides 2, 7, and 12), this is the economic contribution of a lignin-derived product to a fuel molecule produced from the carbohydrate fraction of biomass in dollars per GGE. This metric therefore measures the extent to which a lignin-derived product contributes positively to biorefinery economics; thus, the MFSP results presented (slide 7) indicate that the production of β-ketoadipic acid from lignin can offset the selling price of carbohydrate-derived fuels by $2/GGE, increasing biorefining economics. Regarding risks and mitigation strategies for "potential toxicity and other variables affecting strain performance," we agree that this is a risk (slide 5), and thus are actively identifying and overcoming toxicity and titer challenges (slide 16). To this end, we have used adaptive laboratory evolution, systems biology tools, and genome-wide screening tools (e.g., randomly barcoded transposon insertion sequencing [RB-TnSeq]) to identify nonintuitive targets for strain tolerance improvements, and we have adopted fed-batch bioreactor cultivations as a primary means to ameliorate substrate toxicity. A related reviewer's comment also asked about the toxicity of non-bioavailable aromatic compounds. This is an excellent point, and we very briefly showed this on slide 11, for example, where acetovanillone accumulates in a bioreactor cultivation. Wherein our strain does not have catabolic capabilities, including in this case, we are actively engineering the catabolic pathways, which will both reduce substrate toxicity and increase overall carbon conversion efficiency. For the glucose consumption and ATP generation, we agree that glucose (or another supplementary carbon and energy source) will generate energy for non-growth-associated maintenance (e.g., coping with toxic compounds). To quantify this, we are actively engaged in fluxomics experiments with β-ketoadipate and muconate production strains that are measuring ATP/adenosine diphosphate (ADP) ratios, CO_2 generation, import/export rates, and carbon flux from glucose across the bioreactor cultivation phases; however, we note that the glucose loading is quite low, at an 8:1 aromatic compound:glucose molar ratio, and we achieve equivalent strain performance to a 2:1 molar ratio. We have also quantified the economic impacts of glucose feeding on the overall economics, as shown on slide 7. We agree with the comment that "the project could take additional, incremental steps to support programmatic DEI goals" and plan on formally incorporating DEI milestones in the proposal for future project work; however, we have many DEI activities that were not mentioned on slide 5, including mentoring interns for workforce development, allocating funds for early-career staff to present at conferences (promotes networking and scientific outreach), and following recruiting DEI best practices. In terms of the overall process yields, this is driven by both deconstruction and bioconversion yields. As we have achieved strains with 100 mol % biological conversion of aromatic monomers to product (slides 8–13), the reviewer is correct that overall process yields are now principally driven by the generation of bioavailable monomers from lignin. Monomer yields vary by the substrate and deconstruction approach and are shown on slides 4 and 10–14. The Lignin Utilization project and other projects in the BETO-funded lignin portfolio are working toward higher yields from several lignin streams. Excitingly, we are now able to obtain approximately 50%–80% yield of bioavailable monomers from lignin streams, the extent of which depends on the upstream catalytic process, and we are engineering and adapting strains for 100 mol % conversion of these monomer mixtures to this end now (slides 13–14).

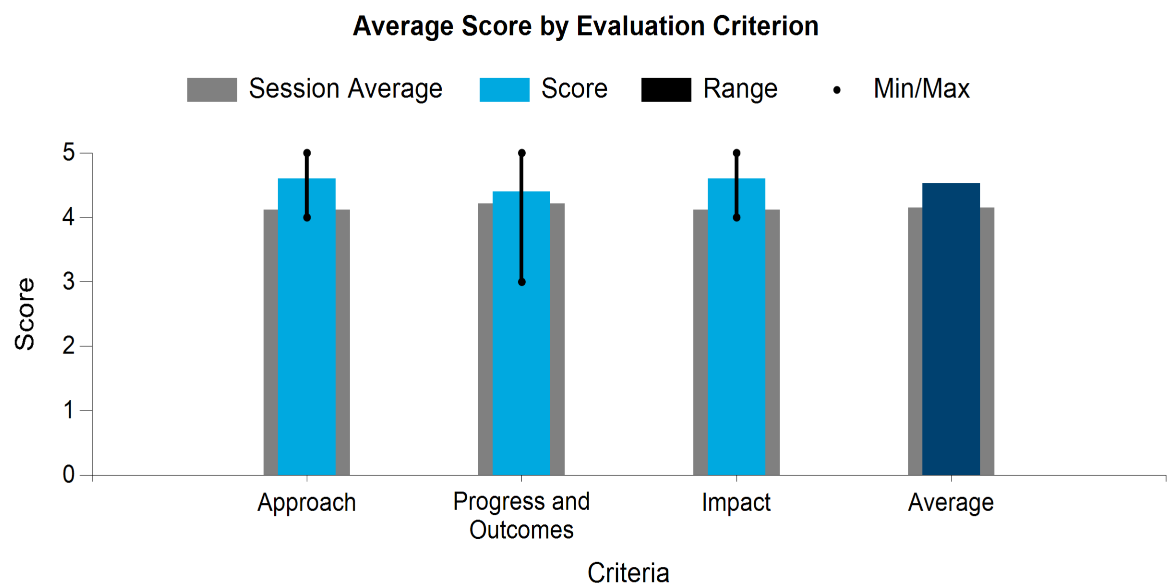
BIOLOGICAL UPGRADING OF SUGARS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.2.105
Presenter(s):	Jeffrey Linger; Laura Hollingsworth; Megan Krysiak
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$2,850,000

The Biological Upgrading of Sugars project aims to produce SAF from lignocellulosic feedstocks through the anaerobic conversion of sugars into butyric acid, which can be further upgraded into various fuels and chemicals. In this presentation, we showcase a fully integrated bench-scale process that utilizes *Clostridium tyrobutyricum* as the biocatalyst for the production of bio-butyric acid. We discuss the genetic improvements made to the biocatalyst that have led to process enhancements as well as the design and initial operation of a pilot-scale reactor capable of 100-L fermentations coupled with *in situ* product recovery, which enables the production of 5–10 kgs of bio-butyric acid and other carboxylic acids per run. Additionally, we share our recent progress in commercializing this technology through collaborations with external partners. Our integrated approach to R&D has significantly advanced the technology of carboxylic acid production and has brought us closer to achieving our goal of cost-effective SAF production.



COMMENTS

- The goal of this project is to provide a pilot-plant process for producing butyric acid from lignocellulosic hydrolysate using *in situ* product recovery. A key strength of this project is a focus on downstream separation, which is a major cost in biofuel production. In this regard, a pilot plant could provide a nice platform for de-risking this keystone project for the BETO portfolio.

- Overall, this program appears to be well managed with a solid risk management plan in place. The team is also making good progress, both on strain development (e.g., co-sugar utilization) and developing the pilot-scale process. It would have helped to provide more detail on the solvent selection and separation train, but progress looks to be good. That said, the team is able to produce purified butyric acid while running the fermenter above the pKa, which is an impressive accomplishment. Another key strength is multiple partnerships with companies, which demonstrates the impact of the project. The next key step will be to integrate the different unit operations and demonstrate sustained production. No major weaknesses were noted.

- This project supports BETO's goals for SAF production.
- The project management is strong; a large team is in place to lead the complementary components of the project. Risks and mitigation strategies are clearly identified. The project benefits from multiple collaborations with BETO-funded consortia and commercial companies. The program considers DEI goals.
- In terms of the technical approach, it is interesting to see the use of three approaches to strain development (genetic engineering, mutagenic selection, and adaptive laboratory evolution) in parallel, each with different preliminary successes. The PI indicated that future areas of opportunity could include greater emphasis on new genetic tools to emphasize new and more complex products.
- The project is demonstrating adequate progress toward goals.
- The project has demonstrated significant advancements in TRL through a combination of *C. tyrobutyricum* strain engineering (i.e., addressing challenges in xylose utilization and addressing potential intracellular pH challenges via arginine decarboxylase expression) and process development (i.e., hybrid extraction distillation). The net economic impact of the estimated production costs for the hybrid process at scale is substantially below that for competitive bio-based butyric acid (i.e., approximately $1/kg compared to $1.80/kg).
- The project has demonstrated the potential to deliver low-cost, bio-based butyric acid (and derived compounds) commercially, as evidenced by collaborations with industry partners working toward SAF, chemicals, and derivates beneficial for human health and wellness.
- Of note, there is some degree of risk that the production of butyrate at extracellular pH values at or below the pKa will lead to technical challenges, limiting the overall fermentation performance. At low pH, extracellular butyric acid (protonated form) may diffuse into the cell, upon which butyrate is formed (due to the neutral cytosolic pH). This phenomenon may lead to high levels of ATP being expended, resulting in a titer ceiling that makes achieving yield and productivity targets challenging.
- Looking forward, the project may benefit from a shift in the level of effort from strain engineering and fermentation process development toward integrated process development, including *in situ* product removal. A number of downstream processing challenges may be encountered as the process shifts from batch toward continuous that can only be accurately identified through long process runs.
- With the project ending in 6 months, what is the project's current TRL? Solvent toxicity is an issue for both processes (liquid liquid extraction and fermentation). What steps are taken to address that issue? Will that be part of the units of operations integration scheduled for the next 6 months?
- This project includes strain development, fermentation with online product separation, and pilot process development, all in a single project. If successful, low-cost butyrate produced using C5/C6 sugar mixtures demonstrated in a fully integrated pilot system will significantly impact biofuels and biochemical production. The project approach for identifying key differences between carbon resources and pHs in carbon metabolism and engineering stains to co-utilize mixed sugars is logical. The progress in developing the integrated system is excellent. The team designed and constructed a fully integrated

pilot-scale system to combine fermentation and online product separation/recovery. Testing DMR hydrolysate feedstock in the pilot system allows the team to identify potential scaling problems. The team's efforts for industry engagement and commercialization are excellent. Overall, the project is on track. Although the scientific approach is justified, the progress of strain development is somehow unclear. It will be helpful if the team can comment on the performance of the current strain (e.g., titer, production rate). TEA estimates an MSP of $0.99/kg compared to the current $1.8/kg. What titer and production rates were used in this TEA?

PI RESPONSE TO REVIEWER COMMENTS

- "It would have helped to provide more detail on the solvent selection and separation train, but progress looks to be good." When we pivoted from an NaOH back extraction to the hybrid extraction and distillation mode, we changed solvents from 20% trioctylphosphine oxide with 40% 2-undecanone and 40% mineral oil to 70% Cyanex 923 (a commercially available phosphine oxide extractant) in mineral oil. The TEA presented was based on using Cyanex; however, the toxicity of this is higher than desired, so we are currently, as our highest priority, screening other blends of extractants, seeking a balance of high extraction efficiency with reduced cytotoxicity. "That said, the team is able to produce purified butyric acid while running the fermenter above the pKa, which is an impressive accomplishment" and "Of note, there is some degree of risk that the production of butyrate at extracellular pH values at or below the pKa will lead to technical challenges, limiting the overall fermentation performance. At low pH, extracellular butyric acid (protonated form) may diffuse into the cell, upon which butyrate is formed (due to the neutral cytosolic pH). This phenomenon may lead to high levels of ATP being expended, resulting in a titer ceiling that makes achieving yield and productivity targets challenging." Thank you for the thoughtful commentary on this topic. It has certainly been the key challenge of this project to optimize pH and parameters that are influenced by pH. In particular, we are looking for pH conditions enabling sufficient growth and productivity but low enough to enable sufficient extraction. As pH increases, which helps *C. tyrobutyricum*, extraction is reduced, which, of course, means additional butyric acid in the reactor, which then adds to the toxicity. Given that we are operating close to the pKa, small reductions in pH lead to large swings in the ability of the acid to be extracted. It is a fine balance, but something we view as key to improved overall process performance. "It is interesting to see the use of three approaches to strain development (genetic engineering, mutagenic selection, and adaptive laboratory evolution) in parallel, each with different preliminary successes." We believe in taking an "all-of-the-above" approach, using both classical methodologies and more modern synthetic-biology-based approaches. There are positives and negatives to both, and we have seen positive shifts from both approaches. "Looking forward, the project may benefit from a shift in the level of effort from strain engineering and fermentation process development toward integrated process development, including *in situ* product removal" and "Solvent toxicity is an issue for both processes (liquid liquid extraction and fermentation). What steps are taken to address that issue? Will that be part of the units of operations integration scheduled for the next 6 months?" We agree with the reviewer completely and have essentially stopped all strain development work for the remainder of the fiscal year so that we can focus efforts on system optimization, modification, and safety enhancements. Regarding future solvent selection, we are in the midst of an experimental campaign to test some new organic blends. Additionally, we have some potential system modifications we are experimenting with that would help alleviate some of the trouble of balancing *C. tyrobutyricum*'s physiological challenges with process efficiencies. "With the project ending in 6 months, what is the project's current TRL?" We would estimate that we are in the TRL 6–7 range based on the following descriptions. TRL 6: System/process model or prototype demonstration in a relevant environment. Beta prototype (system): Prototyping implementations are partially integrated with existing systems. Engineering feasibility fully demonstrated in actual or high-fidelity system applications in an environment relevant to the end user. TRL 7: System/process prototype demonstration in an operational environment. Integrated pilot (system): System prototyping demonstration in operational environment. System is at or near full scale (pilot or engineering scale) of the operational system, with most functions available for demonstration and test. The system, component, or process is integrated with collateral and ancillary systems in a near-production-quality prototype. “Although the scientific approach is justified, the progress of strain development is somehow unclear. It will be helpful if the team can comment on the performance of the current strain (e.g., titer, production rate). TEA estimates the MSP of $0.99/kg compared to the current $1.8/kg. What titer and production rates were used in this TEA?” We apologize for the lack of clarity on this front, but it is a bit of a convoluted discussion because of the numerous process configurations we are using. With the bench-scale pertractive setup (where we get the highest overall process metrics), the experimental throughput is slow and personnel heavy. Accordingly, we do the vast majority of our fermentations in batch or fed-batch mode (without pertraction) to assess strain performance, which leads to reduced titers and yields. We are preparing now to evaluate our top strains in the bench-scale pertractive setup and will then be able to accurately describe the overall improvement. For a detailed discussion on the TEA and productivity metrics, please see https://doi.org/10.1016/j.xcrp.2021.100587.

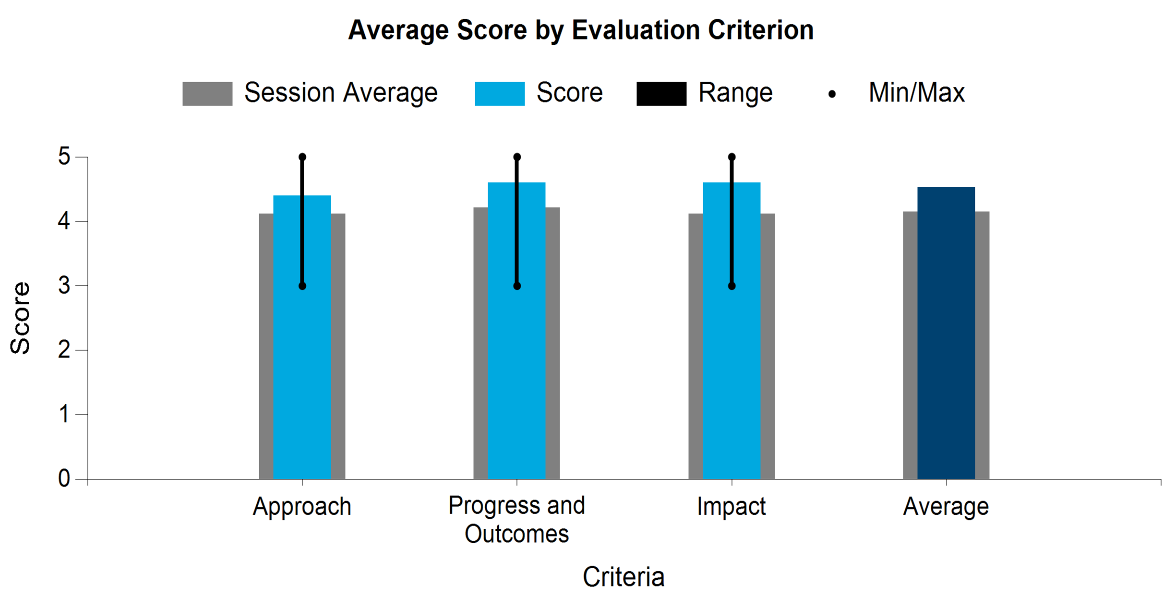
LIGNIN UTILIZATION

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.4.100
Presenter(s):	Gregg Beckham; Laura Hollingsworth; Megan Krysiak
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,875,000

Lignin depolymerization to aromatic monomers is a primary route for myriad lignin valorization strategies. To date, there are many strategies able to cleave aryl–ether linkages in lignin, but the lignin polymer, in both its native and processed forms, contains a substantial fraction of refractory carbon–carbon linkages between aromatic units, which typically limits aromatic monomer yields to about 30–40 wt % or lower, depending on the feedstock. To that end, the Lignin Utilization project addresses the critical challenge of lignin depolymerization catalysis with emphasis on C–C bond cleavage. Being able to achieve cost-effective C–C bond catalysis in lignin depolymerization would enable a substantial increase in the accessible aromatic monomer yields from lignin. Among the catalysis strategies that have been investigated in the project, we have made substantial progress in the use of autoxidation catalysis, inspired by the industrial conversion of p-xylene to terephthalic acid, for C–C bond cleavage in lignin. Using multiple substrates, we have demonstrated that autoxidation catalysis can produce mixtures of bioavailable aromatic monomers for conversion to exemplary bioproducts, such as cis,cis-muconic acid, in collaboration with the Biological Lignin Valorization project. Prior to FY 2023, the Lignin Utilization project also included lignin analytical chemistry method development, lignin analytics for BETO-funded projects, and model compound syntheses, which will also be presented.



COMMENTS

- The goal of this project is to depolymerize lignin with a focus on cracking C–C bonds. The team is making good progress even though the milestones are aggressive. The project is well managed with a clear plan for dealing with risk. A key strength is the development of methods for lignin analytics, which is shared with multiple projects. The technical work is outstanding, in particular the demonstration of C–

C bond cleavage. Progress is outstanding and may lead to a high-yield process for generating monomers. The work also nicely complements a number of existing projects within the BETO portfolio. Overall, the lignin work is the “jewel” within the BETO portfolio.

- This is a strong project that addresses an important problem. Basic feasibility has been established using multiple approaches. The next step is to develop an economically viable process.
- This project is one of a suite of lignin projects supported by BETO and led by NREL. This portfolio of projects fits together well in direct support of BETO’s goals for lignin valorization. The primary aim of this project is to develop catalytic processes for generating aromatic monomers from lignin. The project has identified C–C bonds as an underutilized target for catalytic deconstruction. There are challenges to overcome, but should project goals and scale-up be achieved, the impact of this would be substantial.
- The technical and management approaches are reasonable. The project is making good progress toward its goals. Collaborations with other NREL-led lignin research, as well as industry partnerships, strengthen the research.
- Project impacts are enhanced by efforts to make the analytical tools and protocols it develops publicly available online. It will be interesting to see to what extent these online resources are accessed. Such data may provide insights into whether (1) the posted materials are in demand by other researchers (and by which researchers) and (2) an outreach plan may be necessary to increase awareness that the tools and protocols are available for use.
- The project aims to address a critical technical need in the pursuit of BETO’s goal of valorizing lignin by focusing on C–C bond cleavage in lignin, overcoming the approximately 30%–40% yield limitations faced by current C–O bond cleavage technologies. An innovative approach, autooxidation, is used to generate water-soluble, bioavailable aromatics that can be microbially catabolized. Because the technology should be feedstock agnostic and the output monomers are readily catabolized microbially, this project provides a versatile method to connect upstream lignin to diverse downstream bioconversion technologies (e.g., Biological Lignin Valorization projects).
- Regarding progress to date, in collaboration with the Process Modeling and Simulation project, the team developed analytical methods to track lignin-derived compounds throughout the process. The team also demonstrated proof-of-concept autoxidation of C–C-linked acetylated oligomer, methylated oligomers, and hydrodeoxygenated oligomers. This work sets the stage for introduction of flow-chemistry-based approaches to improve reaction performance.
- The project aims to address the technical problems related to phenol inhibition through three different methods: methylation, acetylation, and HDO. All three routes appear to be viable from a downstream biological perspective, with acetylated products being likely catabolic enzyme substrates; however, concerns were raised about the LCA challenges associated with HDO, and it was intimated that methylation may pose technical challenges. Looking forward, the project would be well served by a rapid determination of how HDO or methylation compete with acetylation from TEA and LCA perspectives. If these approaches are not viable, R&D efficiency cannot solely be increased (i.e., the sole focus is on acetylation); downstream bioconversion projects will have greater clarity on what their input substrates will look like.
- As presented, work to foster DEI is minimal, and additional steps could be taken to support program DEI goals.

- The autooxidation catalytic work performed in collaboration with University of Wisconsin, Madison seems to still be at the proof-of-concept stage, and it is not clear if it has the potential to be economically viable at prepilot or pilot scales. Are plans being made to eventually scale this process up?
- This project is one of the BETO-relevant projects for lignin valorization and complements other projects. The project goals address important aspects of analytical science and lignin valorization. The lack of analytical capability for identifying lignin compounds has been the bottleneck in the field. Gas chromatography/mass spectrometry and nuclear magnetic resonance are insufficient for complex lignin chemistry. Although high-resolution mass spectrometry could provide accurate masses of oligomeric compounds, it is difficult to determine molecular structures. In this context, the energy-resolved mass spectrometry method, Lignin Wrangler library (in collaboration with the computational project), and open-source protocol developed in this project enable the rapid and accurate identification of lignin compounds, broadly benefiting the community. The difficulty of producing chemicals from lignin in high selectivity is addressed by converting lignin into bioavailable monomers and then biologically funneling down to single molecules. Catalytic autooxidation and masking phenolic OH were highly effective in depolymerizing lignin into aromatic acids. The project concept is novel. The risks and mitigation strategies are adequate, and the project management is excellent. The collaborations with multiple parties for TEA/LCA, product separations, product upgrading, and flow-through reaction are commendable. DEIA activities are appropriate. Overall, the project made excellent progress.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the positive feedback on the Lignin Utilization project! We are extremely excited about the C–C bond cleavage efforts and analytics method development efforts in this project. The point about monitoring the views and citations of the posted protocols is excellent. We posted these protocols immediately before the FY 2023 BETO Project Peer Review, and we will monitor these closely going forward to understand if the community is using them. We will also include these posted protocols in external presentations as a resource for the community as well. One reviewer raised the TEA- and LCA-oriented question regarding the choices between acetylation, methylation, and HDO, which we fully agree with as the major question to answer in the C–C bond cleavage chemistry. To that end, we are now actively doing what the reviewer suggested. Regarding the scale-up of autoxidation, we note that the same catalyst system and solvent are used in the Amoco process to make terephthalic acid from p-xylene at 80 million metric tonnes/year, and thus there is considerable precedent for this chemistry at the industrial scale. We intend to conduct TEA and LCA on the autoxidation process in parallel with the experimental transition to flow-based reactor systems. For the comment on future DEI work, we agree, and are working on a larger DEI plan between the NREL lignin projects to make a larger impact.

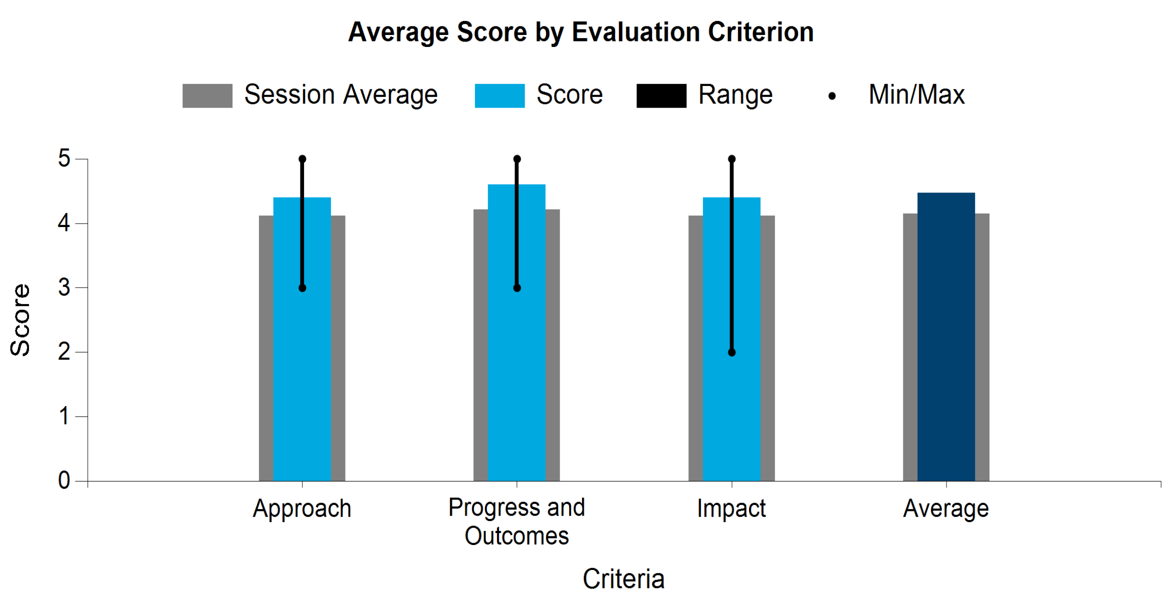
LIGNIN CONVERSION TO SUSTAINABLE AVIATION FUEL BLENDSTOCKS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.4.104
Presenter(s):	Gregg Beckham; Laura Hollingsworth; Megan Krysiak
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$3,600,000

The Lignin Conversion to Sustainable Aviation Fuel Blendstocks project focuses on the conversion of lignin-rich streams to deoxygenated aromatic and cycloalkane blendstocks in the jet fuel range. This work is done in close collaboration with the BETO-funded Lignin-First Biorefinery Development project and industrial scale-up partners, and the work is closely guided by analysis to develop cost-effective and sustainable routes to produce lignin-based SAF blendstocks. To date, we have demonstrated the continuous catalytic conversion of a lignin oil from poplar to deoxygenated aromatic products at approximately 85% C-mol yield. This HDO process uses a stable, earth-abundant catalyst and requires no solvent. We have also established a baseline process model and associated TEA and LCA that together demonstrate the potential to achieve cost parity with fossil carbon-based jet fuel at approximately 70% reduction in GHG emissions. Current work is focused on expanding the slate of feedstocks for HDO to include lignin oils from softwoods, agricultural residues, and grasses, as well as from hydrolysis lignin substrates from biochemical conversion and pulp-and-paper processes. We are also undertaking catalyst development efforts to tune the reaction selectivity from aromatic compounds to cycloalkanes. Last, we are investigating reaction engineering strategies to slurry solids for HDO reactions.



COMMENTS

- The goal of this project is to convert lignin monomers into aromatic and cyclohexane molecules for use in aviation fuel. The key challenge is achieving this goal is to reduce the oxygen content with these molecules. The proposed solution is HDO. The team is making excellent progress, and the technical component is outstanding. The project appears to be well managed with a strong risk management program and is making good progress toward achieving their milestones. A key strength is that TEA and LCA are central to the project goals. The potential impact is huge because it provides a potential route for lignin valorization by targeting the important problem of developing SAF.

- Overall, this is an exciting project and one of the highlights of the BETO portfolio.
- This project is one of a suite of lignin projects supported by BETO and led by NREL. This portfolio of projects fits together well in direct support of BETO's goals for lignin valorization and the SAF Grand Challenge. This project uses substrates from the lignin-first biorefinery project, among other sources, to develop HDO processes to produce performance-advantaged and SAF-relevant products efficiently, economically, and sustainably.
- The approach is well considered. The numerous collaborators involved in the work allow the project to cover a lot of ground in addressing the project's core goals. As with other BETO-funded projects, DEI goals could be strengthened if additional support and guidance were provided.
- Affirming the relevance and potential impact of this work, the project demonstrates multiple collaborations with industry and academic laboratories. The project has achieved early goals and set ambitious future targets. Improving the practicality of the HDO process will require overcoming a number of challenges. The team has identified risks and appropriate mitigation strategies.
- The project has a well-defined management plan that is guided by TEA and LCA. In addition, the combination of product testing through ASTM blending analysis, industry collaborations, and engagement with stakeholders ensures that the project outcomes are relevant and advance the SOA, aligning with BETO's goal of producing SAF.
- From a technical perspective, the decision to focus on developing a benchtop-scale continuous system, rather than a batch reactor, is a strength because it allows for a thorough understanding of how key process performance parameters, such as catalyst total turnover and reactor kinetics, impact the technical feasibility and commercial viability of the technology; however, it is notable that there is no explicit target for reaction kinetics, and it is recommended this be addressed alongside the 500 hours of cumulative time-on-stream target.
- While the project is relatively new, significant progress has been made in completing foundational experiments that set the stage for continuous processing. The data presented in the review are promising, with high C-mol yields (e.g., 86% of theoretical) and low residual oxygen achieved in a two-pass HDO process at the benchtop scale using different feedstocks. Moreover, the output HDO oils show potential as a performance-enhancing component of SAF blends, with approximately two-thirds of the output HDO oil from poplar falling within the jet fuel range and exhibiting superior performance parameters compared to traditional fuels. The LCA results also demonstrate impressive reductions (54%–81%) in GHG emissions associated with the production of RCF HDO oil compared to petroleum-derived Jet A fuel. While the TEA results indicate reasonable MSSPs, further improvement may be targeted in future years to make the sugars cost-competitive with those derived from cane and corn. In sum, if successful, this project has the potential to significantly contribute toward achieving BETO's long-term goals of producing SAF.
- The project is taking steps to support DEI programmatic goals through internships with minority students.
- The retention times seem to be very long. One recommendation would be to find ways to shorten the retention times and subsequently the cost associated with the process as it currently stands.

- The process seems to be expensive as of today. One recommendation would be to put action items in place to find ways to significantly reduce the process cost to meet BETO's metrics and cost targets.
- The project aims to convert lignin to SAF via catalytic HDO. Lignin HDO is an extensively explored research area; however, upgrading RCF oil makes this process an interesting and promising pathway. The team identifies flow reactor setup, catalyst development, and feedstock dependency as the major risks and barriers. The project approaches are very thoughtful and strongly focus on scaling up. Industry engagement is strong. Engaging companies for lignin substrates, reactor scale-up, and end product development will facilitate technology transfer when it is ready for commercialization. Other than SAF, using HDO oil as bio-based lubricants and working fluids is mentioned, which can diversify the product applications. Although the project started recently, the team has already achieved impressive HDO conversion and a high percentage of SAF-range molecules. TEA and LCA support the feasibility of the technology. Overall, the project approach is logical, and the management plan is excellent. DEI activities, such as recruiting interns and holding DEI training workshops, are adequate. It would be helpful if the dependency of HDO conversion and catalyst deactivation on lignin feedstock is elaborated, especially when technical lignins with high molecular weights and impurities are used.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive feedback on the Lignin Conversion to Sustainable Aviation Fuel Blendstocks project. We appreciate the comment on reaction kinetics, and we are pursuing this with real RCF oils as substrates by tracking the reactivity of monomers that can be readily tracked. Regarding the comment about retention times and cost, we showed the estimated economics of the HDO process on residual lignin streams in the presentation at the current residence times, and we note that the estimated economics are quite attractive already. We will continue to use TEA and LCA to evaluate the most impactful process variables, including residence time, to ensure that our focus is maintained on the most important process parameters for beneficial economics, reduced energy use, and reduced GHG emissions. For the comment about using technical lignins, we fully agree that this will be an interesting area to pursue, and we are doing so. In the short time that the project has been running, we have been able to fully conduct HDO on poplar and pine RCF oil, and technical and biorefinery residual lignins are slated to be studied in the future after we are able to reach the scaled-up Tier Beta level for these initial, high-priority feedstocks. For the comment referring to our DEI goals, we would like to elaborate that more work is going on at all institutions than could be highlighted on a slide. All project institutions have the support of institutional DEI plans for hiring, equipment purchases, and workshops. We also focus on the next generation of scientists by allocating funds for early-career researchers to travel and present at conferences as well as funding for research technicians to attend trainings to continue to build their skill sets.

FERMENTATIVE PRODUCTION OF TULIPALIN A: A NEXT-GENERATION, SUSTAINABLE MONOMER THAT DRASTICALLY IMPROVES THE PERFORMANCE OF PMMA

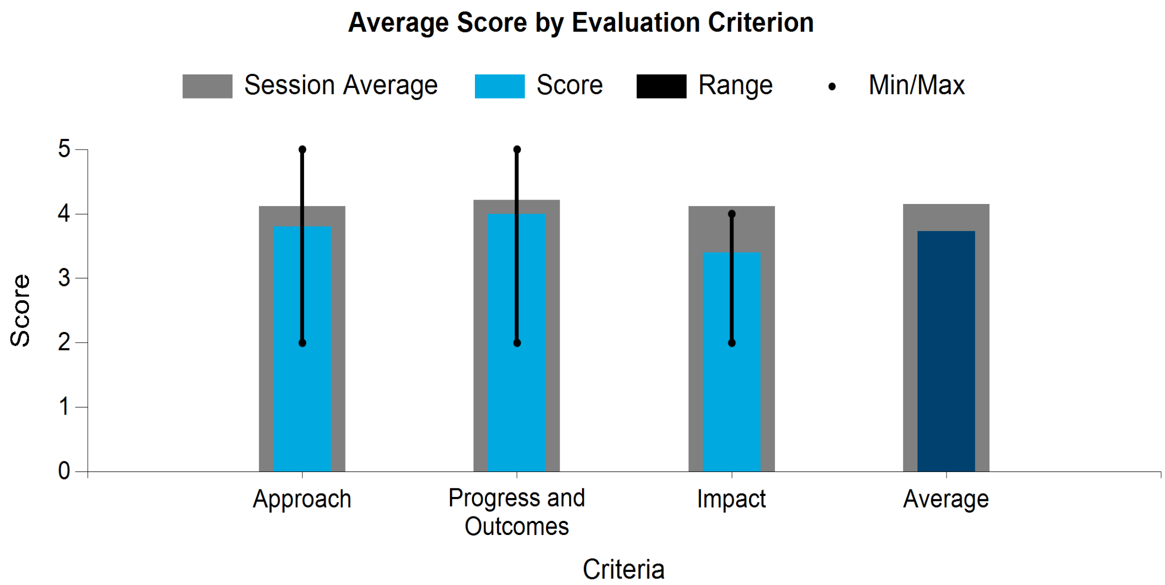
Arzeda Corp.

PROJECT DESCRIPTION

WBS:	2.3.4.208
Presenter(s):	Alex Zanghellini; Aaron Korkegian
Project Start Date:	10/01/2018
Planned Project End Date:	12/31/2022
Total Funding:	$3,704,351

Methyl methacrylate (MMA) is a large-volume petrochemical monomer with a $6 billion/year global market. Its homopolymer, polymethyl methacrylic acid (pMMA), is a transparent plastic with applications in surface coatings, automotive and aerospace casts/sheets, and optical devices. Tulipalin A (i.e., alpha-methylene butyrolactone [MBL]) is a sustainable monomer that as a homopolymer or copolymer with MMA yields materials with similar properties as pMMA but significantly higher Tg (105°C for pMMA, 195°C for poly[alpha-methylene butyrolactone] [pMBL]) and improved scratch and mar resistance, weatherability, and birefringence in optical applications. MBL occurs naturally in small amounts in tulips, the metabolic pathway is only partially known, and the molecule is not produced by any microorganism. Chemical routes are too expensive to reach target prices, so today there are no scalable, cost-effective production routes.

Using proprietary computational pathway and enzyme design techniques, Arzeda has developed an MBL catalytic route. The implementation and development into a fermentation host has produced titers of 5 g/L. Bioprocess development has further demonstrated that the process is amenable to use with sustainable lignocellulosic material. Arzeda has developed a downstream process for the extraction and purification of MBL monomer from fermentation broth at high purity and yield and has demonstrated the ability to polymerize monomer into the clear plastic pMBL. Desirable thermal, mechanical, and optical properties that rival those of its competitor pMMA have been confirmed in collaboration with Pacific Northwest National Laboratory.



COMMENTS

- The goal of this project is to produce tulipalin A, a potential replacement for methyl methacrylate. Details were vague, so it was difficult to evaluate progress; however, the underlying science/technology is impressive and represents the SOA with regard to enzyme and pathway design. While the team is on track, the current results do not suggest that this work will yield an economic process. They are currently making 150 mg/L of tulipalin A, which is at least two orders of magnitude less than required for a commodity chemical. There are not many examples where such increases are possible.

- The reviewer also questions the overall logic of this project. Most successful biological products work with a native producer that for some reason likes to produce high amounts of a fermentation product. It is questionable whether you can start with product and then work backward. Yes, you will be able to establish proof of principle, but generating a strain that will produce a commodity at scale requires high productivities and titers and is an extremely difficult task. There are hundreds of examples of such failures in the literature.

- In summary, this is an interesting project utilizing cutting-edge science that is unlikely to yield a viable product. The key strength is the use of computational enzyme engineering. The key weakness is the lack of TEA or any justification for why tulipalin A can be produced biologically at costs necessary for a commodity chemical replacement.

- The project aims to develop a microbial strain that can produce, via fermentation of lignocellulosic material, a performance-advantaged bioproduct that is otherwise produced in nature via an unknown metabolic pathway. The project is interesting in that the market price for tulipalin A is high, and chemical routes are not cost-effective. Should the team succeed in refining its fermentative production, the product would be valuable. The approaches utilized in this project could expand opportunities to design pathways for other new products.

- The approach of combining computer modeling with wet lab experimentation to develop the catalytic route, strain, and processing approaches is sound.

- The project has achieved some project goals: It has succeeded in producing the target product in small quantities and high quality. The project will need to increase the titer for practical applications. Many technical and management details were unavailable due to the proprietary nature of the research.
- The project aims to develop a biological route to tulipalin A, a monomer used for the production of pMBL as a potential substitute for pMMA. The project has made significant progress to date, achieving key technical milestones such as pathway design and screening achieving, high-throughput optimization, and meeting initial process performance targets with over 99.9% purity monomer precursor at titers of 5 g/L. That said, a more thorough discussion on yield and productivity is warranted because these are typically the primary cost drivers during fermentative small-molecule production.
- The project structure is well developed, leveraging the biodesign capabilities of Arzeda along with the expertise of the national lab (Pacific Northwest National Laboratory) in monomer and polymer characterization. The project's staged management plan, involving design, high-throughput testing, and integrated process development, has contributed to its success by strategically stage-gating resource-intensive aspects such as fermentation process development after achieving key pathway performance targets. The parallelization of certain aspects of the project, such as downstream process development using mock mixtures, has also been pursued to increase overall project efficiency.
- The absence of specific technical details, such as graph axes and the naming of metabolic intermediates or fermentation products, makes it challenging to fully assess the feasibility of future development plans, particularly in achieving commercial yields, titers, and productivities. There may be flux imbalances between different parts of the pathway, and the nature of the remaining technical challenges may be fundamentally different from those addressed in the project to date.
- The potential impact of the project is high because pMBL is a sustainable polymer with potential performance advantages over pMMA, such as increased solvent resistance, high glass transition temperature, and high elastic modulus. The project has also made progress toward industry partnerships and manufacturing agreements, as demonstrated through sampling agreements and a manufacturing letter of intent, which may decrease commercialization risk. Additional integration of downstream partners from industry or national labs could benefit the project because there may be areas where pMBL is advantaged compared to pMMA (such as solvent tolerance) but also areas where it may be deficient (such as elongation at break). While a snapshot of aspirational business development efforts was provided, it is still unclear to what extent pMBL is a true substitute for pMMA in the identified application spaces.
- The project's approach has some potential to provide a more sustainable pathway to producing acrylate.
- Risks/challenges are listed in the presentation, but no mitigation strategies are outlined. How will the challenges outlined be addressed? It would have been helpful to propose potential mitigation to the challenges outlined.
- There is no TEA to support the economic claims. Can a TEA be provided to assess the economic impact, if any?
- No DEI plan was outlined in the presentation. How and where does DEI fit in this project?
- Some collaboration with contract manufacturing partners and potential partners at various scales are mentioned, and 2 kg of tulipalin was shipped to 15 companies. What is the current TRL? Is the project still at such a small scale since 2018?

- What is the intermediate metabolite? It seems to be more concentrated than the desired target product. Future work should look at ways to produce more of the target products and less of the intermediate. Maybe focus on another pathway that produces less intermediate metabolite and more of the product? What is the benefit of focusing on the current pathway if it is not quite satisfactory?
- The project presents a structure with no timeline. It is difficult to assess progress with no timeline.
- It is challenging to accurately review the data presented when the axes in the graphs have no units and are not labeled, the culture times are not disclosed, and the metrics are not clear. What is the productivity? What is the process yield? How much does the natural enzyme produce versus the designed enzyme?
- What is the commercial-scale viability for this project?
- The project goal is to deliver a commercially viable synthesis of bio-based pMBL. pMBL can be a performance-advanced polymer counterpart of MMA; however, tulipalin is difficult to obtain in sufficient quality at low costs. Thus, biosynthesizing tulipalin from sugars for cost-competitive pMBL makes this project attractive. The risks are thoroughly discussed. The project approach is adequate, and the progress is on track. The proof-of-concept enzyme is developed, and pMBL is synthesized to characterize its polymer properties. The resulting MBL and pMBL show excellent properties; MBL at 99% purity was obtained, and pMBL had impressive thermal, mechanical, optical, and solvent resistance properties, better than that of pMMA and the literature-reported pMBL. MBL was also demonstrated using deacetylated and disc-refined hydrolysate, which can greatly improve its commercial potential. The team is actively developing commercial partnerships for product manufacturing and market development. Overall, the project approaches and progress are appropriate. Although the product titer is still much lower than the commercially viable titer level (5 g/L compared to 20 g/L), the results are encouraging. It would be helpful if TEA is given to discuss the cost of pMBL compared to pMMA.

PI RESPONSE TO REVIEWER COMMENTS

- The vagueness in describing the specific pathway and strain utilized was done intentionally to protect confidentiality, and we understand and sympathize with how that can make a thorough review difficult. Details of the pathway were shared with and reviewed by the DOE technical team privately. As a point of clarification, our current achieved experimental titers are at 5 grams of tulipalin A per liter of broth and not 150 mg per liter. This is still short of our estimated 20 g/L needed for initial engagement; however, we are off by four times and not orders of magnitude. I would agree that the goal of creating a novel strain to produce a product that is not produced biologically in nature by any known microorganism is indeed challenging; however, having reached 5-g/L titers while still operating from plasmid without significant optimization of expression, strain, or fermentation, or encountering any issues with toxicity from production in the current host, I believe there is reason to be optimistic that there is a path forward to continue to improve titers. Granted, this is a significantly more difficult problem than optimizing the production of a native pathway in a given host. We appreciate and agree with the concept that the approaches described in our presentation are generalizable to any biologically produced performance-advantaged product, and we are always looking for new potential applications of our platform. We agree that titers will need to be further increased by at least fourfold for any practical commercial engagement and tenfold to further open up the market opportunities to a broader range of applications. Lab-scale research is still required before it would make sense to attempt any scaling for manufacture, although TEA should be taken into account. We agree with the reviewer that measurements of yield and a clear TEA of market opportunities are needed metrics for evaluating the likelihood of success or identifying key risks to be addressed. We are tracking these; however, for the purpose of confidentiality, we were not able to share them in a public setting. We recognize that this answer is not particularly satisfying. Similarly, we understand that not disclosing specifics with regard to our pathway, strain, or production rates makes suggestions and constructive criticisms at times difficult. For each slide presented, we considered what we felt we could share at the time given the public nature of the presentation. We agree that there is risk in pathway engineering for losing yield due to issues of relative flux or the production of off-target products, and as a means of mitigating that risk, we are measuring yield and carbon utilization to monitor for off-pathway products. Although we were not able to share the specifics of those results for confidentiality, we have not yet encountered an insurmountable issue to date, and we have shared that information privately with the DOE technical team. We recognize that additional research in the application space is required before it is clear if applications of tulipalin are commercially viable, and we are in negotiations with several potential application business partners to supply them with sufficient bio-acrylate products for them to conduct their testing for evaluation once fermentation titers and purified yields are sufficient to supply. Potential project risks were identified and used as a means of crafting the project plan, which was reviewed and accepted by the DOE technical team. As part of the de-risking effort, a TEA was produced and shared with the DOE technical team; however, for purposes of confidentiality, we did not wish to disclose the findings in a public setting. The project TRL is still in a research phase to prove feasibility, which will require sufficient (kilogram) quantities of bio-produced MBL to be supplied to potential business partners. We are currently engaged with partners for the applications testing required before they would commit to purchasing at a certain volume and price point. Once a commercial agreement is reached, the project will move to a TRL for reaching the price point required to sell with adequate margin for that application space. The intermediate metabolite is a natural product generated by an engineered strain and is the starting point for the engineered tulipalin pathway. The identity of the intermediate metabolite is confidential and was thus not shared publicly but was shared and vetted with the DOE technical team. This reviewer astutely points out that the intermediate is at higher concentration in the production broth than the target. This is an indicator that the pathway producing intermediate is faster than the pathway producing product. Further refining the full pathway will be the primary focus for improving production by increasing flux through the pathway leading to the target from intermediate to increase target titers while decreasing intermediate titers. We believe that the current engineered pathway to tulipalin is satisfactory, as demonstrated *in vitro*; however, the enzyme production and/or activities need refinement to improve flux through to the final target over the intermediate. We understand the difficulty in critically evaluating the project progress and timelines when information such as productivity and yield are not disclosed in the presentation due to confidentiality. We have presented those metrics to the DOE technical team, and they are part of our validation review process. Currently, the pathway flux is pulled by the designed last-step enzyme from the two initial-step natural enzymes. The natural enzymes are not annotated as having this specific substrate to product conversion; however, we demonstrated *in vitro* that they were capable of conducting the reaction to completion at viable rates, though the production/rate of the enzyme in strain likely needs further refinement. Commercial scales depend on application, and we gave examples of low-, mid-, and high-volume potential applications for the product that would require a range of production scales and production yields/rates. Initial commercial engagement could be done in a low-volume application where tulipalin is used as a copolymer or is used for a high-value application such as photoresist polymers for chip manufacturing. Further refinement of yields, rates, and processing could reach additional application spaces, requiring higher production volumes and lower costs. As the reviewer highlights, there is a gap between the current production and the production required for commercial engagement. Therefore, the current focus of the project is to further improve production titers/rates/yield to achieve the amounts needed for initial commercial engagement. That number was determined through the production of a TEA for some of the lower-volume, higher-value applications identified for which we are in discussions with business partners. A TEA was shared with the DOE technical team as part of the validation but was not shared during the public presentation for reasons of confidentiality.

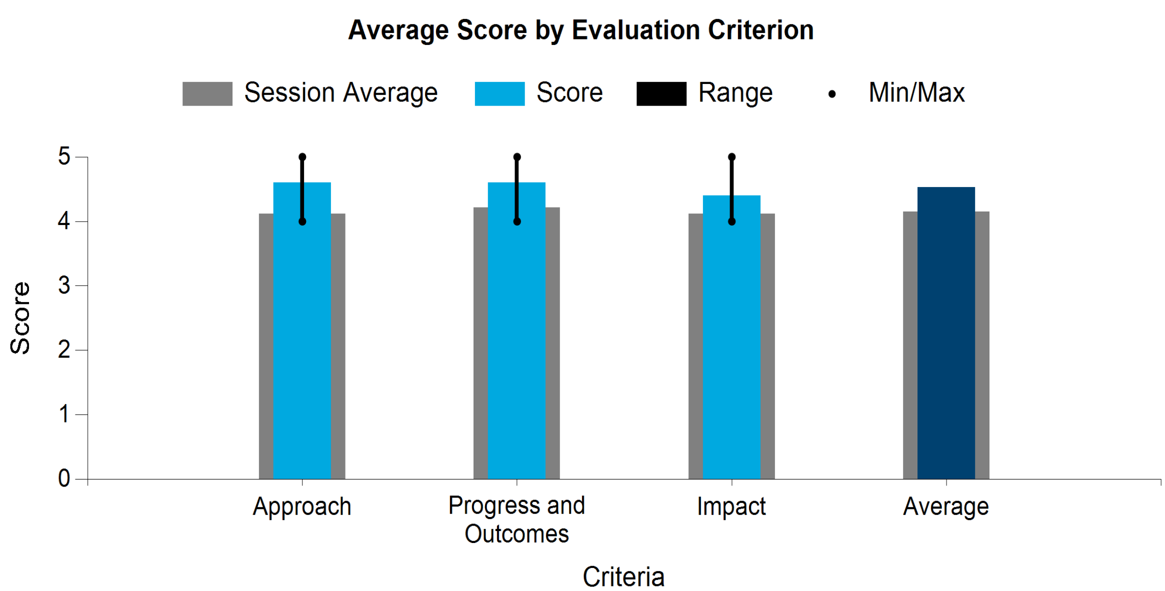
BENCH-SCALE RESEARCH AND DEVELOPMENT

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.4.1.100
Presenter(s):	Laura Hollingsworth; Megan Krysiak; Nancy Dowe
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2023
Total Funding:	$2,250,000

Bench-Scale Research and Development develops and optimizes fermentation processes to produce bio-based fuels and chemicals for commercial scale-up. The project uses fermentation science to achieve high titers and rates and develops online control strategies for better fermentation operations. For this review, we continued developing a commercial-ready 2,3-BDO fermentation from biomass sugars using NREL's proprietary *Zymomonas mobilis* microorganism. 2,3-BDO is a versatile, low-carbon chemical that can be catalytically upgraded to a variety of hydrocarbon fuels and chemicals. The project had three goals: Evaluate the technical feasibility of using whole-slurry pretreated corn stover, optimize a liquor-based fed-batch fermentation for high titer, and develop strategies to enable scale-up. After evaluating different iterations of a whole-slurry fermentation, a go/no-go decision was made to pivot to liquor only with new TEA performance targets, the main one being a 140-g/L titer. We successfully met this goal, producing 170 g/L of 2,3-BDO at 1-g/L-h productivity and 86% process yield. We developed a near-infrared spectroscopy method for rapid analysis, which was used to maximize 2,3-BDO production. We are preparing to scale by mapping the oxygen transfer coefficient (kLa) and oxygen transfer rate in larger vessels to match our optimized bench system. Our end-of-project goal is to meet the design target 2,3-BDO titer (140–150 g/L) from corn stover liquor at 1,000 L to demonstrate scalability.



COMMENTS

- The goal of this project is to produce 2,3-BDO from hydrolyzed, DMR-pretreated corn stover. 2,3-BDO is a potential platform molecule. The only weakness is that 2,3-BDO is a fairly easy target in the field of metabolic engineering: it has been produced at high titer in a number of microorganisms. That said, it is a valuable target and one with potential for commercialization, whether in *Zymomonas* or any number of other microorganisms. Perhaps it would help for the team to benchmark their work against other approaches in the literature.

- With regard to this specific project, it appears to be well managed. The team is making good progress reaching various metrics. The development of the near-infrared probe is a key advance, and it will greatly help with process optimization and scale-up. The latter is also a key strength of the project, and it is good to see that the team is considering these challenges in their plans.
- Overall, this has been a productive though not especially exciting project. The team has exceeded their milestones and demonstrated that a process based on *Zymomonas* can be used to produce 2,3-BDO at high rates and titers. It is unclear what fermentation parameters are needed for an economically viable process.
- This project focuses on scale-up and optimizing fermentation to produce 2,3-BDO from corn stover in support of BETO's SAF goals. The potential for impact is high.
- The project approach is sound, with risks and mitigation strategies appropriately identified. The team reached a go/no-go decision on starting material and pivoted to focus on liquor fermentation only rather than continue to pursue high-solids hydrolyzed DMR and non-hydrolyzed DMR corn stover.
- The team exhibited creativity when addressing challenges related to monitoring reactor conditions in fermentation scale-up. A handheld, near-infrared spectrometer allows for the rapid analysis of ongoing fermentation. They report successes in using this device. Questions remain regarding how reliable the data from such a device will be should scale-up continue.
- The progress and outcomes are positive. The project has achieved remarkable improvements in titer, exceeding project goals.
- Overall, the team has demonstrated significant advancements in the fermentative production of 2,3-BDO using engineering *Z. mobilis* strains with both purified glucose and DMR-derived substrates, achieving best-in-class product titers and yields. The project has also exhibited, or plans to pursue, collaborative projects with other NREL groups (e.g., separations and upgrading consortiums) to develop integrated processes.
- The management approach (e.g., risk register) appears to have done an effective job guiding the R&D objectives. For example, the use of DMR streams comprising solids presented challenges with materials handling, water content, or enzyme loading requirements that made them unfeasible. By focusing on concentrated DMR liquors, the team was able to circumvent these issues and achieve both high product titers and yields.
- The project has the potential to help facilitate the development of 2,3-BDO as a novel bio-based chemical intermediate, as demonstrated by industry partnerships with BioBrincipia (process scaling) and partners working to convert 2,3-BDO to finished chemicals and products. This could be particularly impactful given bio-based 2,3-BDO's negative carbon intensity value.
- The reviewer encourages the project to embrace fermentation goals other than titer, particularly because 2,3-BDO is nontoxic and exhibits little to no end product inhibition. Particularly as the team now explores process intensification, it may be more appropriate to include a combination of yield and productivity goals.

- The project has made significant progress since the last Project Peer Review and has maintained the process efficiency on pure sugars and cellulosic hydrolysates while increasing 2,3-BDO titer. A 170-g/L titer on pure sugar is impressive, and the PI foresees a similar performance with cellulosic sugars.
- We look forward to reading what the focus on de-risking the fermentation technology for scaling will achieve.
- This is an important project in the BETO portfolio for developing commercially relevant technology and enabling low-cost SAF. Choosing 2,3-BDO as the product is well justified (not too toxic to industrial enzymes, not too many byproducts). A multidisciplinary team consisting of chemical/mechanical engineers, microbiologists, and analytical chemists work together, and their roles are reflected in the project approaches and tasks. The project management and industry engagement are adequate. The challenges in scaling up are logically presented, and various mitigation strategies are developed. The team's approaches to overcoming low sugar concentration and insufficient titer are commendable. 2,3-BDO titer increased to 170 g/L using glucose, showing their effective approach. The online analytical capability was developed to aid process control and optimization. The oxygen transfer rate/kLa maps have been developed for reactor scales from 500 mL up to 1,000 L, suggesting the near-infrared analysis can be extended in a commercial-scale process. Overall, the project approach is excellent, and the project is on track. It will be helpful if the team comments on how the 2,3-BDO productions were affected by the different reactor scales they tested. This information is important in developing reliable TEA to guide commercialization.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive comments and appreciate their acknowledgement of the significant advances the project has made in developing a commercially viable fermentation process to produce 2,3-BDO from lignocellulosic sugars for SAF. For future work, we agree with the reviewers to include other fermentation metrics beyond titer, like yield and productivity, as we work with our industry partner to scale the process and develop a relevant techno-economic model. The near-infrared rapid analysis will continue to play a role in scaling, and we are producing data on 2,3-BDO production in different reactors to validate the oxygen transfer rate/kLa mapping work for scale-up.

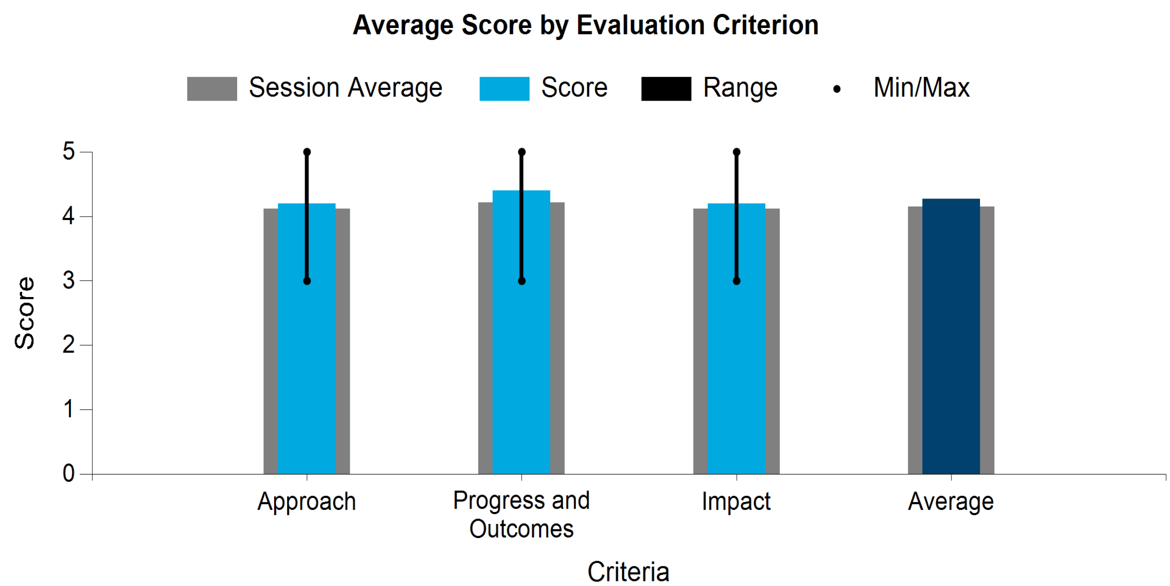
CONTINUOUS ENZYMATIC HYDROLYSIS DEVELOPMENT

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.4.1.101
Presenter(s):	Mike Himmel
Project Start Date:	10/01/2017
Planned Project End Date:	09/30/2023
Total Funding:	$1,650,000

The Continuous Enzymatic Hydrolysis Development project aims to reduce the cost and commercialization risks of second-generation biorefinery sugar/lignin/ethanol production through the development of a readily deployable CEH process. Recent changes in the technical landscape of the commercial enzymatic hydrolysis of second-generation pretreated biomass dictate that the existing hybrid SSF approach be reconsidered. Most importantly, the current practice of "finishing hydrolysis" in SSF must be abandoned. We have recently demonstrated at the bench scale that CEH permits optimal saccharification performance with NREL's DMR solids, because unlike simultaneous saccharification and fermentation with yeast or *Zymomonas*, the pH, temperature, oxygen tension, lytic polysaccharide monooxegenase mediator concentration, and removal of end product inhibitors can be optimized precisely. In scale-up, the goal is to use existing commercial cross-flow ceramic membrane filtration external loops coupled to enzymatic hydrolysis reactors. Pretreated biomass solids and enzymes are retained for reaction while solubilized product sugars are removed *in situ*, with high extents of conversion and longer enzyme lifetimes achieved through a series of reactor-membrane unit stages. The project is focused on advancing CEH as a transformational, process-intensified, lower-cost method for producing soluble clarified biomass sugars and insoluble lignin-rich streams. In summary, the CEH project's primary objective is to reduce the cost of enzymatic hydrolysis by optimizing operating conditions acellularly. Our provisional goals are 10% lower in Year 1 and 20% lower in Year 3 (end of project). This project was reviewed in FY 2020. It is now in its third year of a new 3-year plan spanning FY 2021–FY 2023.



COMMENTS

- This project addresses a key challenge in biochemical conversion by reducing the cost of sugars obtained from biomass through the development of a continuous/intensified process. The development of the pilot plant connecting multiple unit operations is a strength of the project, as are detailed costs calculated. The team has made excellent progress, as evidenced with a cost reduction of 25% through the combined effect of higher yields and lower enzyme loadings. While the science is not especially exciting or cutting edge, the project addresses an important problem that could have wide impact. In these regards, it is an important problem that addresses a central problem in biofuel production: enzymatic hydrolysis.

- Overall, the project has been successful. Ideally, further support could be provided so that long-term runs could be performed to establish both the stability and viability of the pilot plant.
- The project supports BETO's goals with respect to cellulosic sugars.
- The project exercised due diligence in reviewing and refining the project approaches and goals with the onboarding of a new PI. The project demonstrates interest and engagement of industry partners. The project exemplifies creativity and consideration of DEI opportunities with its emphasis on supporting women- and minority-owned industry partners and vendors. As DEI goals become more common among BETO-funded projects, this may serve as an example among many possibilities of how to further DEI goals.
- The project review shows careful consideration of risks and successes in overcoming some and beginning to overcome others.
- The successful development of CEH at larger scales has the potential for significant impact.
- The project aims to develop a CEH process to address issues associated with batch enzyme hydrolysis (i.e., rate limitations and product inhibition of enzyme activity). The goal of the project is to improve the economics of an integrated process from DMR feedstocks through finished end products, including traditional biofuels/chemicals and SAF, by reducing enzymatic hydrolysis operating and capital expenses through process intensification. Overall, the project has the potential to significantly contribute to addressing the challenges associated with enzymatic hydrolysis and promoting sustainable processes for biofuel production from DMR slurries in the future.
- The team has made significant progress in implementing the CEH process. Utilizing a benchtop-scale unit, they have achieved a 24% reduction in MSP associated with CEH, primarily through reduced hydrolysis and conditioning costs, as well as cellulase enzyme cost. The team has also shown that even enzymes evolved for reduced product inhibition still benefit from diafiltration, suggesting that kinetic phenomena and increased time to failure of the enzyme may be contributing factors.
- The project's achievements include a near-theoretical yield of glucose and close to 90% xylose yield with low enzyme loading in a mock or semicontinuous process. Here, the collaboration with Novozymes for enzyme production should also be highlighted as a positive technical approach indicator as the limitation in xylose production is being addressed through enzyme formulation adjustments. At the pilot scale, the assembly of a skid comprising a high-capacity tangential flow filtration membrane with a 1,000-L saccharification tank is a significant milestone because it allows for processing the slurry with high rheological value, addressing the challenges associated with DMR slurries at a smaller scale.
- Regarding DEI, it would be nice to see a stronger commitment (i.e., more definitive language around these goals), but it is noted the project is taking positive steps toward supporting this objective.
- During enzymatic hydrolysis, enzymes tend to bind to the solids, and some go with the liquid. The PI mentioned that most of the enzymes stay with solids in the CEH process. Is that percentage known? Is enzyme recycling being considered? If not, it would be something to consider given the enzyme dosage used in the process.

- The project results demonstrate several advantages of CEH over batch enzymatic hydrolysis. The TEA shows that reduced enzyme costs and increased sugar conversion are the main contributors to the reduced MSSP. Increasing glucan yield by 20% using a lower enzyme loading is impressive. There was a recent project leadership change. The new management plan is in place, and it seems to be reasonable. The modified risks and mitigation strategies are adequate. Several approaches are employed to improve the technology transition in the commercial process, such as using commercial enzymes and a commercial-scale membrane for CEH demonstration, identifying new stakeholders for generating reliable TEA and performing the preliminary TEA. It seems like solid mass loading and the rheology of the slurry are the problem. Because it was mentioned that dilute acid pulp could achieve a higher solid loading than DMR pulp due to the lower viscosity, it will be interesting to know how this affects their TEAs.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate your support. I do consider the diafiltration-assisted enzymatic hydrolysis of pretreated biomass to be the next level of process evolution; however, as I mentioned, fully relieving even the best commercial enzyme formulation of end product inhibition will deliver the best economics for this second-generation sugar production unit operation. And the macro/microporous ceramic membranes available today make this possible. We are planning, in the next 3-year funding cycle, to demonstrate the reliability and feasibility of the long-term CEH operation at a large scale.

- Thank you for your support.

- Very thorough and accurate summary, thank you. We are indeed working on bringing more focus on DEI to the project. The only student working on the project is a woman, and we have made a commitment to employ only woman-owned companies, where possible, to outside services when needed for reactor repair/modification. Going beyond this planning, I do see opportunities to reach out to students with underrepresented backgrounds for rotating assignments working with the CEH system, especially those from the NREL Student Training in Applied Research (STAR) program.

- This is a very interesting topic and one that is not entirely known at the molecular scale. It is true that the most active individual enzymes are thought to remain bound to the substrate until hydrolysis is complete; however, the "duty cycle" of cellulases is to function processively on a strand of cellodextrin until further processing is not possible, and then release from the surface. It is assumed that each enzyme then quickly reacquires another binding site and continues on, releasing more cellobiose and glucose. Once the enzyme has been sufficiently "damaged," it can no longer bind to cellulose and is considered inactive. So, this is really an effect defined by the time period of observation. In the process-level timescale, active enzymes remain associated with biomass and inactive enmesh do not. This also means that attempts to recycle cellulases by classical means fail. Of course, one must be certain that enzymes are not lost through membrane pores that are too large or to membrane surfaces that bind proteins (such as PVDF polyvinylidene difluoride membranes).

- Yes, this is true, but overall the DMR pretreatment is much superior to the dilute acid pretreatment. Specially, DMR results in a much more hydrolysable substrate. When acid hydrolysis is used, there is always some replating of lignin onto the cellulose microfibrils. Even with the best process control, this is unavoidable. When alkali pretreatments are used, lignin remains fully soluble and is more completely removed through a series of washing steps. Put another way, 0.1 M NaOH is essentially a true theta solvent for lignin. The other concern for acid pretreatment is the degradation observed for lignin at pH 1.5 and 160°C compared to DMR. Finally, acid pretreatments often result in the generation of fermentation inhibitors from reversion and other reactions. So, we took on the challenge of adapting ultrafiltration with small-scale but commercially relevant systems to handle the rheology exhibited by DMR solids. We also note that when these ultrafiltration systems are scaled to the true commercial scale, the larger piping, pumps, membranes casings, etc., will reduce most of these concerns. This is the dilemma of doing bench-scale or small pilot-scale work with slurries—some of the flowability issues will disappear upon final scale-up.

SUGAR IS THE NEW CRUDE

AVAPCO LLC

PROJECT DESCRIPTION

WBS:	2.4.3.201
Presenter(s):	Kim Nelson
Project Start Date:	10/01/2021
Planned Project End Date:	05/31/2025
Total Funding:	$3,500,000

The Sugar is the New Crude project will demonstrate the production of lignocellulosic sugars with three levels of purity from three low-cost feedstocks—construction waste, energy cane, and forest residues—using AVAPCO's patented AVAP biorefinery process. These feedstocks have been identified by DOE, USDA, and the bioeconomy industry as offering cost-advantaged production of biofuels and bioproducts, as well as additional advantages, including:

- Reduction of escalating, costly forest fires (forest residues)
- Landfill CO_2 emissions (construction waste)
- Exceptional carbon sequestration (high-productivity energy cane).

With the growing commercial interest in sustainable aviation and marine fuels, a wide variety of low-cost biomass feedstocks will be required to satisfy extremely large aviation fuel markets.

AVAP's downstream partners—BASF, Arbiom, and Corbion—will evaluate the quality and convertibility of the sugars to a proprietary biochemical, a second-generation feed protein, and lactic acid to gain a diverse understanding of the quality of the substrates and market potential. In addition, an established alcohol-to-jet technology partner will evaluate the technical specifications of cellulosic ethanol produced by AVAPCO from the various AVAP sugars to confirm if the ethanol from each source meets their quality requirements for conversion to SAF. Students and professors from Clark Atlanta University—a historically Black University—will perform data science analysis of project data.

Goals of the project include:

- Reducing the specific manufacturing cost of AVAP sugars to <$0.20/lb through utilization of three low-cost feedstocks and process intensification
- Confirming the TEA and LCA benefits of low-cost feedstocks and AVAP process intensification for production of high-conversion second-generation sugars
- Incorporating underserved communities on the project team and STEM mentorship.

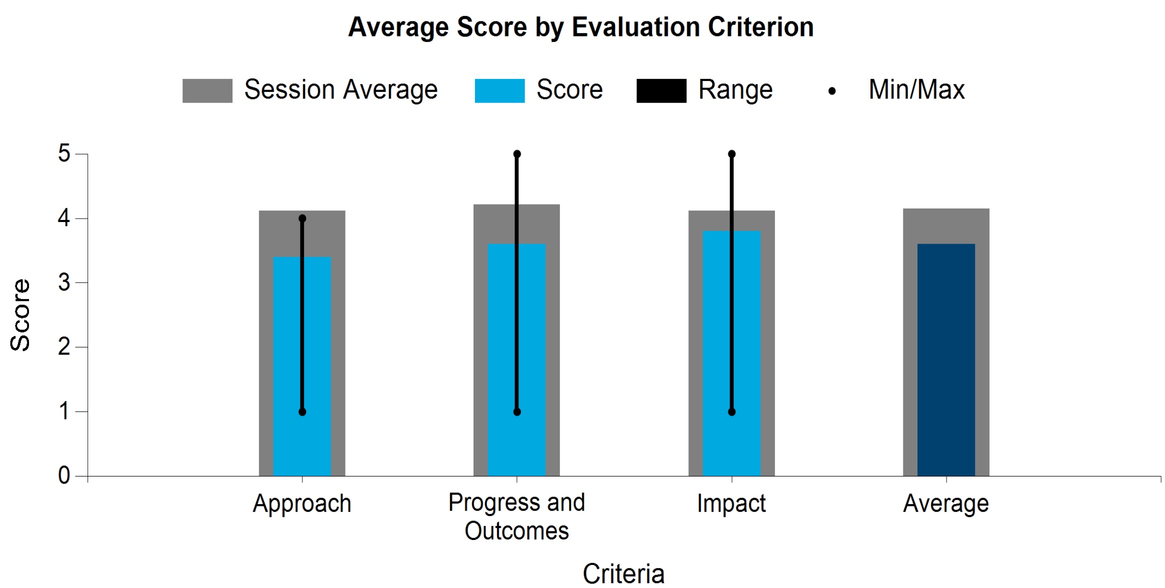
The project passed the initial verification gate in December 2022. The baseline LCA considering hardwood chips gives an 82% reduction in GHG emissions (g CO_2eq/kg sugar) for AVAP sugars over corn dextrose sugars. The baseline MSSP estimate of AVAP sugars falls below $0.20/lb for all feedstocks to be evaluated in this project. Process intensification is anticipated to further decrease the prices by about $0.02/lb.

Potential challenges that the project may encounter include:

- Inflation-related price escalation of equipment
- Extended equipment delivery time due to COVID-related backups.

By proving the technical and economic viability of low-cost residual feedstocks, this project will help AVAPCO reach its goal of securing 3% of the world's anticipated SAF demand by 2050, which would require approximately the same daily consumption of biomass as currently utilized by the U.S. pulp and paper industry.

The low-cost residual feedstocks and AVAP process intensification could reduce the MSSP of alcohol-to-jet SAF by 30% compared to current estimates using woody biomass.



COMMENTS

- This project mostly seems to be about the verification and benchmarking of the AVAPCO process. They are already up and running. They will then validate their process for the production of different grades of sugars. The project also includes detailed TEA and LCA for their process. It is not clear why the milestones are necessary because they can already produce the target sugars.

- Overall, this is a solid project that supports an existing industrial process and will provide detailed data regarding the AVAPCO process. This will enable their pretreatment process to be compared with other processes. This is a strength of this industrial project, which lacks technical details like the others. Looking forward, these sorts of validation projects are the ideal ones for BETO to support. In particular, provide the support so that companies can demonstrate their existing technology rather than develop new technologies.

- AVAPCO has long produced cellulosic sugars using its proprietary biorefinery process. This project aims to refine this process for low-cost and waste feedstocks: energy cane, construction waste, and forest residues. This objective aligns with BETO's sustainability goals. The project advances DEI goals through AVAPCO's long-running collaborative relationship with an MSI, which is analyzing project data.

- The presentation was light on technical details, and as such it is challenging to evaluate technical concerns. The project is demonstrating on-time progress toward its goals.

- Should this research succeed, questions remain regarding scale-up. For example, AVAPCO has identified a local supplier of aggregated and sorted construction waste with sufficient material to supply their process. To what extent are similar supplies available nationally, both currently and if demand grows?
- To date, this project has demonstrated an ability to produce high-quality sugars with excellent process metrics (e.g., 87% sugar yields); now, the project aims to build on the SOA through process intensification (chip pre-steaming and post-fractionation separation) and demonstration of the technology with low-cost, abundant biomass feedstocks.
- There is no mention of process yields in the presentation, just conversion yields. Because the process is feedstock agnostic, what are the overall process yields for each feedstock to be tested? What were the TEA model predictions, and do they match the results at lab scale?
- TEA/LCA and DEI are carried out, but experimental work has yet to be started because the project is working on equipment acquisition and installation. The company has a successful history of producing cellulosic sugars from various biomass based on the AVAP process. Third parties previously demonstrated the utilization of sugars for chemicals. The risks are identified. The project company partners with several feedstock suppliers and chemical companies for sugar utilization, which is commendable. The project goals are excellent: developing a commercially relevant process using non-ideal, low-cost feedstock and developing TEA to include the interplay among the feedstock inhibitor profile, sugar purification costs, and sugar performance in its conversion. Including construction and demolition wastes in their feedstock lists will expand the impact of the project from biomass conversion to waste recycling. AVAP sugars are compared with corn sugars to show a significant GHG reduction. How do AVAP sugars compare to other cellulosic sugar processes? In the TEA, construction and demolition feedstock had the lowest MSSP due to the lowest feedstock price from using the waste material. It would be helpful if the team could comment on what levels of preprocessing and decontamination are required for this waste to become an acceptable feedstock in this project. Was the cost for preprocessing construction and demolition waste considered in the TEA?

BIOCHEMICAL PROCESS MODELING AND SIMULATION

National Renewable Energy Laboratory

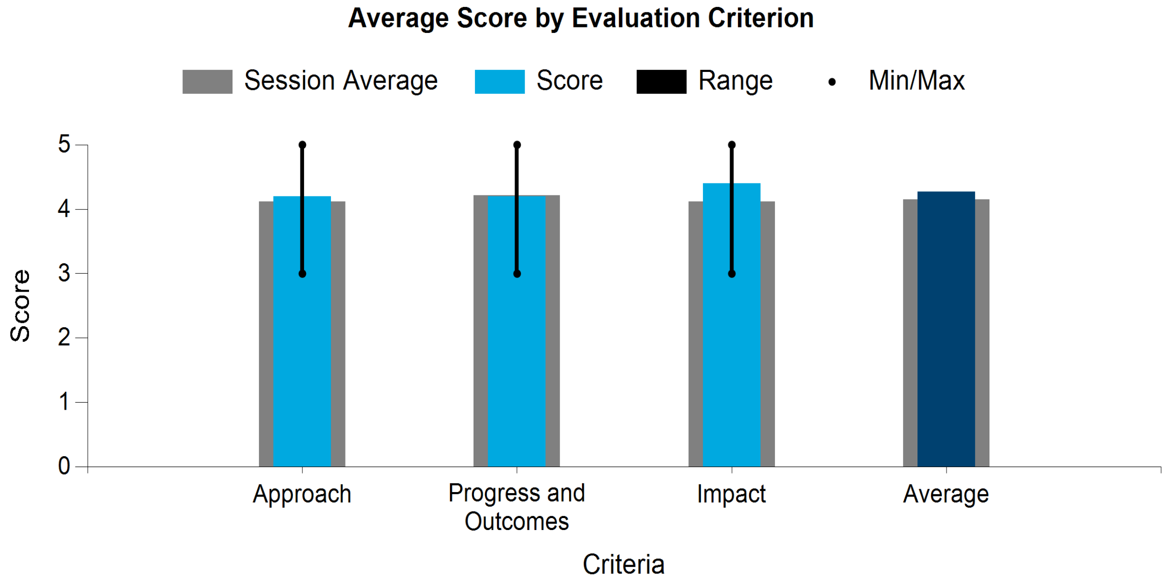
PROJECT DESCRIPTION

WBS:	2.5.1.100
Presenter(s):	Yannick Bomble
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$3,000,000

The Biochemical Process Modeling and Simulation project aims to reduce the cost and time of research by applying theory, modeling, and simulation to the most relevant bottlenecks in the biochemical process. We use molecular modeling, quantum mechanics, metabolic modeling, fluid dynamics, and reaction-diffusion methods in close collaboration with pretreatment, hydrolysis, upgrading, and TEA. The project's outcomes are increased yields and efficiency of the biochemical process, added value to products, and reduced price of fuels by specifically targeting catalytic efficiency, reactor design, enzyme efficiency, and microbial design.

We work closely with experimental projects to identify problems and iterate with experiments to find and refine solutions. By working with experimentalists, we decide on problems that can be solved with simulations that could otherwise not be solved or would take too long with experiments alone to reach BETO's targets. Over the years, we have produced solutions that have resulted in determining the most likely fatty acid derivative for passive transport out of bacteria that upgrades biomass, and we have also designed enzyme mutations for enhanced lignin upgrading. Metabolic models have been developed to tune the activity of 2,3-BDO production for the 2022 target. A computational method to deliver understanding of how complex omics data can be interpreted in the metabolic pathways of organisms is used in the Agile BioFoundry. We have found methods to overcome specific barriers and continue to develop those methods. Our reactor studies have guided the design of both the microbes and reactors for aerobic and micro-aerobic production at all scales and have been instrumental in improving the accuracy of TEA models. This project is essential in the process of selecting the final processes for 2040 SAF production targets.

More specifically, we have recently (1) predicted the strength of the basic structural interactions in commodity plastics to provide guidance for plastic upcycling strategies; (2) developed computational tools to improve the characterization of lignin-derived compounds; (3) developed new methodologies to enable machine learning-based directed evolution for protein engineering; (4) developed machine learning methods to predict protein promiscuity and mutations to further improve microbial and enzymatic-driven processes and demonstrated the utility of machine learning approaches to engineering proteins from sparse experimental datasets; (5) developed new methods to enable high-fidelity simulation of aerobic fermentation at the industrial scale and resolve the mismatch of timescales through subcycling/operator splitting; and (7) identified the difficulty in preventing local high-oxygen conditions in industrial bubble columns, which leads to less desirable acetoin production, suggesting future research directions in alternative reactor configurations (e.g., loop reactors, shallow-channel reactors).



COMMENTS

- This project provides computational tools to support projects within the BETO/NREL portfolio. While computer modeling still has not achieved equivalent success in biotechnology as it has in other technical fields, it is a potential game changer in that it can dramatically accelerate progress. BETO, in particular, can take a leading role in developing accurate computer-aided design tools for biofuel/chemical production. Another key strength of the program is the development of tools from the molecular to macro scale.

- The key outcome of the program is the development of the LigninWrangler tool. This will greatly aid lignin analytics. The other is the use of computational fluid dynamics (CFD) for assessing the performance of different fermenter configurations. The use of timescale coupling is a key outcome because it addresses some of the challenges of CFD simulations over longer timescales. While the work on machine learning and pathway modeling is useful, it is less impressive than the other two initiatives compared to what has been done in the past.

- This project is extremely useful. Its main impact is to provide foundational tools for bioprocess development. While modeling still has a far way to go in biotechnology, it can potentially be a game changer like in other fields. One suggestion is to increase support for CFD modeling because this area is generally underfunded in the United States compared to molecular and pathway modeling. Bioprocess scale-up is still one of the major barriers to commercialization, and this is where CFD can have a huge impact. Another suggestion would be to develop a plan for the long-term support of these computational tools, either by making a source or at least having a plan for eventual loss of support.

- The project provides a valuable service in developing modeling and simulation approaches to challenges in biochemical processes. The project has developed a strategic approach to providing modeling and simulations that will be of most value to the community they serve, within the constraints of available financial, human, and capital resources.

- The project has made remarkable progress with limited funding and significant staff turnover. The project managers have identified staff turnover as a significant risk and ongoing concern. Increasing emphasis on recruiting graduate students is a reasonable near-term mitigation strategy. Ultimately, the project will need to consider how to recruit and retain more senior staff to maintain continuity of operations and provide strategic direction going forward.

- The project's impacts are clear. High among these impacts is the project's development of LigninWrangler, a publicly available computational tool that has seen substantial uptake by the community. It would be useful to see a strategy for developing and making publicly available additional tools and knowledge. Providing opportunities for public feedback or consultations on what tools are most needed can assist in shaping future directions.
- This project has the potential to significantly impact biofuel/bioproduct R&D across BETO's project portfolio. When successfully employed, modeling- and simulation-based guidance can increase R&D efficiency by shortening timelines and reducing overall project cost. While some examples of direct impact were provided, more detailed information would be beneficial to assess the full extent of the project's effectiveness in this regard. An increase in interproject engagement would help magnify the impact of the tools developed.
- One weakness of the project's approach is that its focus is quite diffuse, with work spread across four different research areas. This may be exacerbated by challenges in attracting and retaining top talent in this competitive field. To address this, it may be appropriate to prioritize a smaller number of research areas that address unmet needs in industry or academic research. For example, LigninWrangler appears to be a successful example where a unique tool was developed that addresses a challenging technical problem in the area of biomass deconstruction and lignin valorization.
- A project strength is that its models, tools, and libraries have been made publicly available, providing a way for this work to support the advancement of biofuel and bioproduct research outside of just the national labs. This open approach to sharing resources may promote future collaborations and further increase overall project impact.
- Regarding DEI, the team has made some steps to increase minority student engagement by working with the Graduate Education for Minority Students (GEM) program.
- The project was able to successfully develop tools that facilitate machine learning techniques to guide enzyme engineering with model-based data that have been reproduced at the small scale to validate the model predictions.
- The project has also been able to predict reactor models for 2,3-BDO fermentation yields at the small scale that translate in experimental data. One recommendation would be to improve the model predictions to match the fermentation yields at the large scale.
- The team's approach to working with BETO overall to determine where modeling is applicable and using multiscale approaches to assist and provide guidance for the BETO-relevant processes is excellent. The benefits and impact of this project are clear. Using modeling to overcome experimentally inaccessible space and to guide the system designs improves scientific understanding and can significantly reduce the cycle of technology development. The team supports projects with a wide bandwidth, from bio-based SAF and plastic degradation to cell-free synthesis. The project management is adequate, and the outcomes are commendable. For example, LigninWrangler, a publicly available computational tool developed by the team in collaboration with another BETO project, resolved the long-standing challenge of identifying lignin compounds using a computational and experimental combined approach. Overall, the project made great progress.

PI RESPONSE TO REVIEWER COMMENTS

- We would first like to thank the reviewers for their effort to carefully evaluate this project. Their feedback will help us redirect some of our efforts and consider details we had overlooked. We agree that we always need to remind other projects of the value of modeling and what improvements were or could be obtained from modeling to improve processes. CFD is indeed an area of our project that we think has a lot of promise, notably to help with reactor design for atypical production routes, including complex fermentations and cell-free biocatalysis. We do have budget constraints in terms of our total funding, but we do intend to increase the share of CFD in the next few years. We realize that it can really help evaluate scale-up potential for a variety of processes. We do aim to focus on research projects where modeling could have the most impact, and to do so we are in constant discussion with experimental project leads to demonstrate that modeling can help improve their bottom line. We have tried to refocus over the years and have made progress doing so by wrapping up several ongoing projects. We believe that in 1–2 years we will be able to be more focused than we are now and therefore quicker to deliver on the most important problems. Additionally, regarding the development of publicly available tools and getting public feedback, we try to focus on the tools for which there is a clear need and lack of development; however, we must also be aware of the fact that we have limited funds to achieve our goals and help with near-term experimental projects. Nevertheless, we will make an effort to reach out to the community and see if we have the bandwidth to help. Finally, we are indeed trying to develop more robust approaches to predict the fermentation yields at a large scale using a combination of metabolic modeling and CFD. This approach shows promise when used to predict 2,3-BDO yields, so we are hopeful that we can further improve and apply it to other processes and products.

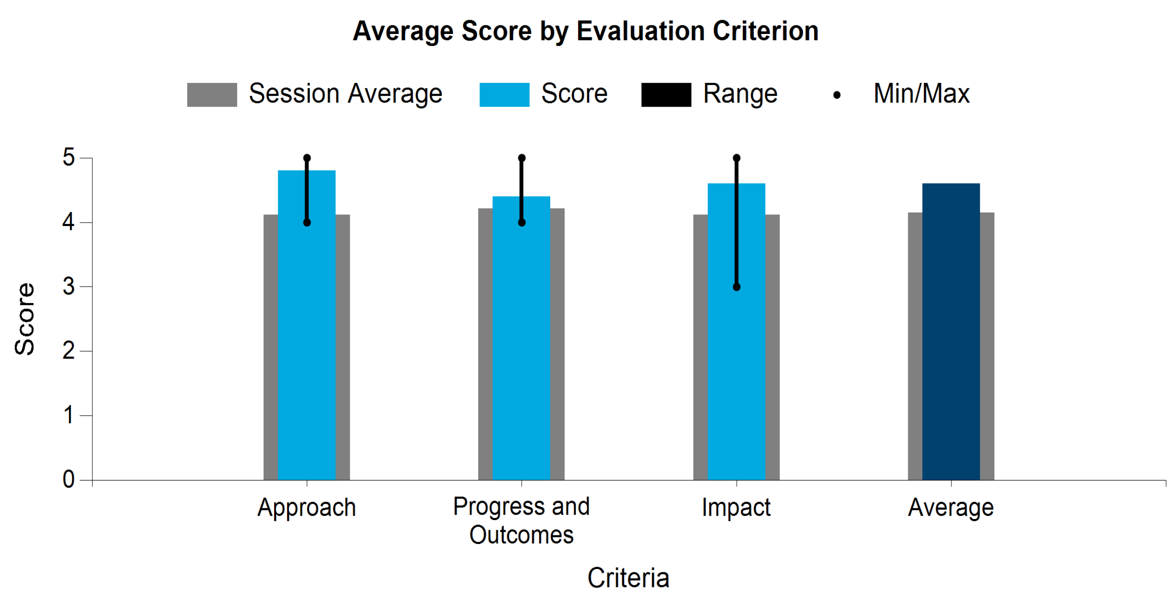
ANALYTICAL DEVELOPMENT AND SUPPORT

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.5.1.101
Presenter(s):	Justin Sluiter
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,025,000

The objective of the Analytical Development and Support project is to produce and maintain the critical analytical methods and tools that enable the evaluation of emerging biofuels R&D within BETO and within the broader biofuels community. Our project is divided into two parts: The development task develops novel analytical techniques and improves existing methods, and the support task maintains existing analytical capabilities at NREL and provides outreach to the wider community. The project is world-recognized for our laboratory analytical procedures, which provide detailed procedures for the compositional analysis of biomass and have been adopted as the de facto standards within the biofuels community, largely due to the transparency of the methods and the high reputation of NREL's research. Our dialogue with stakeholders allows us to provide robust, precise, accurate, and publicly available analytical procedures for better valuation of scientific tools. Our focus is on developing characterization methods to support the conversion of cost-advantaged feedstocks to a variety of fuels including SAF. This project also has four ongoing industry-led agreements for method development that will have a direct impact on biofuel production.



COMMENTS

- The goal of this project is to provide analytical support for 20 different projects within the BETO/NREL portfolio. In addition, the program develops new methods and protocols that benefit the field at large. A key strength is that the team provides detailed merits demonstrating their progress and impact within the field. Another key strength is that the team is working with a number of companies, demonstrating their impact to the field. A final strength of note is the project management and resource allocation: The team has a clear vision on the type of problem that they wish to develop and their unique skill set. Overall, this is an impressive, productive, and well-run project.

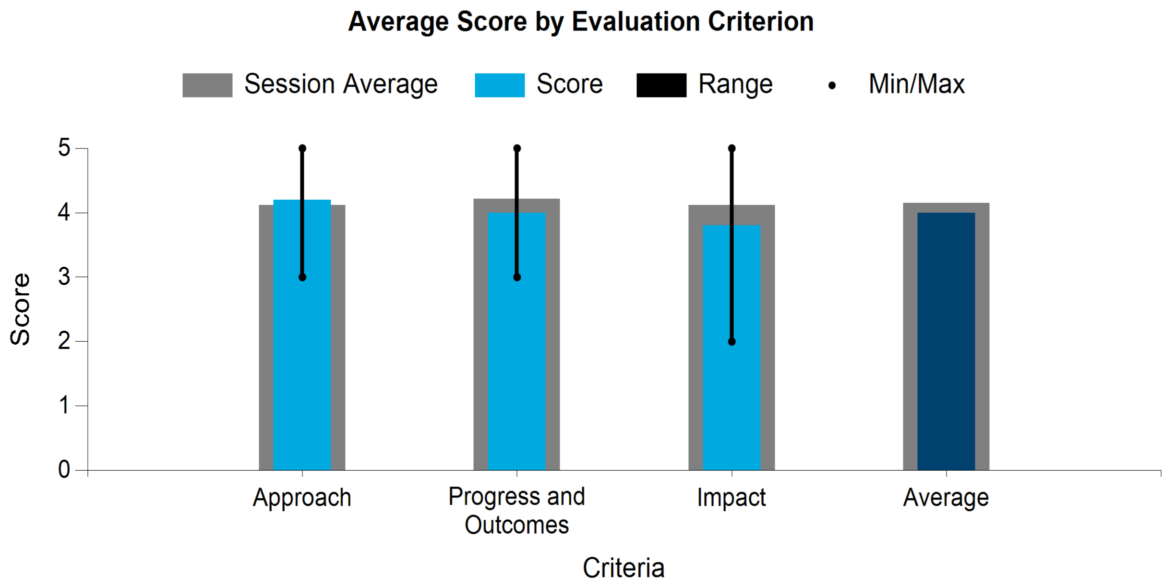
- This is a very important project that supports multiple BETO projects. In addition, this project also develops standards for the broader community and has an impressive working relationship with industry and other federal agencies.
- The project serves a valuable crosscutting purpose, providing support to existing projects, improvements of existing analytical techniques, and the development of new analytical techniques. The project approach maximizes impact for its small team and limited budget. Most collaborative work has been with NREL. The project approach is sound and forward-looking. For example, the group's forecasting anticipates growth in interest in using municipal solid waste as a feedstock, and it has applied appropriate emphasis to prepare for this. A small team implements the project, and as such, staff turnover is a risk. Cross-training staff and developing partnerships are appropriate mitigation strategies. The project has successfully developed partnerships with industry and other groups to maximize impact. Successful industry collaborations demonstrate the value of the project's activities.
- The project's DEI strategy leverages its long-standing relationship with an MSI, and it works to deepen the opportunities that those ties provide.
- The project has a demonstrated track record of delivering novel analytical methods in support of new technologies, both in industry and at NREL, and it serves as a central and shared analytical, quality assurance/quality control, and instrumentation resource to BETO projects. This approach adds value to the BETO (and specifically NREL) portfolio of projects by providing centralized quality and control, coordinating samples between projects, maintaining instrumentation, and training/supporting staff using the equipment.
- The management approach is well thought out and developed, ensuring that the methods being developed are (1) not duplicative with ongoing method development work within BETO or industry and (2) broadly applicable (through work with ASTM) and can be practiced outside the national labs.
- Regarding the progress made, the team has demonstrated excellent progress toward developing a suite of analytical methods enabling good (90%) mass closure on a set of municipal solid waste substreams (e.g., papers and dairy products) and has developed a set of actionable steps to help increase mass balance closure in areas where it is currently lacking. More broadly, the team has demonstrated success supporting both BETO's internal goals (e.g., SAF) and addressing challenges in industry (e.g., cellulose assay for Gen 1.5 ethanol).
- Of note, the collaborations and partnerships are heavily skewed toward NREL projects, which is likely due to project collocation (i.e., it is easy to transfer samples between labs). Project impact could be increased if the team's unique capabilities were being leveraged by projects at other national labs; this could be realized, for example, by continued development of unique and/or specialized analytical methods unavailable at other sites.
- Regarding DEI, the project could elaborate further on how it is engaging Metro State University (a Hispanic-serving institution) and the potential impact of this effort.
- This three-person team has achieved satisfactory milestones and developed new methods that are useful and industry relevant.
- Focusing on wastes streams, this funding cycle is very useful and is helping the current efforts aimed at valorizing those streams.
- Analytical capability and data accuracy are essential parts of research. In this context, this is an important project for the BETO portfolio. The number and diversity of the projects this project supports

are impressive. Another important contribution of this project is developing standard analytical methods and making them available to the public at no cost. The team's approach to creating procedure FAQs and training videos is also an excellent way to help the industry and academia adopt the procedures. The project impact is visible; the laboratory analytical procedures are broadly downloaded internationally. The project also develops analytical capability for low-cost, complex feedstocks (e.g., municipal solid wastes, organic wastes). Such work aligns well with BETO's goal for low-cost SAF and supports increasing efforts in waste utilization. The project also helps industries solve analytical challenges, which is commendable. Overall, this is a high-demand project, and the team did an excellent job. The project approach, risk identification, and mitigation plans are appropriate. The DEI activities are adequate.

ENGINEERED REVERSAL OF THE Β-OXIDATION CYCLE IN *CLOSTRIDIA* FOR THE SYNTHESIS OF FUELS AND CHEMICALS

Northwestern University

WBS:	2.5.3.206
Presenter(s):	Shivani Garg
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2023
Total Funding:	$2,000,000



COMMENTS

- The goal of this project is to produce a range of promising chemicals such as hexanol from syngas by reversing beta-oxidation in *Clostridia*. A key component of the project is the use of cell-free systems for pathway optimization, which is a promising application of this technology. The team appears to be making good progress, though few technical details were provided, making it hard to determine whether this work will result in a viable process. The LCA results are also questionable: How can hydrocarbon-based process require more water than a biological one? This makes no sense, and the team was unable to answer this question.

- Overall, the main impact of this project is to demonstrate the utility of cell-free systems for pathway optimization. Whether its resulting designs yield an economic process is unknown. To answer this question, more details would be required about titers, yields, etc.

- The project aims to develop *Clostridia* to ferment syngas into a variety of advanced bioproducts at the pilot scale. This goal supports sustainability goals. It combines *in vitro* (cell-free) and *in vivo* approaches to assist in pathway design, validation, and production. A project strength is the collaboration among university and industry researchers to advance interdisciplinary objectives.

- The project is continuing to pursue the final milestone under a no-cost extension, after achieving all other project milestones on time.
- To date, the project has efficiently and effectively demonstrated the team's ability to translate an R&D objective (i.e., rapid pathway prototyping for new product biosynthesis) from design through near-pilot-scale application with a potential near-term commercialization with an industry partner. This is likely a testament to the high-quality management of the project and the interdisciplinary team (including expertise in techno-economics). While the team has not yet achieved their end-of-project goal (due August 2023), this appears to be more of a logistical challenge and not due to a technical hurdle.
- The work has the potential to be highly impactful in at least two areas. First, the *in vitro* pathway prototyping approach has the potential to serve as a general model for metabolic pathway optimization, an impact facilitated by the recent publication. Second, the engineered strains provide a route to access a relatively broad suite of small-molecule products from an abundant, inexpensive feedstock.
- As the team aims to wrap up their research, it may be helpful to disseminate more information on where there's room for additional optimization in this pathway prototyping approach. For example, it appears there were some issues translating enzymes from *E. coli* (where they may express well) to *Clostridium* (where they may not), or where specific enzymes may function only in aerobic contexts with glucose.
- Even though the TEA seems not to have been a requirement, it would have been very beneficial to have a sense of the project's economics and have some TEA output to assess if the project meets BETO's cost targets. How economically viable is this process?
- One highlight of this project is producing multiple platform molecules from syngas based on a cell-free system approach. Because syngas is less dependent on feedstock type, developing diverse advanced biochemicals from syngas has a clear advantage compared to other approaches. Although biomass gasification-derived syngas is mentioned in this project, this technology can be extended to syngas based on waste resources (municipal solid waste, waste plastics). The project is scientifically meritorious. By combining the reversal b-oxidation and cell-free system, versatile molecules can be available at high production rates. These molecules could be used as drop-in fuels, fuel additives, and chemical building blocks. The project is currently under a no-cost extension. The progress toward the new project's ending date is excellent. It is impressive that the team far exceeded the milestone targets. The project demonstrated 10 biochemicals but narrowed the products down to butanol and hexanol for pilot-scale development. LCA of the two molecules is completed, and the assessment of infrastructure and biomass supply chains is also performed. Overall, enabling versatile platform biochemicals and the ability to utilize diverse, low-cost feedstock make this project highly attractive. The presenter mentioned that syngas composition is currently standard CO_2, CO, and H_2 but may vary in commercialization depending on conditions. Discussing the potential risks associated with syngas conditions would be helpful. The project is ready for pilot-scale production. Thus, a TEA to evaluate commercial viability will be helpful.

PI RESPONSE TO REVIEWER COMMENTS

- "Subject to disclaimers on the associated presentation." Response: We appreciate the reviewer's comments and questions. Regarding water consumption, an important aspect of LanzaTech's process is water recycling to reduce freshwater use. Further, because LanzaTech's process is decoupled from photosynthesis, the input water requirements are very low. Moreover, the use of water in petroleum extraction is included in the hydrocarbon-sourced chemicals. The LCA system boundary is well-to-chemical. The project has indeed leveraged cell-free systems for pathway validation and optimization; however, in this instance, a whole-cell biocatalyst is advantaged when gases are used as feedstock. Considering the stage of the project, we are not reporting titers and yields because we have yet to begin pilot-scale fermentations. We thank the reviewer for highlighting that all the milestones on the project (except for the final piloting milestone) have been achieved on time. At this time, it remains LanzaTech's intent to assess the performance of our top strain at the pilot scale. Pilot-scale performance is a more accurate representation of strain performance at the commercial scale (versus continuous stirred-tank reactors). We want to thank the reviewer for the encouraging and positive feedback. The reviewer brought up a very valuable point, and the teams are working on further strengthening the correlation between cell-free data and *in vivo* data. This will further help us to predict future experimental designs. Looking ahead, there is an opportunity to develop anaerobic cell-free systems. The advantages and disadvantages of the current cell-free system are captured in previously disseminated manuscripts (e.g., https://doi.org/10.1038/s41589-020-0559-0). LanzaTech appreciates the reviewer's comment. Even though TEA is not a project deliverable, TEA was used to help define the project's performance targets. Further, LanzaTech uses TEA to quantify the impact of performance metrics such as selectivity and productivity on the cost of production. TEA is a tool and one of many inputs into specific business case development scenarios, which ultimately will help define the economic viability of a commercial project. This effort will be carried out downstream of the DOE project. We thank the reviewer for pointing out the scientific merit of the project and for acknowledging the excellent progress that the project has made so far. One strength of LanzaTech's bioprocess is the robustness of the biocatalyst to variable gas flows, gas component ratios, and even potential contaminates. Additionally, LanzaTech has significant experience evaluating myriad gas sources and has developed intellectual property and know-how to address risks that may be attributed to the gas sources. We have operated our ethanol process with a wide range of syngas feedstocks, and we understand the impacts. Another example is the previous DOE-funded acetone project, DE-EE000756, that resulted in the scaling up of acetone production from syngas at the pilot scale. Regarding TEA, as mentioned in the response to a prior question, LanzaTech uses TEA to quantify the impact of performance metrics, such as selectivity and productivity, on the cost of production. TEA is a tool and one of many inputs into specific business case development scenarios, which ultimately will help define the economic viability of a commercial project. This effort will be carried out downstream of the DOE project.

CELL-FREE AND IMMOBILIZATION TECHNOLOGIES TO PRODUCE SUSTAINABLE AVIATION FUELS AND OTHER BIOPRODUCTS

National Renewable Energy Laboratory

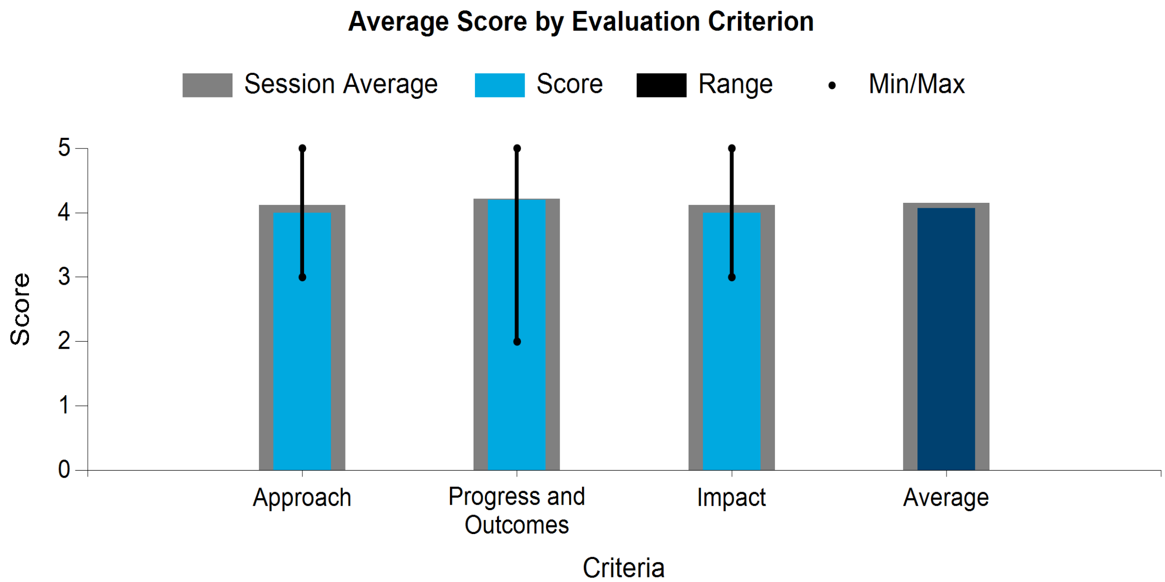
PROJECT DESCRIPTION

WBS:	2.5.4.101
Presenter(s):	Yannick Bomble
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$3,685,000

Today, several key factors negatively impact the production of fuels and chemicals from renewable sources. Common hindrances in the biological production of biochemicals are: (1) end product or intermediate toxicity to the microbial biocatalyst, (2) the diversion of carbon to biomass formation, and (3) coproduction of undesired byproducts. A particularly attractive alternative is to eliminate the biocatalyst entirely and instead operate the desired metabolic pathways in isolation, thus circumventing the roadblocks of biological toxicity, lower yields, and lack of specificity; however, cell-free enzyme systems still suffer from low productivities, owing in part to the effects of free diffusion of intermediates, lack of long-term enzyme stability, cofactor cost or inefficient recycling rates, and, finally, the cost of enzyme production/purification. This project represents a new effort to propose innovative and cost-competitive routes to producing biochemicals from a variety of feedstocks using cell-free approaches. These routes will help reduce the current risk and cost associated with classical cell-free production. Cell-free technologies show promise for application to the production of toxic/inhibitory products or products difficult to separate from microbial growth media and can help reduce the production barriers in multiple areas of the biological conversion of feedstocks to biochemicals.

More specifically, we are developing new technologies and routes that could be used to produce high-value biochemicals such as 2,3-BDO and terpenes (among many others) from biomass-derived C5/C6 sugars or lignin but also from waste byproducts such as glycerol. This project will lead to significant innovation and also new concepts and the rational design of pathways and enzymes. Within this project, we will develop new metabolic enzyme cascades that will represent natural or artificial combinations of enzymes to produce the desired biochemicals from a variety of feedstocks. We are also developing basic design principles for constructing synthetic metabolons, using fusion proteins and synthetic protein scaffolds, to promote substrate channeling and stability while conserving peak activity. Additionally, our efforts include a TEA of cell-free approaches to provide the sensitivities of the process to enzyme loading, activity, pH, reactor volumes, and cofactor recycling rates. Finally, we are focusing on further increasing the stability, operating lifetime, and efficiency of the pathway enzymes by immobilization on support surfaces. We are also focusing on immobilizing pathway enzymes or combinations of enzymes on several different conducting polymers and evaluating the effect on stability and operating lifetime. As more combinations become available, we will conduct a more systematic study of the means of immobilizing these enzymes. This preliminary work will enable the in-depth study of cofactor recycling at these interfaces using mediators for electron transfer. Together, these approaches will enable process intensification, continuous operation, lower capital and separations costs, and end product flexibility, and thus they have the potential to significantly contribute to BETO's goals of cost-competitive biofuels and bioproducts.

To date, we have (1) demonstrated the conversion of pyruvate to 2,3-BDO (four enzymes with cofactor recycling; no additional cofactors needed) at >100 g/L (>3 g/L/h) using our enzyme tethering approach; (2) generated mutants of a key redox enzyme with >180-fold improvement in nicotinamide adenine dinucleotide (NADH) utilization over wild type to >85% of NADPH utilization; (3) produced mevalonate at >10 g/L from glucose, limonene at >10 g/L from mevalonate, and >5 g/L from glucose with crude enzyme preparations and complete cofactor recycling; (4) successfully generated fully active cross-linked aggregates of NOX, a cofactor-regenerating water-forming oxidase that is key to our process with increased stability; and (5) engineered and identified enzymes able to use the biomimetic cofactor NMN and synthesized new synthetic cofactors.



COMMENTS

- The goal of this project is to produce terpenes using a cell-free system. In addition, 2,3-BDO is being pursued, presumably as a proof of principle because it can already be produced at high titers using microorganisms. With regard to terpenes, the team is making good progress with a strong risk mitigation plan. The work on immobilization and biomimetic cofactors is really nice and exciting science, though this is still a low-TRL project relative to others within the BETO portfolio.

- One question concerns the impact of cell-free technologies. There is no question that these technologies can be useful for pathway optimization. The question is whether cell-free systems can be used to produce chemicals economically due to the cost of enzymes (the reviewer is skeptical). In the reviewer's mind, this is a key question. Rather than trying to produce complex chemicals, why not first see whether you can produce a redox-balanced chemical like ethanol or lactic acid from glucose at some intermediate scale (e.g., >100 L)? Such a project would be useful for demonstrating the potential of cell-free systems and would directly address these recurrent questions. Otherwise, this project is a bit of an outlier in the BETO portfolio and seems more appropriate for a different program more focused on basic science/technology. Despite these criticisms, the team is making good progress and developing some promising approaches. They are accomplishing what they proposed to do.

- This project aims to develop new science and technologies to produce fuels and chemicals in cell-free systems. This goal supports BETO's goals for SAF. This research has high potential for impact, but it must overcome many challenges to achieve that potential. The team has developed a reasonable approach and engaged in active management of the research to maintain focus on the most promising opportunities. Collaborations with other BETO-funded projects, academic researchers, and industry contacts strengthen the approach.

- Cell-free systems promise advantages over traditional biological conversion, including the potential for improved predictability and yield and elimination of toxicity concerns; however, cost and scale-up are ongoing concerns at this early stage in the development of the technology and into the future. This project acknowledges those concerns and uses TEA to guide the research. Details of the TEA were not presented.

- The strategy of focusing on terpenes as products ripe for production in a cell-free system, due to their toxicity, reasonably explores a need unmet by traditional biological conversion.
- The project provides an innovative technical approach, cell-free biosynthesis, to address issues with traditional, microbial production systems (e.g., limitations on productivity and titer). In addition to enabling the production of molecules that may be too toxic for living cells (e.g., many short-chain alcohols), the technology has the potential to achieve substantially higher productivities than typically witnessed in microbial fermentations. Thus, long-term, cell-free technologies may help not only expand the range of products accessible from lignin and sugars but also decrease production costs and simplify process scale-up.
- The team has demonstrated that they are actively managing the project to ensure that the research directives are advancing the technology (i.e., increasing TRL level) and/or addressing major cost centers associated with cell-free systems (e.g., cofactor and enzyme cost). As an example, management discontinued work on cofactor recycling via electrochemistry approaches and increased partnerships with industry experts to help address specific areas of risk.
- Substantial progress has been made to date, including directed evolution of a NAD-utilizing GapN (achieving 80% of activity compared to the wild-type enzyme with NADPH) and the production of terpene pathway intermediates (mevalonate) and products (limonene) at >90% yields. The planned work to produce synthetic mimetics of NAD(P)H has the potential to address one of the most significant disadvantages to current cell-free reaction schemes; if successful, this alone would be broadly useful given the ubiquity of NAD(P)H-dependent redox reactions in microbial metabolism.
- The project would benefit from a rigorous assessment of enzyme performance parameters, namely, the total turnover number and the specific rate to determine what, if any, additional work needs to be performed to engineer (or select for) more stable variants.
- The project has outlined specific steps to be taken to support programmatic DEI objectives, mainly along recruiting students and staff from underrepresented communities.
- The proposed project could help reduce costs, but the entire enzyme pathway seems to be more intensive for capital expenses. An apples-to-apples TEA comparison of both processes (conventional and cell-free and immobilization technologies) would be helpful to assess the process viability.
- How is the product separated at the end? What does the downstream process look like?
- One recommendation would be to test more cellulosic hydrolysates to test the process robustness. Will sugars/hydrolysate cleanup be necessary or not?
- This project aims to demonstrate the viability of cell-free-based approaches by producing terpenes as SAF and diesel intermediates or as direct replacements. One novel aspect of this project is their research approach, which will greatly advance conventional cell-free technologies. The project approach has strong scientific merit. The project team carries out very thoughtful research, investigating nearly all aspects of the cell-free system—from pathway, enzyme engineering, cofactor engineering, immobilization, and cofactor recycling—to TEA-assisted technology development. The approaches for reducing cofactors and enzyme costs are excellent. The project has made excellent progress. A computational approach was adopted for cofactor synthesis, and several low-cost synthetic cofactors

were developed with high yields. The impact of the successful project is significant—it will not only enable SAF molecules but also greatly advance science for cell-free systems. The project also interacts with other BETO-relevant projects and collaborates with academia, national labs, and industry. Risks are identified, and multiple mitigation strategies are discussed. The DEI plan is adequate. Because no TEA was given, it is difficult to understand how far the technology is from being commercially viable.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for all their efforts to carefully evaluate this project, its strengths, and its weaknesses. It is very clear that these reviewers carefully considered our project and took the time to provide valuable feedback. We also appreciate the fact that the reviewers pointed out the promise of cell-free biomanufacturing and the impact it could have on the bioeconomy. We do realize that there are still significant hurdles for the technology to be viable, and this is exactly what our project is trying to help overcome. The reviewers have raised several important and valid points that we would like to address. Regarding enzyme production and costs (and therefore if we could produce chemicals economically using cell-free systems), we are confident that scale-up production can be achieved using dedicated production strains. We have now demonstrated extracellular production of some of these enzymes at high titers without optimization in a complementary Technology Commercialization Fund project. Therefore, we are confident that experts in enzyme expression would be able to greatly improve these titers. Of course, some enzymes will need to be expressed intracellularly, but they would only require crude purifications such as heat precipitation when thermophilic enzymes are used. The contribution of enzyme cost to the overall process can also be mitigated by increasing their operating lifetime, which we are trying to achieve using a combination of enzyme prospecting, engineering, and immobilization. We already know that some enzymes remain active for days in solvents without immobilization, which bodes well for the prospects of enzymes operating for 30+ days once stabilization approaches are put in place to enable continuous operation. Regarding concerns about scale-up, we appreciate those concerns, and they are legitimate; however, we believe that this technology can scale with a few changes to the way the reactions are conducted—for example, our collaborators have now shown that high titers of terpenes can be achieved when scaling up to 10 L, which is, of course, still pre pilot but significant. Additionally, there are other processes in Japan and Scandinavia that have been shown to scale for the cell-free production of biodiesel (though these processes did not have the challenge of using cofactors). Regarding the benefit from a rigorous assessment of enzyme performance parameters, we agree with the reviewer, and it is something that we continuously do to pick the best biocatalysts for our applications. We may not go into as many details for all enzymes, but we do for the key and problematic enzyme targets. We realize that this work was not part of the presentation due to the limited amount of time allocated. Regarding the fact that the TEA model was not presented, we do realize that a full TEA would be useful, especially to assess whether a low-TRL technology would be viable. We have been developing a TEA model for terpene production, and even though this model is preliminary and does not include all the benefits that cell-free systems can offer, this model shows that if scientific and technological advances are made to lower the cost of cofactors and increase the operating lifetime (and production cost) of enzymes, then our technology would lower the MFSP for the production of terpenes compared to microbial counterparts. Additionally, we are also working on an LCA model that we believe will also show the benefit of cell-free systems over microbial systems for terpene production. Regarding post-processing and the utilization of hydrolysates, we are currently using an organic overlay for extraction. Of course, we know that this is difficult to realize at scale, and we are currently evaluating liquid-liquid extraction methods with the separation consortium, which are more industrially relevant. We believe that these approaches will be compatible with our processes and products. The reviewer is correct to point out that hydrolysates represent a challenge. In the previous iteration of this project, the use of hydrolysates led to a reduction in titers (for 2,3-BDO in this case). We will be testing hydrolysates for our current pathway in FY 2024, and we will try to identify the compounds that could be inhibitory.

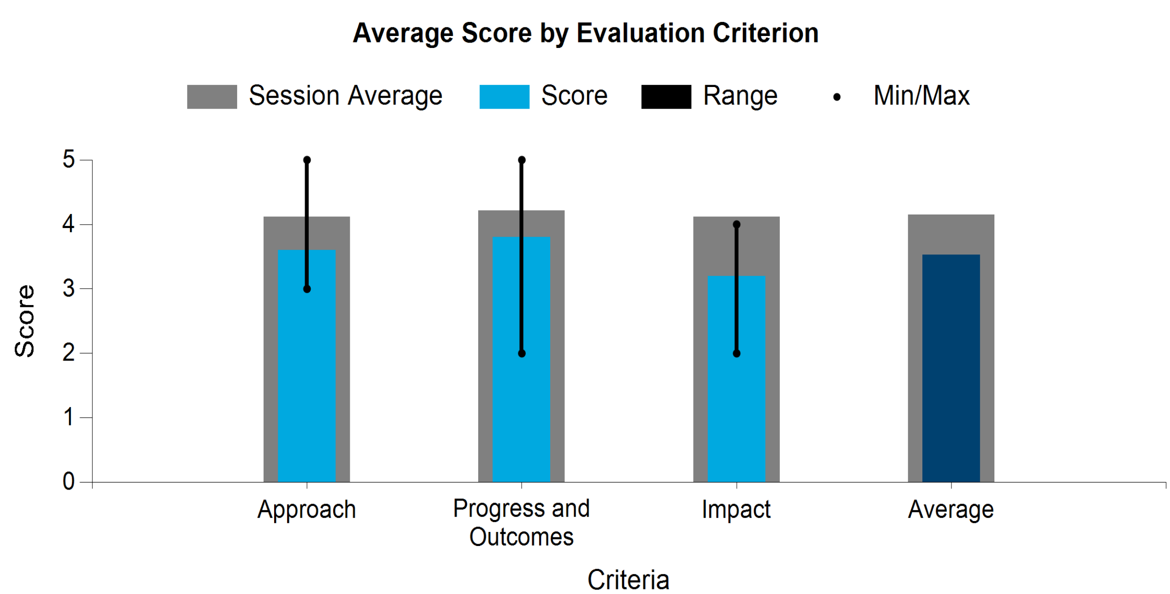
TOWARDS ECONOMICAL CELL-FREE ISOBUTANOL PRODUCTION

Invizyne Technologies Inc.

PROJECT DESCRIPTION

WBS:	2.5.6.203
Presenter(s):	Paul Opgenorth
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2023
Total Funding:	$2,628,610

Cell-free enzymatic systems are an increasingly promising alternative to performing biochemical conversions in live cells. In this approach, metabolic pathways are reconstituted using purified enzyme activities (not necessarily pure enzymes) in bioreactors. This presentation will highlight two projects that advance the concept and TRL of cell-free systems. The first project is titled “Towards Economical Cell-Free Isobutanol Production.” This project pushes the upper limit of productivity demonstrated in cell-free systems by utilizing sugars found in hydrolysates for conversion into isobutanol. The second project is titled “Cell-Free Biochemical Production of Terpenoid Chemical Astaxanthin Using Crude Cofactor Lysates.” This project focuses on utilizing low-cost cofactor mixes from microbial waste steam lysates to produce long-chain terpenes.

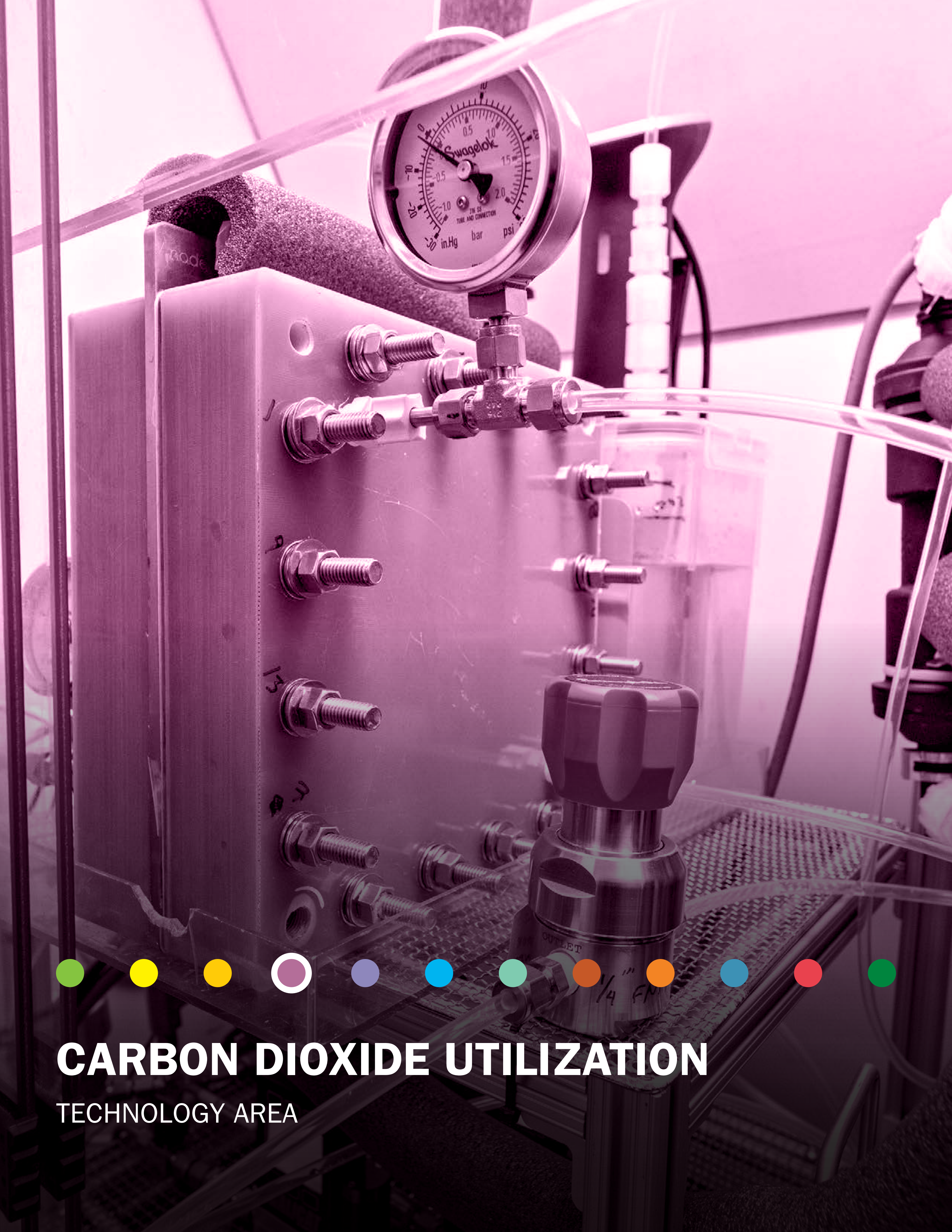


COMMENTS

- The goal of this project is to produce isobutanol and astaxanthin from sugar (both pure glucose and hydrolysate). With regard to isobutanol, the team has made excellent progress producing this chemical at high titers and yields, thus demonstrating the potential of cell-free systems. The choice of astaxanthin is puzzling. Why not first demonstrate that they can scale up the isobutanol process to 100 L before embarking on a new target? The major criticism of cell-free systems is that they will be too expensive at scale. Why not directly address this concern by developing a pilot-scale process? A number of promising results—namely, low enzyme loadings—suggests that this may be possible. Criticisms aside, this team is making excellent process. The reviewer also appreciates that unambiguous results were presented so that a technical evaluation is possible.

- With regard to the management of the project, the team is making excellent progress and meeting their milestones/objectives. The science and technology supporting this work are impressive. In these regards, the project is on track toward successful outcomes; however, the impact would be greatly enhanced if they focused more on the issue of cost because this is the big unknown with cell-free systems being used to produce commodity chemicals and fuels.
- Invizyne presented two cell-free projects in this session. The first project, nearing a close, aims to develop a new route to producing isobutanol. The second project, which began last year, aims to produce a long-chain terpene using microbial waste stream lysates. Cell-free technologies have high potential for impact, but they must overcome many challenges to achieve that potential.
- The presentation included few details on the project management approaches (an additional slide details a management overview for the first project) and certain technical details. The slides were difficult to follow (e.g., unclear sequencing of slides for Project 1 versus Project 2; charts are generally helpful, but font sizes are too small; many slides are too busy). The project strengths include an ongoing and long-term university collaboration. Progress is on track for all, and the team states that they have published in high-impact journals (citations?).
- This project provides an innovative approach to address the issues with more traditional, microbial production systems (e.g., limitations on productivity and titer). This is well demonstrated by progress made to date on isobutanol production, including yields (>95%), titers (>250 g/L), and productivities (4 g/L/h) from glucose that far exceed what microbial systems are capable of. The control systems used (i.e., NADH rheostat and ATP purge valve) provide a novel and broadly useful approach to addressing issues with maintaining sufficient ATP while ensuring the pathway is redox balanced.
- From the information presented, it was difficult to determine if the team has addressed the stated goal of de-risking cell-free, small-molecule production processes and economics. First, insufficient detail was provided in the presentation on cofactor optimization to address the challenges with cofactor cost. Second, there appears to be challenges producing sufficient enzyme to run reactions at greater than the 200-mL scale. The overall impact of the technology and project could be increased by addressing these two limitations.
- Last, the project may benefit from greater detail and/or sensitivity analyses on the various cost centers in the TEA to help better assess progress toward achieving higher TRLs and cost-competitive economics.
- No DEI plan was outlined in either project.
- Project 1: Project completed.
    - Experiments with pure glucose are performed at a 200-mL scale. It is not clear at what scale cellulosic hydrolysates are performed. Bigger or smaller scale?
    - What action items will be put in place to improve the titer with cellulosic sugars? Does the PI foresee challenges/risks associated with scaling this process to the bench scale and subsequently at process development unit and/or pilot scale?
- Project 2: Terpenes production.
    - It would be insightful to have the TEA for this project and assess how the project meets BETO's target metrics and cost.
    - This is a project for a cell-free system, and the target product is isobutanol. The project aims to reduce production costs by achieving high titer and productivity of isobutanol (in the first project)

and developing low-cost cofactors (in the Small Business Innovation Research project). The team demonstrated isobutanol production exceeding the target titer (60 g/L versus 40 g/L) using a C5 and C6 mixture. The scaled system is currently being tested. The team also demonstrated comparable isobutanol titers using lower-cost and standard higher-cost cofactors. ATP production using microbial waste stream is an interesting idea that can reduce the cofactor costs. The project included a product cost estimation to show the effect of cofactor costs on the product cost, which justifies the importance of developing low-cost cofactors. The project approach is adequate. The risks and mitigations are not specifically discussed, but I assume they are related to enzyme engineering and developing cheap cofactors. The end project goal is 500 g/L from glucose, while the current titer is 250 g/L. Because the project is ending, it would be helpful if additional information is provided to explain how the gap will be addressed.



CARBON DIOXIDE UTILIZATION

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The CO_2 Utilization Technology Area is one of 12 technology areas that were reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 18 presentations were reviewed in the CO_2 Utilization session by six external experts from industry, academia, and other government agencies. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks (https://www.energy.gov/eere/bioenergy/carbon-dioxide-utilization).

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $18,026,188, which represents approximately 3% of the BETO portfolio reviewed during the 2023 Project Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project management, approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Ian Rowe as the CO_2 Utilization Technology Area review lead, with contractor support from Anthony Sorbera. In this capacity, Ian Rowe was responsible for all aspects of review planning and implementation.

CO_2 UTILIZATION REVIEW PANEL

Name	Affiliation
Charles McCrory*	University of Michigan
Ataeres Antoniuk-Pablant	Carbon Direct
Amishi Claros	U.S. Department of Energy
Cao-Thang Dinh	Queen's University
Mark Held	Air Protein
Grigorii Soloveichik	SolEXS Consulting, LLC

* Lead Reviewer

CO_2 UTILIZATION REVIEW PANEL SUMMARY REPORT

Prepared by the CO_2 Review Panel

INTRODUCTION

The CO_2 Utilization program was established by BETO in Fiscal Year (FY) 2017 with the goal of developing new biological and artificial strategies for upgrading waste CO_2 into value-added chemicals and fuels using renewable energy and CO_2 and water (H_2O) as feedstocks. The unique aspect of the CO_2 Utilization program's approach to CO_2 upgrading is the integration of electrocatalytic CO_2 reduction and biocatalytic upgrading to convert CO_2 into highly reduced, valuable chemicals and fuels. The review panel agrees that the CO_2 Utilization program is a crucial component of the DOE mission to decarbonize hard-to-electrify sectors, such as sustainable aviation fuel (SAF), and the production of commodity chemicals.

The review panel reviewed 17 projects in total: 11 were conducted at national labs, three were conducted at academic institutions, and three were conducted in industry labs. The review panel also reviewed a presentation overview of the management strategy for the CO_2 Reduction and Upgrading for e-Fuels Consortium (CO_2RUe), a group of 11 projects within the program led by national labs that regularly meet to synergize research approaches. The panelists engaged in rigorous discussions with project presenters, principal investigators (PIs), BETO program managers, and other participants. Overall, the review panel was impressed with the breadth and depth of research within the program and felt that the programmatic goals are likely to be met with the project portfolio. The projects within the program have generated important knowledge toward scaling and implementing CO_2 utilization technologies. Although the review panel's overall impressions of the program were very positive, the panel recommends improving focus within the center by tailoring research milestones to individual projects and improving communication between projects, especially those that are not part of the CO_2RUe. In this report, the review panel provides summarized review comments and recommendations on program development.

STRATEGY

Impact

To mitigate the worst effects of climate change, governments throughout the world, including the United States, have pledged to reduce carbon emissions in the coming decades and achieve net-zero emissions by 2050. This commitment has been mirrored by numerous companies in the manufacturing, technology, transportation, and energy sectors. The production of renewable carbon is a crucial component of the decarbonization strategy for hard-to-electrify sectors, including air transportation, long-distance shipping, and commodity chemical production. In particular, converting CO_2 into value-added chemicals and fuels is a particularly useful mechanism to recycle waste carbon into renewable carbon to help decarbonize these sectors; however, CO_2 conversion technologies still remain at middle to low technology readiness levels (TRLs). There have been some moderate-scale demonstrations of CO_2 conversion to one-carbon (C1) products, such as carbon monoxide and formic acid, but not for the production of large concentrations of other two-carbon-plus (C2+) products.

The BETO CO_2 Utilization program is well poised to facilitate the discovery and implementation of scalable, practical CO_2 conversion technologies for the production of high-value and high-energy chemicals, such as SAF. The strategy of the CO_2 Utilization program combines electrochemical CO_2 conversion to intermediate C1 feedstocks with downstream biological upgrading into C2+ fuels and commodity chemicals. This program fits well within the broader BETO funding portfolio, and it is unique compared to the other programs under the BETO umbrella. Moreover, this strategy is well considered for eventual practical CO_2 conversion to high-value and high-energy chemicals, such as SAF. By coupling these C1 conversion products to biological upgrading, the projects in this technology area have the potential to lead the world in developing technology for the conversion of CO_2 to fuels and commodity chemicals through sustainable, non-hydrogenation pathways.

The projects within the CO_2 Utilization program are well aligned with the broader BETO mission, and they are responsive to its strategic priorities, especially decarbonizing transportation and decarbonizing industry. The projects are all at approximate TRLs from 2–5, which well matches the target TRL for BETO-supported applied research. Many of the teams in the program are part of the larger CO_2RUe, which involves the National Renewable Energy Laboratory (NREL), Argonne National Laboratory (ANL), and Lawrence Berkeley National Laboratory (LBNL). The projects outside the consortium included projects led by a combination of academic institutions, including Montana State University (MSU), Johns Hopkins University, and the University of Delaware; and industry teams from LanzaTech, Dioxide Materials, and Twelve.

Overall, six projects focused on developing and scaling CO_2 electrolyzer technology. These projects covered a broad spectrum of approaches—from early-stage projects focused on validating novel CO_2 electrolyzer technologies at a small scale to projects focused on scaling more well-established CO_2 electrolyzer technology for CO or formic acid production. The review panel felt that the projects in this section were on the cutting edge of research within their respective fields. Three projects in this topic area specifically focused on scaling CO_2-to-CO electrolysis using membrane electrode assembly (MEA) electrolyzers: one from NREL, one from Dioxide Materials, and one from Twelve. Electrochemical CO_2 reduction (ECO_2R) to CO or CO:H_2 blends is a rapidly maturing field, but the review panel felt that these projects successfully differentiated themselves from other work by specifically focusing on durability, degradation, scalability, and integration rather than fundamental technology development. The review panel identified the work by Dioxide Materials focusing on degradation mechanisms and mitigation strategies in CO_2 electrolyzers as particularly impactful and highlighted that funding projects looking into these types of failure processes is critical for scaling processes that are vital to the success of the CO_2 Utilization program. Another project, from NREL, focused on scaling MEA electrolyzers for formic acid production to the 25-mA cm^{-2} scale. The remaining two projects in this topic area were early-stage projects focused on developing novel electrolyzer technology and included the development of a solid-state electrolyzer for formic acid production, led by the University of Delaware, and new catalyst designs for CO_2 electrolysis to methanol, led by ANL. The review panel considered these projects important areas of research that are breaking new ground in their topics and was supportive of their inclusion in the broader CO_2 utilization research portfolio.

An additional eight projects focused on biologically upgrading CO_2-derived intermediates into valuable chemicals and fuels. Two of these projects focused on engineering microbial systems for the biocatalytic conversion of pure input streams. An additional project focused on scaling bioreactor designs to enable large-scale fermentation for biofuel production from gaseous CO_2:CO:H_2 streams. The final five projects in this topic area focused on integrating CO_2 electrolysis and biocatalytic processes. These projects focused on engineering biocatalytic processes to be specifically compatible with inputs from CO_2 electrolysis and on integrating the CO_2 electrolysis directly with the biocatalytic reactors. Overall, the review panel was supportive of the research in this topic area and felt that the projects in this topic area were making good progress. The review panel recommends that each bioconversion project provides a more comprehensive justification of their choice of the starting microbe for engineering and their choice of production target. For example, in the project from NREL focused on engineering acetogens for conversion of CO:H_2 syngas into 3-hydroxybutyric acid, the review panel suggests the researchers better justify why they are focusing on acetogen as the target microbe rather than engineering native strains that already produce the target. In another example, in the project from NREL focused on biological conversion of formic acid to fatty acids, the review panel was unclear how the target fatty acids could be converted downstream into sustainable fuels. In some cases, the review panel was also concerned about the feasibility of scaling some biological conversion processes to meet midterm targets. For example, in the case of the project led by MSU focused on integrating CO_2 electrolysis to formic acid with the bioconversion of formic acid to ethylene glycol, the project was able to achieve midterm production goals only by adding high concentrations of reducing equivalents and coenzyme A (CoA) donors into the system, limiting the scalability of the approach. In general, the review panel recommends the use of techno-economic analysis (TEA) and life cycle analysis (LCA) to justify the use of co-additives in microbial metabolism where applicable and to justify target products at target performance metrics; however, the review panel recognizes that TEA and LCA tied to current production values are not useful for some lower-TRL projects until they can convert C1 inputs into the desired products at fast production rates and high titer. The review panel commends the focus on integrating electrolysis and bioconversion into many projects and notes that this renewed focus on integration is responsive to the recommendations from the 2021 Project Peer Review.

The remaining three projects in the program focus on developing TEAs and LCAs to help guide research directions and inform production targets. Although each individual project within the CO_2 Utilization program had some level of TEA and LCA, the three projects in this topic area focus instead on program-level goals. For example, one project from NREL focuses on combining TEA and LCA in feasibility studies of current and emerging CO_2-to-fuel technologies to identify knowledge gaps and future technological targets. A second project from NREL focuses on using location-specific resource availability to determine viable markets for implementing CO_2-to-fuels conversion technologies. A third project from the portfolio compares the TEA and LCA of different CO_2 utilization pathways for SAF production. The projects in this topic area were seen as a strength of the CO_2 Utilization program. One suggestion of the review panel was to encourage greater collaboration between the analysis groups and the researchers in the first two topic areas. This could help standardize the TEA and LCA modeling and facilitate participation by experimental groups that do not have experience in TEA and LCA.

Innovation

The review panel was impressed with the research output and directions of the projects within the CO_2 Utilization program. Overall, the projects are tied to the strategic direction of the program and are at the forefront of their fields. The projects regarding CO_2 electrolysis were mostly focused on scaling and durability and have identified key technology gaps and possible solutions regarding membrane durability, degradation mechanism, reactant transport, and product crossover upon scaling. A small subset of projects in this area are early-stage projects focused on validating novel electrolyzer technology at a very small scale, but that could eventually lead to important new research directions. The projects regarding biological conversion included two projects focused on developing new strains for CO and formic acid conversion, five projects focused on integrating electrolysis and biocatalytic reactors, and one project focused on scaling continuous stirred-tank reactors (CSTRs). The projects focused on integration highlighted numerous important knowledge gaps, most of which were not present in the individual electrolysis and biocatalytic processes and only presented when the processes were integrated. The projects focused on TEA, LCA, and feasibility analysis set important and realistic performance targets and provided important insights into the technological and economic viability of the eventual implementation of CO_2 utilization technologies.

STRATEGY IMPLEMENTATION AND PROGRESS

Synergies

In response to a specific recommendation in the 2021 Project Peer Review to improve communication between projects in different research areas, the CO_2 Utilization program created the CO_2RUe in 2022. Eleven projects within the CO_2 Utilization program (~65%) are part of the CO_2RUe, with researchers in five national labs. As discussed in the first presentation of the review, the CO_2RUe has a formal leadership structure, with a consortium lead that is advised by the program and both an internal advisory board and an external advisory board of leading researchers in academia and industry. The consortium hosts regular meetings between PIs, regularly interacts with the advisory boards, and works to establish research pathways to achieve the broader programmatic targets of the CO_2 Utilization program.

The review panel saw the creation of the CO_2RUe as a game-changing strategic advance that strengthens the overall CO_2 Utilization program by dramatically increasing communication between projects, leading to increased synergy and better integration of project goals. Collecting projects from all topic areas within one consortium has increased the likelihood that the projects will address important challenges unique to the CO_2 Utilization program.

Despite the success of the CO_2RUe, there is still room to improve communication across the different projects within the program to ensure beneficial outcomes for the performer and the government. For example, there was substantive overlap across projects focused on electrolyzer development that would have benefited from cross-pollination. Specific examples are the distinct projects led by ANL and Johns Hopkins University that both focused on integrating molecular catalysts into electrolyzers for CO_2 electrolysis. It was clear that the two projects were developing very similar technology but had not met to discuss challenges and generate solutions. To further improve synergy within the program, the review panel suggests that other projects not within the consortium be invited and encouraged to participate in regular discussions with the CO_2RUe.

Focus

The review panel was impressed by the diverse and ambitious research portfolio within the CO_2 Utilization program. Research being conducted in the program fits well into BETO's strategic plan to decarbonize industrial and transportation sectors through targeted, applied research focused on recycling waste CO_2 into value-added chemicals and fuels through a combination of electrocatalytic and biocatalytic processes. Technical targets were well defined, and projects are responsive to these targets.

Projects funded in this program fell into three broad topic areas: (1) developing and scaling electrolyzer technology for CO_2 reduction to C1+ intermediates, (2) biocatalytic upgrading CO_2-derived intermediates to valuable products, and (3) developing TEAs and LCAs to inform research goals and product targets.

In the first topic area, four of the six projects specifically focused on scaling electrolyzer technologies to the necessary output rate and product concentrations for downstream biological upgrading and on determining their durability under practical operational conditions. This focus on electrolyzer scaling and durability testing is directly responsive to the recommendations from the 2021 Project Peer Review, and it allowed the project teams to determine the knowledge gaps that are being bridged through targeted, applied research. The remaining two projects in this topic area focused on developing new electrolyzer technologies. The inclusion of these more exploratory, lower-TRL projects was seen as a promising addition to the program that, if successful, could provide additional research avenues in the coming years; however, the review panel felt that the target metrics should be de-emphasized for these early-stage, high-risk/high-reward projects to allow the project teams to focus on technology development rather than scaling and integration. The balance of the research portfolio seemed about right to the review panel, with most projects focused on the scaling and durability of higher-TRL technologies for nearer-term progress and a smaller contingent focused on lower-TRL research that has the potential to advance in the future.

In the second topic area, most projects focused on integrating electrolyzer and biocatalytic processes. The focus on integration in the current funding portfolio was directly responsive to the 2021 Project Peer Review recommendation that the program focus on integrated scale-up approaches that more fully combine electrocatalytic and biocatalytic processes. This topic area also included a project focused on scaling CSTRs, which was another recommendation from the 2021 Project Peer Review. Overall, the review panel felt that the shift in this topic area toward the integration and scaling of biological conversion with real, intermediate feeds from electrolyzers was appropriate and aligns with the goals of the CO_2 Utilization program.

In the third topic area, the projects focused on program-level LCA and TEA for CO_2 upgrading using the combined electrochemical and biocatalytic strategy supported by the CO_2 Utilization program. This program was part of the CO_2RUe, and as such, it was well aligned with the goals of the consortium and the individual projects. This close alignment of the analysis with the experimental research is responsive to the 2021 Project Peer Review feedback and is seen as a success of the program by the review panel. The analysis projects are able to assess the feasibility of implementing the technologies being developed within the program and provide important feedback to the research projects regarding target inputs, products, and performance metrics. The review panel suggests maintaining a focus on these types of program-level analysis projects within the broader program research portfolio.

Overall, the review panel felt that the projects within the CO_2 Utilization program aligned with programmatic strategy and goals. The implementation of the CO_2RUe dramatically enhanced communication between projects within the consortium, which has helped focus research directions. Improving communication between CO_2RUe projects and those outside the consortium, especially regarding feasibility assessment, could further enhance research focus toward the most promising technologies and reduce research overlaps. Another concern of the review panel is that sometimes projects spend effort and resources on unproductive research directions simply to meet short-term and midterm milestones, even if these research directions are not important for the success of the project. For instance, some projects used recirculation to meet CO_2 conversion efficiency milestones or introduced co-additives into biocatalytic reactors to improve yields and titer milestones, even if these additions are not scalable. The review panel felt that the milestone target goals might be more effective if they were tailored to the needs of each individual project, or the program should more effectively communicate to the projects that it is okay to miss some performance milestones as long as the projects are making progress and increasing knowledge.

RECOMMENDATIONS

Recommendation 1: Improve communication between projects to prevent overlap of effort.

The creation and implementation of the CO_2RUe has dramatically enhanced communication and synergy for projects within the consortium; however, this improved communication has not benefited projects outside the CO_2RUe but rather those that are still within the CO_2 Utilization program's research portfolio. To further improve synergy with the program, the review panel suggests that projects outside the consortium be invited and encouraged to participate in regular meetings with CO_2RUe projects. Taking this step will help improve communication among all projects within the program and will help ensure that projects are collectively working to achieve the broader program goals.

Recommendation 2: Tailor project milestones to each project.

The CO_2 Utilization program has set uniform performance milestones for projects operating in the various technology areas. In some cases, projects have spent time and effort to develop unscalable approaches or otherwise unproductive research paths for the sole purpose of meeting these milestones. The program should work with the projects to develop specific performance milestones tailored to each individual project. The program should also clearly communicate that although it is important to strive toward performance milestones, the overall purpose of each project is knowledge generation, and it is okay to occasionally miss performance milestones as long as the project is making research progress and generating important knowledge in its field.

Recommendation 3: Develop a facility to help test CO_2 electrolysis under "real-world" conditions.

A common roadblock to testing ECO_2R is the inability to run and do onstream testing and analysis for long durations of time with the full system. A facility for CO_2 electrolysis scaling could help mitigate risks by discovering challenges that are difficult to see in conventional bench-scale setups and experimental time frames. Such a facility could help normalize long-duration, "real-world" stress tests and degradation studies for the different electrolyzer technologies being developed within the program.

CO_2 UTILIZATION PROGRAMMATIC RESPONSE

INTRODUCTION

The Conversion Research and Development (R&D) Program Area is quite thankful for the valuable insights and engaging discussion on this subject provided by the CO_2 Utilization review panel. This type of critical assessment continues to be a driving force in the development of this portfolio. As stated by the Review Panel Summary Report, this portfolio has significantly grown since its inception, and it would not have been possible without such expert involvement from the private and academic sectors. BETO is indebted to the reviewers, both new and returning members.

The panel agrees that a program such as this—that focuses on leveraging CO_2 as a feedstock for fuels and chemicals—is a "crucial component of the DOE mission to decarbonize hard-to-electrify sectors" of the economy. As with all R&D endeavors, striking the right balance between the quantity of areas explored and the depth within specific topics is difficult. The review panel stated that the CO_2 Utilization portfolio achieves an impressive breadth and depth of research.

The areas being researched by BETO were generally seen as appropriate for the challenge of enabling CO_2 conversion, which generally remain at low to middle TRLs today. The panel described the portfolio as consisting of three broad areas: electrolyzer technology, biocatalytic conversion of intermediates, and TEA and LCA. The review panel spoke highly of the newly formed CO_2 consortium and saw it as the appropriate way to increase communication among these efforts and allow for integration where needed. Establishing this consortium was a major accomplishment of the CO_2 Utilization portfolio during the past 2 years, and it was influenced by feedback from the 2021 Project Peer Review.

The electrocatalytic applied R&D work occurring in the portfolio, a combination of national lab projects within the consortium as well as those occurring externally, were seen as cutting-edge efforts that are helping to advance the start of technology in this area. The biocatalytic work was also assessed to be making good progress in the field; however, projects could benefit from additional justification for the choice of host organisms and the production target as well as deeper investigation into whether they could scale to hit ambitious climate targets within a reasonable time. Last, the analysis projects in the portfolio were also seen as a strength that can inform program-level goals and identify technical gaps, though they could be better leveraged to inform the researchers on the electrocatalytic and biocatalytic projects.

The reviewers pointed out the synergistic opportunity for combining researchers who work on catalyst development with their counterparts who are engaged in process engineering and biological strain development. Such interdisciplinary collaboration was seen as key to developing robust conversion systems. Similarly, additional collaboration between those at the national labs and their university and industrial counterparts could be leveraged to overcome major barriers in CO_2 utilization. Overall, the reviewers saw room to improve communication across the portfolio, both within the consortium and with other projects in industry and academia. The following section specifically addresses the three major recommendations from the review panel.

Recommendation 1: Improve communication between projects to prevent overlap of effort.

BETO agrees with the panel on the importance of communication across the portfolio. Although the consortium has been successfully established and readily communicates among relevant projects across the national labs, it has minimal interaction with projects that are not within this group, such as funding opportunity announcement (FOA) awardees at companies and universities. This blind spot misses an opportunity to allow learnings to filter into the public. Per the review panel's recommendation, BETO and the CO_2 consortium are exploring mechanisms to allow and encourage external awardees to participate in consortium activities and share their work with that group.

Recommendation 2: Tailor project milestones to each project.

The program appreciates and agrees with this recommendation. Milestones should be tailored to the specific project work, and there is room for improvement in the BETO CO_2 Utilization portfolio on this front. Specifically, certain projects selected from an earlier FOA have goals and milestones that adhere to specific targets that were outlined in the initial FOA language, but some of those milestones proved not to be very relevant once the projects were underway. To meet the review panel recommendations, BETO will set more flexible targets in future FOAs and, through active project management, will ensure that awardees work toward answering important scientific questions related to the spirit of the project, not simply hitting arbitrary metrics to technically meet the stated requirements within the financial agreement.

Recommendation 3: Develop a facility to help test CO_2 electrolysis under "real-world" conditions.

BETO agrees with this assessment and is actively exploring the subject. As stated by the reviewers, the lack of access to long-duration electrocatalytic testing is a major hurdle in the field. There is an opportunity to help advance the field by providing a mechanism for stakeholders to address things like catalyst durability, accelerated testing, protocol standardizing, and electrolyzer scale-up. Although such an effort is difficult to establish under current BETO funding, some future efforts within the consortium could be dedicated to answering some of these questions. In addition, BETO will explore collaborations on this subject with other applied R&D offices across DOE that are interested in CO_2 conversion.

FEASIBILITY STUDY OF UTILIZING ELECTRICITY TO PRODUCE INTERMEDIATES FROM CO_2 AND BIOMASS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.1.0.304
Presenter(s):	Gary Grim
Project Start Date:	11/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$400,000

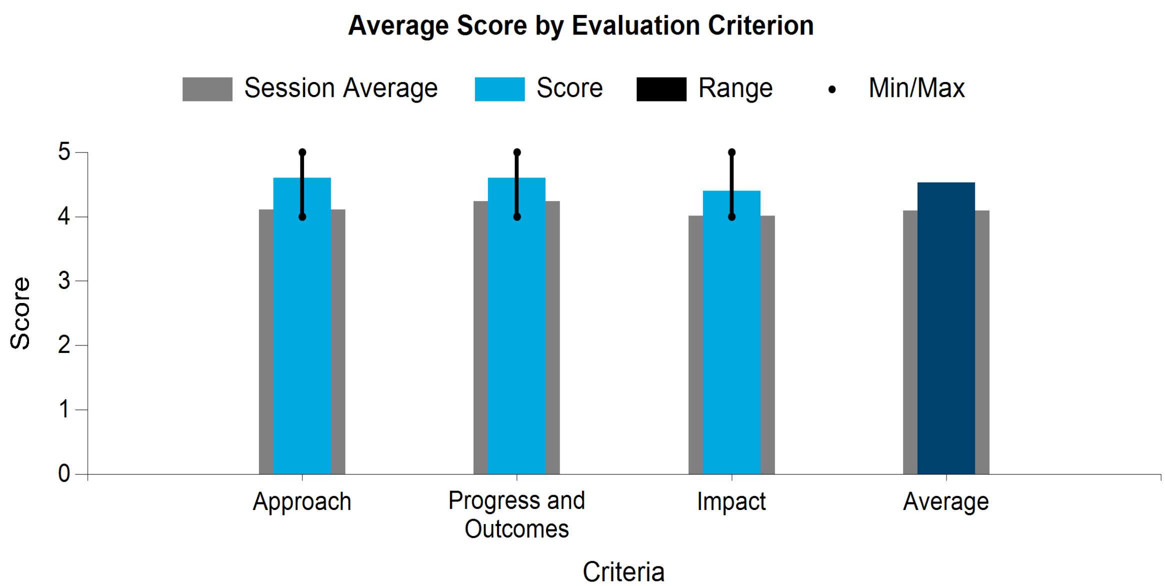
The increasing availability of renewable electricity at costs competitive with, and even lower than, electricity from fossil fuel sources, along with increasing interest and recent technological advancements in reducing carbon emissions through CO_2 capture (whether from point sources or the air), is challenging the status quo in the way that we produce and consume energy and products. Renewable electricity can be leveraged to produce fuels and chemicals from CO_2 via CO_2 reduction, offering sustainable routes to reduce the carbon intensity of our energy and products-driven economy. It has been estimated that the annual market opportunity for CO_2 utilization (all products and pathways, not only electricity-driven CO_2 reduction) is on the order of $1 trillion. More specific to CO_2 reduction, a recent study from 2019 estimated that producing chemicals such as methanol, polyolefins, and aromatics from CO_2 and renewable electricity instead of fossil fuel-based resources could reduce annual greenhouse gas (GHG) emissions by up to 3.5 gigatons of CO_2-equivalents in 2030, albeit at a cost of hundreds of billions of U.S. dollars per year. In most existing biorefineries in the United States and in BETO's conceptual biorefinery designs, CO_2 is released to the atmosphere either as a concentrated stream (i.e., ethanol fermentation) or as a component of flue gas (e.g., gasification and pyrolysis). As of 2018, the 216 existing biorefineries in the United States emit 45 million tons of CO_2 annually. Capturing and converting this CO_2 into valuable products, leveraging renewable electricity as the primary energy input, could increase overall biorefinery CO_2 utilization by as much as 40%; however, due to the diversity of CO_2 capture and conversion technologies (many of which are at low TRLs) and the trade-off between improved biogenic carbon yield at the expense of additional energy input, considerable uncertainty exists around the impact of these electron-driven CO_2 utilization strategies on the minimum fuel selling price (MFSP) and the overall carbon intensity of the process.

This project combines TEA and risk evaluation to address this uncertainty. More specifically, this project evaluates the conceptual stand-alone, electricity-driven CO_2 utilization technologies (i.e., CO_2 reduction strategies) and their integration into existing biorefinery designs to quantify the impact on the MFSP. The key differentiators of this project are as follows: (1) We take a holistic approach to addressing this uncertainty (most studies in the literature focus on a single technology, e.g., thermochemical hydrogenation of CO_2, whereas our study spans existing technologies and evaluates the integration of these technologies into existing biorefinery designs), (2) we maintain a strict focus on the intersection of electricity and biorefinery streams (CO_2), (3) we have a world-class analysis team with deep expertise in modeling emerging technologies (low TRL) with complex chemistry, and (4) we leverage in-house chemical and biological conversion experts.

Our FY 2021–FY 2023 scope focused on (1) specific CO_2 reduction technologies that represent the greatest potential to reduce the MFSP for SAF and generating out-year technical targets and comprehensive reports, and (2) providing crosscutting, technology-agnostic guidance to the field of CO_2 reduction. Further, we aim to address key feedback from the 2019 Peer Review regarding process parameters that need more in-depth assessment of carbon intensity and process risk. The key innovations of this project include (1) establishing state-of-technology (SOT) and waterfall projections based on ongoing BETO-supported experimental work, (2) integrating with LCA to assess carbon intensity, (3) evaluating technological risk (especially for low TRLs) via a node-by-node and complex systems-level approach, and (4) evaluating opportunities for process intensification (combining CO_2 capture and conversion) and coupling CO_2 with other biorefinery streams. Our project will extensively collaborate with other ongoing and proposed new-start projects supported by BETO, including the newly formed CO_2RUe.

The key outcome of this work is to inform and guide stakeholders toward the effective utilization of electricity to improve biorefinery CO_2 utilization. The specific stakeholders for this work are (1) researchers, (2) technology developers, and (3) biorefinery owners/operators. For researchers, this project identifies opportunities for transformational research, i.e., research that will result in significant reductions in cost and/or risk, and it guides R&D efforts by setting future targets for key technical metrics. Integration of this project with experimental teams working on CO_2 utilization technologies will result in tangible technological advancements and cost reductions through analysis-guided R&D. For technology developers, this project identifies and assesses technological barriers and risks that are limiting the commercial viability of these CO_2 utilization processes. For biorefinery owners/operators, this project helps them understand the trade-offs of implementing these CO_2 utilization technologies (i.e., energy requirements, capital costs, and product yield and quality captured in comprehensive design reports) so that they can assess the value proposition based on their specific needs.

Since the 2021 Project Peer Review, this project has directly authored or contributed to five peer-reviewed journal publications: (1) https://doi.org/10.1021/acsenergylett.0c02692, (2) https://doi.org/10.1039/D0EE03525D, (3) https://doi.org/10.1039/D2EE02439J, (4) https://doi.org/10.1016/j.apenergy.2021.117637, and (5) https://doi.org/10.1002/9783527833634.ch3.



COMMENTS

- The information gained from this complex project—pulling multiple key aspects of technology, economics, modeling, and LCA—is key to guiding research efforts. Analyzing information from current projects can help mitigate risk and increase the chances of successful scaling and implementation. The online tool that was developed can increase awareness in a broader audience.

  Potential impact:

  - More outreach to industry with the knowledge gained from their research and the online tool could help normalize the LCA/TEA in this field
  - Increased communication with specific projects within the CO_2RUe could assist with guiding the target goals of each project—e.g., additional guidance on the effect of the per-pass CO_2 conversion

on the TEA versus recycle loop, limits to venting the recycle loop, tuning the conditions in the reactor affects the major cost drivers, target products, scenarios where the focus should be on formate versus MeOH versus CO/H_2.

- This project aims to combine TEA and LCA to provide technological guidance for CO_2-to-SAF technologies. It evaluates the production cost and carbon intensity of various CO_2-to-SAF processes based on the SOT performance and highlights key cost drivers of these processes. Overall, the project has a significant impact and offers key insights to move CO_2-to-SAF forward. The project has been managed well, with interactions/contributions from all key parties. The progress and outcomes are excellent, as demonstrated by multiple publications and the launch of an interactive website. It is not clear how various steps in the CO_2-to-SAF processes are integrated. The level of integration between various steps (e.g., ECO_2R, fermentation of syngas, catalytic ethanol upgrading) would significantly influence both production cost and carbon intensity. It is also not clear how the target performance values for each individual step are determined based on the target value of the final SAF product.

- This project is well executed and an important component of the CO_2RUe. The goal of the project is to use the TEA and LCA of current and emerging technologies to identify existing technology gaps and future technical targets for CO_2 utilization. Assumptions used in the models were largely pulled from the literature, but crucially, the project also leveraged key industry partners to provide validation for key assumptions. A significant strength of the project is its integration of emerging technologies within the CO_2RUe into its TEA/LCA to help ensure that the project's analyses are responsive to the changing landscape of CO_2 utilization. The integrated TEA/LCA approach is an important and unique component of the project that allows for simultaneous optimization for price and environmental parameters. This integrated TEA/LCA approach is a strength of the project that helps identify economic and environmental trade-offs, although it would be useful for the project to provide more guidance on how LCA and TEA should be weighted in these analyses to help define the technical targets for research components. Overall, this is a successful project that has already demonstrated significant impact through peer-reviewed publications, the launch of an interactive website, and engagement both within and external to the CO_2RUe.

- The project goal of the integration of TEA and LCA models is very important because it will guide the development of different technologies and will allow for excluding non-promising products from consideration at early stages. Strangely, in some examples, future and theoretical costs are about the same, which assumes (highly unlikely) zero losses. A cost analysis was performed on a $/kg basis, though for energy purposes it would be useful to also represent this in $/kWh ($/Btu) units. The performed Monte Carlo analysis is definitely a plus of this project; however, some used parameters are questionable—e.g., capacity factor (should go as low as 25%) and electrolyzer cost (it is better to present this in $/kW units). It is not clear how the team plans to perform the optimization of the integrated TEA/LCA model: What will the optimization target be—cost, carbon intensity, etc.? What weight for different factors will be used? Setting future targets is undoubtedly a plus, but the analysis of current trajectories for the most important products would be useful.

- This was an excellent presentation that gave a clear, tangible sense of the progress and outcomes. The work is a critical component of the CO_2 utilization consortia because it informs the group of the current pain points and therefore where to focus the research. The durability, cost, efficiency, and lifetime of electrolyzer units were highlighted as important variables affecting the success of a CO_2-derived product. This was good to see because the clear majority of projects funded in the CO_2 utilization consortia focused on electrolyzer development. The authors have also published four peer-reviewed articles and generated an interactive website to help communicate their work. One important consideration for the group and BETO as a whole is how to ensure that this sort of analysis and *in silico* tools live on. Are there plans to diversify the products analyzed using similar analysis pipelines?

PI RESPONSE TO REVIEWER COMMENTS

- We thank the subject matter expert panel for taking the time to review this project and provide thoughtful and constructive feedback. Moving forward, we will apply this feedback to (1) continue to guide and inform our partner programs within the CO_2RUe, (2) provide transparent and actionable information on CO_2 conversion through peer-reviewed publications and online tool kits, (3) provide multicriteria decision analysis as a means to weigh the outcomes of our integrated TEA/LCA, and (4) balance our approach between the production of intermediate products and fully integrated pathways to fuels.

MARKETS, RESOURCES, AND ENVIRONMENTAL AND ENERGY JUSTICE OF CO_2-TO-FUELS TECHNOLOGIES

National Renewable Energy Laboratory

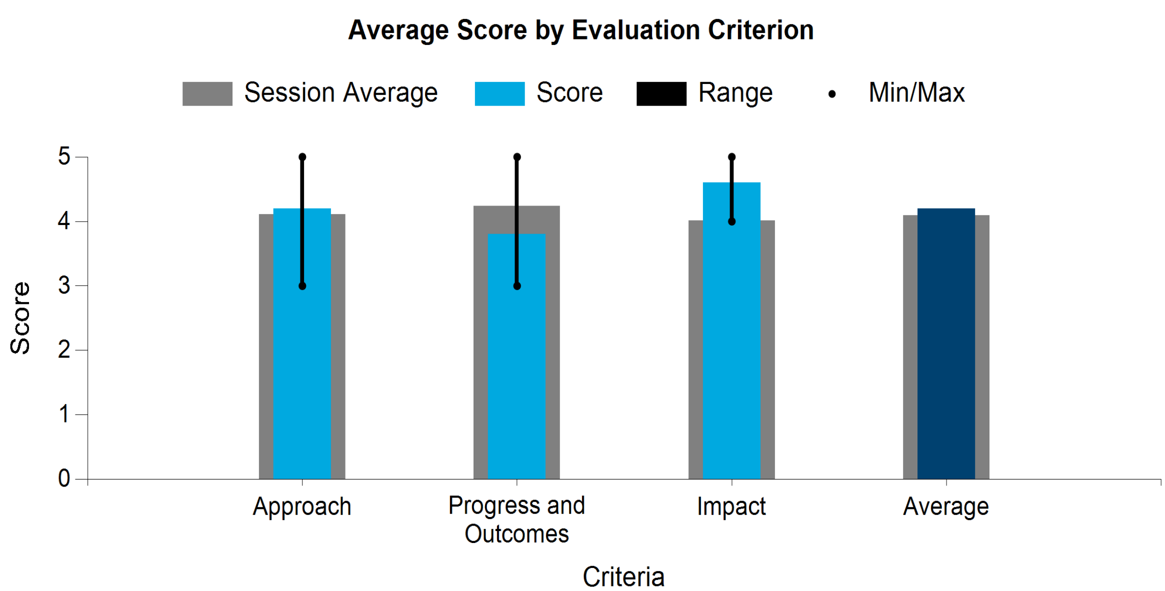
PROJECT DESCRIPTION

WBS:	2.1.0.504
Presenter(s):	Ella Zhou; Jiazi Zhang
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$950,000

Today's production and market locations for fuels and chemicals are largely determined by fossil fuel resources and existing infrastructure (e.g., natural gas and petroleum oil).

To achieve DOE's decarbonization and energy justice objectives, at-scale investment in CO_2 utilization technologies needs to be informed by detailed analyses of CO_2 and H_2 resources and costs, non-fossil fuel electricity availability and prices, air emissions, job and gross domestic product impacts, and other factors.

This project informs the development of the CO_2 utilization industry by (1) assessing the resource potential, market potential, and infrastructure requirements for the near-term (2030) and long-term (2050) deployment of CO_2 utilization technologies; and (2) evaluating the energy equity and environmental justice (EEEJ) implications. The insights can be used across a large portfolio of CO_2 utilization technologies so that stakeholders can make decisions according to both economic and societal factors.



COMMENTS

- This project shows impactful research on resource availability, CO_2 markets, and EEEJ analysis. Their research is key to strategically scale CO_2 technology and identify focus areas while addressing EEEJ. Can they communicate their work to a broader audience? Additional information/questions for further assessment include:

  Risk management:

  - Additional information regarding how they are measuring health impacts and exposure disparity

- Additional information regarding the scenarios they chose to focus on.

Potential impact:

- Additional information regarding other potential unforeseen consequences and mitigation strategies.

- The project aims to quantify the effect of carbon sources (capture cost and transportation) and energy sources (cost and carbon footprint) on CO_2-to-SAF conversion. The goal is to identify possible locations for CO_2-to-SAF based on two key paths: (1) low-temperature electrolysis to produce syngas followed by fermentation and (2) water-gas shift followed by the Fischer-Tropsch process. Progress has been made in identifying CO_2 and energy sources at different locations. It is unclear how the final goal can be achieved within the timeline of the project. It is also unclear how societal impacts are evaluated. Some aspects that may affect the overall process, including CO_2 purity and product distribution, have not been considered/discussed.

- The project uses a cross-sector modeling framework assessing location-specific resource availability to determine viable markets for CO_2 utilization technologies for SAF production. A key strength of this project is the close collaboration with other projects in the CO_2RUe, especially the other modeling and analysis groups, which provided the 2233 TEA/LCA metrics used in the cross-sector modeling. The project has already made significant progress, identifying three preliminary sites for CO_2 utilization with the correct balance of grid electricity capacity and cost, proximity to CO_2 resources, and proximity to jet fuel refineries. Future immediate plans appropriately focus on expanding the model to include emissions inventory analysis and estimated delivery and storage costs for hydrogen and reduced CO_2 intermediates. It remains unclear how the EEEJ component will be integrated into the cross-sector modeling. The timeline for onboarding this component is not until Year 3 of the project, but no approach was discussed as to how this would be integrated and weighted into the current cost-based models. Although pilot-scale implementation of CO_2 utilization is not part of the CO_2RUe portfolio, this project nonetheless provides an important and impactful contribution to the consortium by assessing the feasibility of implementing CO_2 utilization technologies at scale in optimal location-specific markets based on technology performance targets.

- Quantification of resource (feedstock and renewable electricity) availability and costs for CO_2 conversion to fuels is extremely important to guide development and deployment, and the project is moving in the right direction. A couple of comments are as follows: The team showed the advantages of the preferred pathway (LTE – syngas fermentation – EtOH to SAF) with the pathway based on reverse water-gas shift reaction. It seems that another pathway (LTE – CO_2 H_2 – MeOH) may be more cost-competitive and should be used as a base case. Second, localization of the distributed SAF production (close proximity to major airports, delivery infrastructure) should be analyzed. I also recommend considering water resources.

- The specific goals of this project were not clearly communicated. Slide 9 sets the stage at a very high level, but beyond that, the reviewers need to go to the quad chart to see the goals. Because this project followed WBS 2.1.0.304, it would have been useful to hear more about how this project differed from the previous one. I was left wondering if the work was significantly distinct or simply looking at the same issue in a slightly different way. More collaboration and communication between these two projects would have helped highlight and differentiate their added value to the program. I see that mentioned on Slide 20, but it was not clear from the presentation.

  In regard to progress and outcomes, I've given this project a three because although they have made good progress toward their goals, little mention was made of risk mitigation and challenges. This left me with the impression that the work could have been more challenging.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the valuable feedback provided by the reviewers and their insightful comments. We are grateful for their contribution to the refinement of our methodology. In the following sections, we break down the questions and provide detailed answers.

  Comments 1: Impactful research on resource availability, CO_2 markets, and EEEJ analysis. Their research is key to strategically scale CO_2 technology and identify focus areas while addressing EEEJ. Can they communicate their work to a broader audience? Additional information/questions for further assessment: risk management—additional information regarding how they are measuring health impacts and exposure disparity, additional information regarding the scenarios they chose to focus on; potential impact—additional information regarding other potential unforeseen consequences and mitigation strategies.

  Answers:

  - 1.1 Communicate our work to a broader audience. We will continue to present and publish the key findings in conferences, peer-reviewed journals, and reports to inform stakeholders, industry partners, and the public.

  - 1.2 Risk management. Insufficient transmission capacity to meet the increasing electrolyzer demand resulting from SAF targets is a potential risk. This risk can be managed by investigating other future capacity and transmission expansion scenarios that consider new technologies, such as long-duration energy storage build-out and high-voltage direct current. Decreasing the CO_2 available from sources by industrial decarbonation is a potential risk. The risk can be managed by including additional potential CO_2 from direct air capture (DAC) or bioenergy production that may replace petroleum fuels. In particular, DAC provides a direct way to decrease CO_2 concentration from atmosphere. Green hydrogen shortage due to the low-carbon electricity supply shortage is another potential risk. NREL is addressing this risk through the electricity market analysis. Hydrogen production by polymer electrolyte membrane (PEM) electrolysis may face material supply barriers, such as for platinum or iridium. This is investigated by a separate supply chain study. CO_2 pipeline construction might be a bottleneck due to the permit application/approval and construction hurdles. This will not be a risk if DAC is used for CO_2 source.

  - 1.3 Additional information regarding how they are measuring health impacts and exposure disparity. The NREL team will estimate the EEEJ factors, including impacts on human health and job distribution, using the results from the TEA/LCA project. To estimate high-spatial-resolution human health impacts of air emissions, the Intervention Model for Air Pollution (InMAP) will be used. Its results will be combined with demographic data to evaluate the impacts to specific communities. Outputs include changes in the annual average concentration of particulate matter (PM) 2.5 (particulate matter with diameter 2.5 µm or smaller) and avoided (or additional) annual average mortality by demographic. Socioeconomic impacts, including regional wealth and job distribution, will be estimated using the Bio-based circular carbon economy Environmentally-extended Input-Output Model (BEIOM) with regional supply and demand conditions and electricity generation mix developed in this project and process-level TEA and LCA data provided by the TEA/LCA project team.

  - 1.4 Additional information regarding the scenarios they chose to focus on. We have analyzed high- and medium-purity process CO_2 sources from six industries (ethanol, ammonia, natural gas processing, steam methane reforming [SMR] hydrogen, cement, and iron and steel). For these potential CO_2 sources in the future, we have two scenarios: one in the near future, i.e., 2030, and another longer term, in 2050. The 2030 CO_2 scenario is based on available data obtained from the Annual Energy Outlook by the U.S. Energy Information Administration. The 2022 Annual Energy

Outlook projected an amount of CO_2 emissions in 2030 similar to that in 2022 from the six selected industries. For the considered 2050 CO_2 sources, we adopted a scenario in which the considered industries would achieve the net-zero CO_2 emissions target; thus, we assumed that ammonia, hydrogen, and iron and steel will be decarbonized via clean hydrogen production and use in current and emerging technologies, such as Haber-Bosch and direct reduction of iron. We assumed reduced CO_2 emissions from the cement industry due to switching from fossil fuels to alternative low-carbon fuels for combustion. We also assumed reduced CO_2 emissions from natural gas processing because less natural gas will be used by 2050 (especially in residential and commercial sectors). The grid-mix simulation with additional electricity demand for CO_2 utilization is based on the available CO_2 sources in 2030 and 2050 as well as the corresponding SAF production potentials via selected CO_2 utilization pathways. The NREL team has used the Regional Energy Deployment System (ReEDS™) model to conduct capacity expansion modeling and outline the U.S. power sector planning from the present day to 2050. A standard power grid capacity expansion scenario with a high energy demand growth projection has been chosen as the baseline scenario, and a net-zero CO_2 emissions target for 2035 has been enforced. The SAF Pathway 1 facilities in each balancing area, accounting for 27% of the SAF target in 2050 as provided by the ANL team, have been converted to the energy demand for SAF fuel production and incorporated into ReEDS. Additionally, a sensitivity analysis has been conducted considering SAF targets of 10%, 15%, and 20% in 2050 to compare the power grid impacts of different SAF targets. The outputs of power system capacity and transmission expansion, along with the identified SAF demands, have been passed to the power system production cost model for daily grid operation analysis. The resulting electricity costs, locational marginal prices, and marginal generation mix will be provided to the TEA/LCA project to adjust the TEA and LCA factors. Further, the SAF facility siting constraints identified through the grid analysis will be provided to the ANL team to optimize the selection of the SAF facility siting.

- 1.5 Potential impact. This study quantifies the potential CO_2 reductions in the aviation sector by producing low-carbon SAF. Such a methodology can be adopted to decarbonization scenarios of other fuels and chemical markets. This study will provide information on key external factors that will impact the market potential for CO_2 utilization technologies. The project's outcomes, in conjunction with the TEA/LCA project's outcomes, will provide understanding of the market potential of a CO_2 utilization industry, the associated costs and environmental implications, and the potential technical and market barriers to inform future R&D decisions. This project's outcomes will also provide DOE and other stakeholders with an understanding of CO_2 sources; impacts on the grid by increasing loads; and the trade-offs between transporting CO_2, electricity, possible intermediates (e.g., H_2), and CO_2 utilization products that are necessary for siting. It will quantify regional and national environmental benefits and trade-offs as well as potential impacts on human health, gross domestic product, and job distribution. All these factors provide the essential information necessary to determine the priority for future CO_2 utilization research, development, and demonstration projects, whether funded by the government or private industry. Because this project is analyzing both mid- and long-term time frames, the information will be useful in considering the evolution of a CO_2 utilization industry over the next 30 years.
- 1.6 Additional information regarding other potential unforeseen consequences and mitigation strategies. A significant amount of clean electricity demand may increase the electricity cost. This is a major cost driver for CO_2 utilization products. This is being investigated by NREL as part of grid simulations.

Comments 2: The project aims to quantify the effect of carbon sources (capture cost and transportation) and energy sources (cost and carbon footprint) on CO_2 to SAF conversion. The goal is to identify possible locations for CO_2-to-SAF based on two key paths: (1) low-temperature electrolysis to produce syngas followed by fermentation and (2) water-gas shift followed by the Fischer-Tropsch process.

Progress has been made in identifying CO_2 and energy sources at different locations. It is unclear how the final goal can be achieved within the timeline of the project. It is also unclear how societal impacts are evaluated. Some aspects that may affect the overall process, including CO_2 purity and product distribution, have not been considered/discussed.

Answers:

- 2.1 It is unclear how the final goal can be achieved within the timeline of the project. The project team is on track to complete tasks according to the project timeline. The project completion date is the end of September 2024. The team has already identified 2050 potential CO_2 sources and is currently modeling the additional electricity demand for the 2050 SAF production scenario. Our target is to complete the 2050 CO_2 utilization SAF production scenario (including electricity costs, marginal generation mix, CO_2 sources, and SAF production potential by CO_2 utilization) by the end of this year. The evaluation of the EEEJ implications of deploying CO_2 utilization technologies is scheduled to start in July 2023 because it requires information from the 2050 modeled scenario.
- 2.2 It is also not clear how societal impacts are evaluated. We appreciate the reviewer for raising this valuable question. In fact, the societal impact assessment can be divided into our proposed Task 5, the assessment of air quality impact and public health impacts, and Task 6, the assessment of socioeconomic impact. These tasks will be addressed in Budget Period 3; however, we are pleased to provide the proposed assessment method here. For Task 5, the focus is on assessing the regional air quality and public health impacts associated with long-term exposure to PM 2.5 emissions from various sources related to CO_2 utilization pathways. This is achieved using the InMAP air quality model. The model provides fine-resolution and demographic-specific estimates of air quality impacts, which are important for EEEJ analysis. The analysis incorporates criteria air pollutant emissions and siting information to create location-specific inputs for InMAP. The concentration-response function is used to estimate health impacts considering changes in PM 2.5 concentration. The output metrics include changes in population-weighted exposure to PM 2.5, net health impacts, and corresponding economic valuations by different demographics and income levels. For Task 6, the socioeconomic impact assessment focuses on evaluating the economywide impacts of industry-scale deployment of preselected CO_2 utilization technologies. This is done using a regional version of the BEIOM macroeconomic model, which considers supply chain interactions and estimates socioeconomic and environmental impacts. Demographic and economic data from official sources are collected and modeled to forecast the baseline U.S. economy. The preselected CO_2 utilization technologies are specified in BEIOM using process-level data from the TEA/LCA project. Additional data collection is conducted to detail the primary supply chain industries and perform sensitivities to scenarios and electricity generation mixes.
- 2.3 Some aspects that may affect the overall process, including CO_2 purity and product distribution, have not been considered/discussed. We have considered the impacts of CO_2 purity and transportation to the CO_2 utilization site as follows. CO_2 purity: CO_2 purity from different industries was considered and reflected by the difference/variation in CO_2 capture costs (i.e., low CO_2 capture cost for high-purity CO_2 and high CO_2 capture cost for medium-purity CO_2). In addition, we considered CO_2 transportation cost with different scales and distances. We analyzed the cost of CO_2 capture, compression, and transportation for various CO_2 sources in the 2030 CO_2 utilization scenario. We are currently analyzing these costs for the 2050 scenario. Product (SAF) distribution: We have selected the potential SAF production locations considering three criteria: (1) electricity cost, (2) proximity to CO_2 sources, and (3) proximity to the jet fuel production in refineries. Criteria (1) and (2) are related to SAF production cost, and criteria (3) considers SAF markets. We can use the current blending facilities and jet fuel pipeline network in the United States by locating SAF facilities near the current refineries producing jet fuel.

Comments 3: The project uses a cross-sector modeling framework assessing location-specific resource availability to determine viable markets for CO_2 utilization technologies for SAF production. A key strength of this project is the close collaboration with other projects in the CO_2RUe, especially the other modeling and analysis groups, which provided the 2233 TEA/LCA metrics used in the cross-sector modeling. The project has already made significant progress, identifying three preliminary sites for CO_2 utilization with the correct balance of grid electricity capacity and cost, proximity to CO_2 resources, and proximity to jet fuel refineries. Future immediate plans appropriately focus on expanding the model to include emissions inventory analysis and estimated delivery and storage costs for hydrogen and reduced CO_2 intermediates. It remains unclear how the EEEJ component will be integrated into the cross-sector modeling. The timeline for onboarding this component is not until Year 3 of the project, but no approach was discussed as to how this would be integrated and weighted into the current cost-based models. Although pilot-scale implementation of CO_2 utilization is not part of the CO_2RUe portfolio, this project nonetheless provides an important and impactful contribution to the consortium by assessing the feasibility of implementing CO_2 utilization technologies at scale in optimal location-specific markets based on technology performance targets.

Answers:

- 3.1 It remains unclear how the E component will be integrated into the cross-sector modeling. The timeline for onboarding this component is not until Year 3 of the project, but there was no approach discussed as to how this would be integrated and weighted into the current cost-based models. We thank the reviewers for raising this question. The integration of the EEEJ components into the cross-sector modeling will be addressed in our proposed Task 5 and Task 6, which will be delivered in Budget Period 3. In Task 5, the focus is on assessing the regional air quality and public health impacts associated with long-term exposure to PM 2.5 emissions from various sources related to CO_2 utilization pathways. This is achieved using the InMAP air quality model. The model provides fine-resolution and demographic-specific estimates of air quality impacts, which are important for EEEJ analysis. The analysis incorporates criteria air pollutant emissions and siting information to create location-specific inputs for InMAP. The concentration-response function is used to estimate health impacts considering changes in PM 2.5 concentration. The output metrics include changes in population-weighted exposure to PM 2.5, net health impacts, and corresponding economic valuations by different demographics and income levels. In Task 6, the socioeconomic impact assessment focuses on evaluating the economywide impacts of the industry-scale deployment of preselected CO_2 utilization technologies. This is done using a regional version of the BEIOM macroeconomic model, which considers supply chain interactions and estimates socioeconomic and environmental impacts. Demographic and economic data from official sources are collected and modeled to forecast the baseline U.S. economy. The preselected CO_2 utilization technologies are specified in BEIOM using process-level data from the TEA/LCA project. Additional data collection is conducted to detail the primary supply chain industries and perform sensitivities to scenarios and electricity generation mixes.

Comments 4: Quantification of resource (feedstock and renewable electricity) availability and costs for CO_2 conversion to fuels is extremely important to guide development and deployment, and the project is moving in the right direction. Following are a couple of comments: The team shows the advantages of the preferred pathway (LTE – syngas fermentation – EtOH to SAF) with the pathway based on reverse water-gas shift reaction. It seems that another pathway (LTE – CO_2 H_2 – MeOH) may be more cost-competitive and should be used as a base case. Second, localization of the distributed SAF production (close proximity to major airports, delivery infrastructure) should be analyzed. I also recommend considering water resources.

Answers:

- 4.1 The team shows the advantages of the preferred pathway (LTE – syngas fermentation – EtOH to SAF) with the pathway based on reverse water-gas shift reaction. It seems that another pathway (LTE – CO_2 H_2 – MeOH) may be more cost-competitive and should be used as a base case. The project is currently scoped to SAF production due to the large size of its market. In the future, we will evaluate CO_2 utilization for chemical production such as methanol because it is an important intermediate with broad applications and also a potential marine fuel decarbonization application.
- 4.2 Second, localization of the distributed SAF production (close proximity to major airports, delivery infrastructure) should be analyzed. We analyzed the SAF markets and infrastructure in our research. In particular, we considered (1) proximity to the current jet fuel distribution infrastructure and (2) proximity to the end users (i.e., blending facilities connected to infrastructure). Because the jet fuel pipeline is already well distributed from the jet fuel refineries to the airports, we assumed that the current jet fuel pipeline network in the United States will be used for SAF transportation to various markets, and hence we located CO_2 utilization SAF facilities near the current jet fuel refineries, where SAF will be replacing or blended with the petroleum jet fuel.
- 4.3 I also recommend considering water resources. Water resources are analyzed in parallel in the other project (WBS 2.1.0.506 and WBS 2.1.0.507) that we are closely working with.

Comments 5: The specific goals of this project were not clearly communicated. Slide 9 sets the stage at a very high level, but beyond that, the reviewers need to go to the quad chart to see the goals. Because this project followed WBS 2.1.0.304, it would have been useful to hear more about how this project differed from the previous one. I was left wondering if the work was significantly distinct or simply looking at the same issue in a slightly different way. More collaboration and communication between these two projects would have helped highlight and differentiate their added value to the program. I see that mentioned on Slide 20, but it was not clear from the presentation. In regard to progress and outcomes, I've given this project a three because although they have made good progress toward their goals, little mention was made of risk mitigation and challenges. This left me with the impression that the work could have been more challenging.

Answers:

- Three projects (WBS 2.1.0.504 and WBS 2.1.0.505, WBS 2.1.0.506 and WBS 2.1.0.507, and WBS 2.1.0.304) are closely coordinated to align and interface their different scopes and system boundaries. This project (WBS 2.1.0.504 and WBS 2.1.0.505) focuses on potential CO_2 and clean power for SAF production, the cost of their supply to SAF production facilities, and SAF market size and distribution to end users. WBS 2.1.0.506 and WBS 2.1.0.507 use the cost of power and CO_2 supply to the SAF facility from the first project and evaluate SAF production cost, water use, and GHG emissions throughout the SAF value chain using a bottom-up TEA, LCA, and water analysis approach. The feasibility study project (WBS 2.1.0.304) evaluates the feasibility of the entire CO_2 utilization landscape by considering the competition among multiple products and using information from the other two projects to complement the development of a comprehensive CO_2 utilization analysis portfolio.

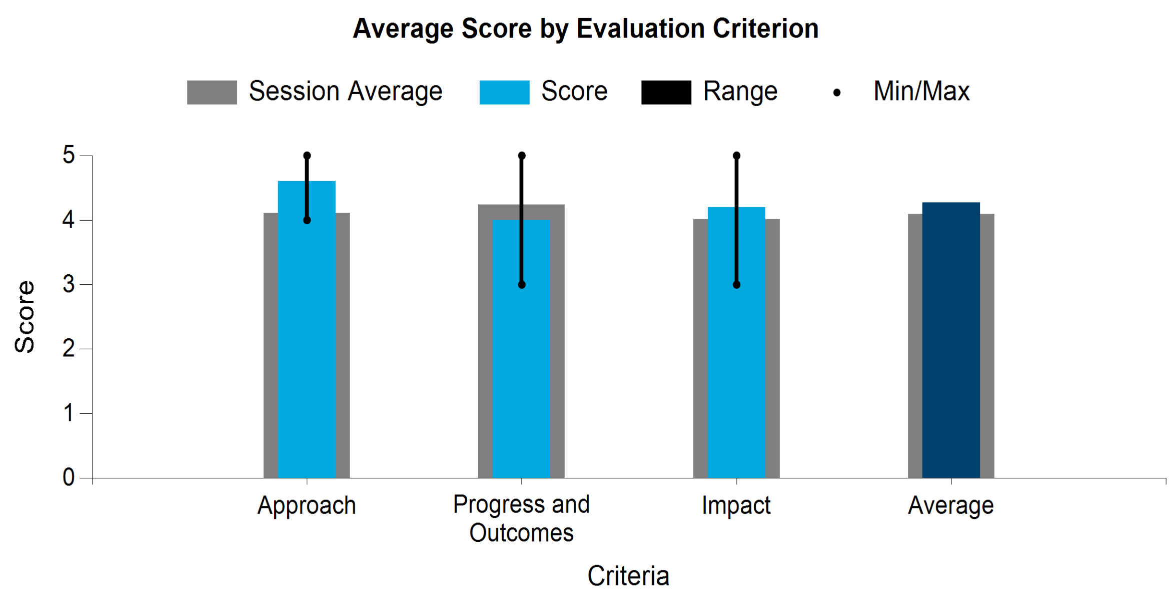
ECONOMICS AND SUSTAINABILITY OF CO_2 UTILIZATION TECHNOLOGIES WITH TEA AND LCA - NREL

Argonne National Laboratory

PROJECT DESCRIPTION

WBS:	2.1.0.507
Presenter(s):	Michael Wang
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$700,000

This project performs TEA, LCA, and water analysis of CO_2 utilization technologies to address their costs and sustainability implications. The project leverages TEA capabilities at NREL; the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) LCA capabilities at ANL; and water modeling capabilities at ANL to develop analytic capabilities of TEA, LCA, and water for the CO_2RUe. The team incorporates the data sets from other projects of the CO_2RUe to produce the cost and energy/environmental results of CO_2 utilization technologies. The outputs of this project have been used by the other two analysis teams and the R&D teams of the CO_2RUe for improving cost and sustainability performance. Specific outcomes include: (1) TEA results with key cost drivers for CO_2 utilization technologies; (2) LCA results with an expanded, updated GREET CO_2 utilization LCA module for relevant CO_2 utilization technologies covering electricity generation, hydrogen production, and CO_2 sourcing; and (3) a compilation of analyses addressing regional water resource availability and stress for CO_2 utilization facilities using the water models. With the results from this project, BETO, CO_2RUe teams, other agencies, and industry will be able to present the value proposition of CO_2 utilization technologies and identify bottlenecks/hot spots of costs and the sustainability of CO_2 utilization technologies for improvements.



COMMENTS

- The approach of incorporating water analysis into the investigation of CO_2 utilization technologies will provide key information to the community. Expanding and updating GREET is extremely important and will make a wide impact. More communication between the groups in the CO_2 consortium could be fruitful. Additional information/questions for further assessment:

Risk management:

- Additional information regarding how the individual unit operations are designed and modeled
- Additional information regarding the analysis of this group and how it guides and communicates with the CO_2 consortium and industry partners regarding their target products, reactor configurations, and operating conditions.

Potential impact:

- More information regarding the analysis of CO_2 electrolysis versus other methods to produce target products
- More information regarding the analysis of CO_2 electrolysis versus other methods to produce SAF.

- This project aims to perform TEA, LCA, and water analysis to analyze CO_2 utilization technologies. Several pathways for CO_2 conversion have been considered. Results for energy inputs and carbon footprint have been discussed; however, the connection between the energy input and carbon footprint with key performance metrics has not been discussed. Therefore, it is unclear how the TEA/LCA can help direct the research direction. It is unclear if the carbon footprint for CO_2 capture is considered. It is also unclear how the performance for each individual step is considered.
- This project represents the third portion of the TEA/LCA component of the CO_2RUe. This project specifically focuses on the TEA and LCA of different CO_2 utilization pathways to SAF. The goal of the project is to address the cost and environmental impacts of the proposed technologies within the CO_2RUe for CO_2 utilization. A specific strength of the project is the close collaboration with the analysis and research teams within the CO_2RUe in defining conversion processes and performance metrics for consortium-relevant modeling. The incorporation of water stress analysis is another key strength of this project and highlights the close collaborations with the other analysis projects in the CO_2RUe, especially with WBS 2.1.0.504. This project is an important component of the CO_2RUe, with significant impact in validating the feasibility of and informing research priorities for proposed CO_2 utilization technologies and processes.
- The team is doing a good job modifying the GREET model to additional conversion pathways. Will this model be available to the public (it was stated only for the consortium teams)? It is good that water availability is included in the analysis, but competition for the resources should be included. It is not clear which capacity factor is included in the cases with $0.02/kWh electricity cost. Negative CO_2 emissions should be taken with a grain of salt because this loophole could be closed in the future. Carbon emissions of renewable natural gas (RNG) are probably underestimated (high fugitive methane leakage due to distributed and poor technology). It is strange that the cost of pathways using renewable H_2 is lower than the baseline. I recommend putting more effort into analyzing Pathway 5 as the most probable promising alternative.
- This project has a very strong plan, with talented researchers invested in addressing questions on which factors impact the competitiveness of CO_2-based SAF production. The analysis is detailed and thorough, leaving little question of the results or their significance. The part where this project suffers is the same as WBS 2.1.0.504: uniqueness. How different is this work from that project? It seems as though the three analysis projects have shared interests (as expected), but more energy spent on differentiating each project would be helpful in assessing how much value the three projects yield for BETO and the public as a whole and individually.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The approach of incorporating water analysis into the investigation of CO_2 utilization technologies will provide key information to the community. Expanding and updating GREET is extremely important and will make a wide impact. More communication between the groups in the CO_2 consortium could be fruitful. Additional information/questions for further assessment: risk management—additional information regarding how the individual unit operations are designed and modeled, additional information regarding the analysis of this group and how it guides and communicates with the CO_2 consortium and industry partners regarding their target products, reactor configurations, and operating conditions; potential impact—more information regarding the analysis of CO_2 electrolysis versus other methods to produce target products, more information regarding the analysis of CO_2 electrolysis versus other methods to produce SAF.

  Responses: The project encompasses key metrics, including economic feasibility and environmental impacts, such as life cycle GHG emissions and water consumption/stress. We aim to develop an extended version of GREET that includes all significant CO_2 utilization pathways with all relevant CO_2 utilization technologies. We will maintain active communication within the consortium and engage with external stakeholders to enhance the value and applicability of our analysis results. When it comes to risk management, a critical issue is associated with data availability. Because CO_2 utilization technologies are still in the early stages of R&D, our analysis heavily relies on process modeling and/or limited experimental data in the literature and as provided by R&D teams. To mitigate this risk, we plan to actively engage with the R&D teams within the consortium. Through the engagement, we will gain deeper insights into conceptual process designs, access timely developed data, refine our parameters, and improve the representation of our analysis. Individual unit operation design is based on both active collaborations between the R&D teams and process engineers and engineering judgment from the TEA team. Additionally, we recognize the importance of engaging with external industry stakeholders who can provide valuable input, expertise, and reality checks. Their inputs will further enhance the quality and reliability of our analysis by validating and enriching the data and process-related knowledge upon which we rely. We follow an iterative process throughout the project with the consortium. Once we generate analysis results for a technology, we inform the corresponding R&D team and engage in discussions to identify opportunities for improving the economic and environmental metrics. These discussions help us refine parameters, update processes, and improve configuration to reflect R&D efforts. Given that the project includes all major CO_2 utilization pathways, this allows us to evaluate and compare their respective benefits, challenges, and opportunities for improvements. The iterative process enables us to continuously refine our methods and results, leading to more informed R&D decision-making and ultimately maximizing the consortium's impact on both economic and environmental fronts.

  Comments: This project aims to perform TEA, LCA, and water analysis to analyze CO_2 utilization technologies. Several pathways for CO_2 conversion have been considered. Results for energy inputs and carbon footprint have been discussed; however, the connection between energy input and carbon footprint with key performance metrics has not been discussed. Therefore, it is unclear how the TEA/LCA can help direct the research direction. It is unclear if the carbon footprint for CO_2 capture is considered. It is also unclear how the performance for each individual step is considered.

  Responses: Our team has been conducting comprehensive analyses of the economic and environmental impacts associated with CO_2 utilization pathways, employing TEA and LCA methodologies. As highlighted by the reviewer, the carbon footprint (life cycle GHG emissions) of these pathways significantly varies based on the type and amount of energy used. As we mentioned in the approach section of our presentation, this is an iterative process, and the TEA/LCA is directly linked with R&D to help guide the research direction. Because of the presentation time limitation, we did not present the details of the TEA and LCA. For instance, key cost drivers and key carbon reduction strategies were analyzed in detail for each selected pathway and have been communicated with the R&D teams to provide specific guidance on cost reduction or sustainability improvement strategies. This communication enables us to identify R&D activities on the major cost and emissions contributors for each pathway and guide discussions on potential strategies for further reducing these key performance metrics. In our LCA, the energy use and associated emissions of CO_2 capture and transportation are included. Note that we used a consistent LCA system boundary and methodology as used in other BETO-funded projects, ensuring comparability and consistency across studies. By employing rigorous analysis methodologies, collaborating with the consortium R&D teams, and using consistent LCA practices, we aim to provide robust and reliable results that will inform R&D decision-making to maximize the effectiveness of CO_2 utilization pathways in reducing emissions and advancing sustainability goals.

Comments: This project represents the third portion of the TEA/LCA component of the CO_2RUe. This project specifically focuses on the TEA and LCA of different CO_2 utilization pathways to SAF. The goal of the project is to address the cost and environmental impacts of the proposed technologies within the CO_2RUe for CO_2 utilization. A specific strength of the project is the close collaboration with the analysis and research teams within the CO_2RUe in defining conversion processes and performance metrics for consortium-relevant modeling. The incorporation of water stress analysis is another key strength of this project and highlights the close collaborations with the other analysis projects in the CO_2RUe, especially with WBS 2.1.0.504. This project is an important component of the CO_2RUe, with significant impact in validating the feasibility of and informing research priorities for proposed CO_2 utilization technologies and processes.

Response: Thank you for your positive comment.

Comments: The team is doing a good job modifying the GREET model to additional conversion pathways. Will this model be available to the public (it was stated only for the consortium teams)? It is good that water availability is included in the analysis, but competition for the resources should be included. It is not clear which capacity factor is included in the cases with $0.02/kWh electricity cost. Negative CO_2 emissions should be taken with a grain of salt because this loophole could be closed in the future. Carbon emissions of RNG are probably underestimated (high fugitive methane leakage due to distributed and poor technology). It is strange that the cost of pathways using renewable H_2 is lower than the baseline. I recommend putting more effort into analyzing Pathway 5 as the most probable promising alternative.

Responses: The main objective of incorporating the CO_2RUe pathways into the GREET model is to assess and enhance the environmental metrics of the CO_2 utilization conversion technologies under consideration by the consortium; however, our team also has plans to include these pathways in the public version of the GREET model, subject to the decision of the consortium and BETO. Thus, these CO_2 utilization pathways will be available to others via public release of the GREET model. We agree that water is a critical component of the sustainable implementation of CO_2 utilization technologies. In response to the reviewer's comments on the competition for water, we agree that the competing water use from all sectors is a key issue. In fact, water tools used in this project are capable of assessing the impact. The Available Water Remaining for the United States model is indeed intended to address the impact on regional water supply and demand by different competing water uses in specific regions; the WATER estimates changes in freshwater available to other economic sectors after meeting water demand from CO_2 utilization technologies at a local level. Further analysis of reclaimed water use by CO_2 utilization technologies represents the degree to which the competing demand can be reduced. Regarding the avoided GHG emissions credits of RNG, we plan to conduct a thorough review of the conditions and parameters to affect the so-called counterfactual scenario emissions of waste management practices. This will help revise RNG avoided emissions credits. As the comment correctly points out, it is essential to prevent overestimating the emissions credits attributed to the production of RNG and to fully account for the methane leakage of the RNG supply chain. The cost of $0.02/kWh for renewable electricity is from the estimated cost of renewable electricity in the next 10 years. The capacity factor is assumed to be 90% onstream. While the cost or the capacity factor for renewable electricity is optimistic, we used it in our TEA as a case of continuing success of renewable power deployment as observed in the past 10 years globally and domestically. In addition, variations of these parameters were included in the sensitivity analysis to address the uncertainty, which is part of the project efforts but was not included in the presentation because of time constraints. Similarly, our use of low-cost renewable hydrogen is based on the premise of low-cost renewable power and significant cost reduction in hydrogen electrolysis that reflect the success of DOE and the federal government's significant R&D investment in renewable hydrogen in the next 10 years. Our FY 2023 analysis has been centric on Pathway 5 and cross-comparing direct or indirect CO_2-to-methanol pathways using a consistent analysis basis. We sincerely appreciate the comment and will definitely put more emphasis on analyzing this pathway.

Comments: This project has a very strong plan, with talented researchers invested in addressing questions on which factors impact the competitiveness of CO_2-based SAF production. The analysis is detailed and thorough, leaving little question of the results or their significance. The part where this project suffers is the same as WBS 2.1.0.504: uniqueness. How different is this work from that project? It seems as though the three analysis projects have shared interests (as expected), but more energy spent on differentiating each project would be helpful in assessing how much value the three projects yield for BETO and the public as a whole and individually.

Responses: The consortium leadership has defined the scope, the boundary, and the interrelationships among the three analysis projects to ensure coordinated efforts and to avoid potential duplication among them. This project covers the TEA, LCA, and water analysis (WBS 2.1.0.506 and WBS 2.1.0.507) with a bottom-up approach, starting with process-level modeling that encompasses CO_2 utilization conversion technologies and other relevant life cycle stages, such as CO_2 capture and transportation. Thus, detailed TEA and LCA are performed to provide guidance to the R&D teams for cost reduction and sustainability improvement strategies. Our goal is to provide information to and incorporate R&D progress data from the R&D teams of the consortium. Also, we aim to bridge data gaps in TEA/LCA with relevant data from industry experts and stakeholders in addition to the data from the consortium's R&D teams. We strive to make the TEA/LCA/water analysis an integral part of the consortium's efforts to develop credible, relevant cost and sustainability results to rally policy and public support of CO_2 utilization technology deployment. The TEA/LCA data from this project are fed to the market/resources assessment project (WBS 2.1.0.504 and WBS 2.1.0.505) to (1) analyze how much renewable power and CO_2 resources would be needed for CO_2 utilization plants to meet BETO's SAF production goal; (2) determine the optimal regional locations of CO_2 utilization plants and potential transportation of CO_2, renewable electricity, and/or renewable hydrogen; and (3) address potential constraints of regional availability for all major resources. Additionally, the feasibility study team (WBS 2.1.0.304) takes a more holistic approach to evaluate the technology feasibility of the entire CO_2 utilization landscape by considering the competition among multiple products, which contributes to the development of a comprehensive portfolio. Detailed TEA/LCA data from this project are also fed to the feasibility study team (WBS 2.1.0.304) so that more holistic conclusions can be distilled for providing road-mapping strategies for major CO_2 utilization potentials.

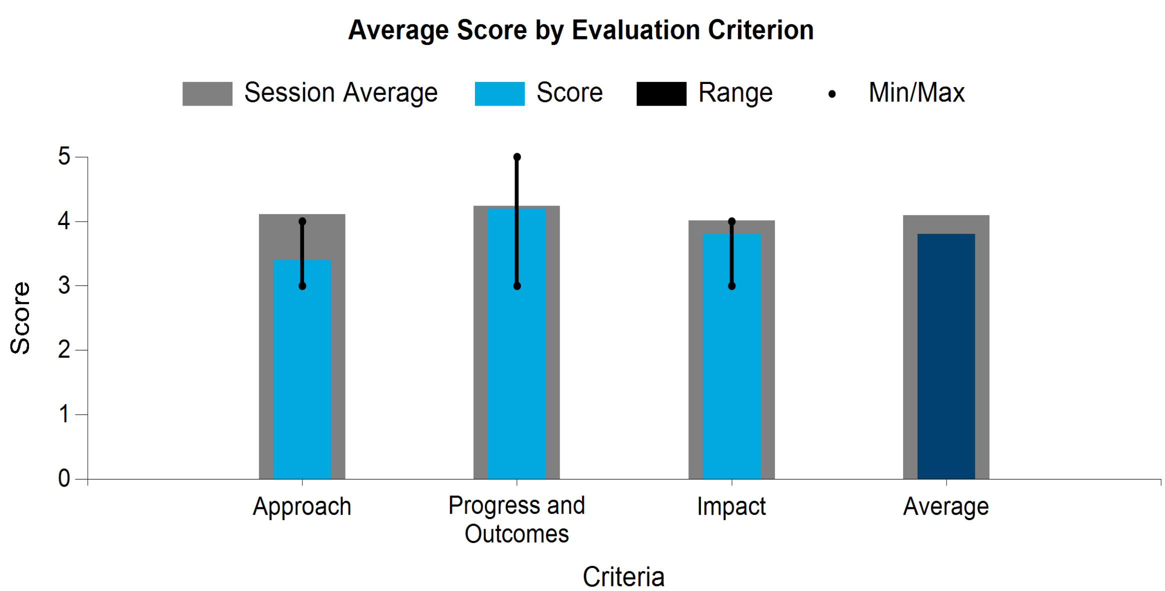
CO_2 UTILIZATION: THERMO- AND ELECTROCATALYTIC ROUTES TO FUELS AND CHEMICALS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.1.316
Presenter(s):	Jack Ferrell
Project Start Date:	11/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$300,000

Existing biomass conversion processes, such as fermentation to produce ethanol, produce very pure industrial sources of CO_2. In fact, domestic ethanol biorefineries are the largest single-sector supplier of CO_2 to the merchant gas markets. This provides a unique opportunity for the bioenergy industry: to reduce the cost (MFSP) of the primary product (ethanol) by valorization of this large CO_2 waste stream. In this project, first, we work closely with TEA/LCA projects to identify/quantify the largest risks for the commercialization of low-temperature CO_2 electrolyzers. Next, we perform targeted experimental work to address the identified risks. While there has been significant recent interest in this field, challenges remain before this process can be performed industrially. The goal of this project is ultimately to enable long-term and stable operation at high current densities for low-temperature CO_2 electrolysis. During the past 2 years, we have helped identify risks, incorporated these risks into TEA/LCA, and published this work in *Energy & Environmental Science*; these risks have also been incorporated into the strategic plan for the CO_2RUe. We have also performed research on cathode electrocatalyst degradation and carbon corrosion. Moving forward, we plan to focus on catalyst degradation. By addressing the persistent issues facing these technologies, we aim to enable the economic electrochemical conversion of CO_2.



COMMENTS

- The approach of doing experimental research guided by TEA is important for risk mitigation, and focusing on various key real-world drivers is valuable. Their work on testing MEAs with online gas chromatography units will provide key information regarding the conversion and migration of CO_2 and the mass balance of the reaction. I would like to see more communication with the other projects that are working on the increased stability of ECO_2R. Additional information/questions for further assessment:

Risk management:

- Additional information on testing and methods to test the system in real-world conditions; R&D road map to achieve their goals
- More information regarding other cost drivers and other target goals used in other groups within the consortium.

Potential impact:

- More information regarding the justification of research on carbon paper and the translatability of their findings to other catalysts.

- The goal of the project is to identify and de-risk low-temperature electrocatalytic CO_2 reduction to CO. Efforts have been made to understand the corrosion of carbon at the anode side. The project also aims to understand the degradation of the catalyst at the anode side using *ex situ* characterization. Carbon corrosion is quite common, and often titanium porous transport has been used to overcome this problem. Would it be more efficient to consider using titanium instead of porous carbon support for the anode? A lifetime of more than 4 years would be challenging for evaluation; would you consider any accelerated testing to understand the catalyst degradation? Catalyst degradation can come from the failure of other parts in the electrolyzer, such as the membrane, or leaching of anode, or salt formation. It would be more impactful if catalyst degradation was studied in parallel with other components.

- The approach of this project is to closely collaborate with the analysis teams in the CO_2RUe to identify key risks in CO_2 electrolysis commercialization and then to conduct targeted experiments to address those risks. Initial studies have focused on MEA durability testing, which has been identified as a key technology gap in CO_2 utilization. To assess durability, the project has developed an MEA testing system with online detection at both the anode and cathode for full mass balance and *ex situ* microscopic and spectroscopic analysis of component degradation. Key findings of the project include 100-hour durability of the catalyst materials during operation within the MEA testing system but appreciable degradation of the carbon support used in the gas diffusion electrode (GDE). One concern with the project approach lays with the scale of the MEAs tested. It is unclear if issues determined at the 5-cm^2 scale are translatable to larger-scale, 100–1,000-cm^2 systems. For example, many (but not all) larger-scale electrolyzers eschew the use of carbon supports in favor of tin, possibly limiting the impact of the initial studies. Another concern is that the timescale of the degradation measurements, 100 hours, is small on the scale of the proposed electrolyzer lifetime needs, meaning that some degradation pathways may be missed due to the short durability testing time. The short testing timeline highlights the need for developing accelerated lifetime testing protocols in the CO_2 electrolysis field, although such work is likely outside the scope of this project. Overall, this project plays an important role in the CO_2RUe of quantifying risks in emerging electrochemical CO_2 utilization pathways being explored within the consortium and in performing important studies to help mitigate these risks.

- Using CO_2 waste from biorefineries may indeed provide early opportunity for the deployment of CO_2 utilization due to the low-cost available feedstock and the possibility of having the single product stream (if the product is ethanol); however, high capital expenditures (CapEx) may be a showstopper for owners (payback period?). The proposed external testing of materials could potentially accelerate the development of durable MEAs; however, the results of the CO_2 electrolyzer generally showed much better durability than can be calculated from the reported *ex situ* tests, which demonstrated extremely fast degradation. So, it is unclear how relevant these results are to real-life electrolyzer durability, and the final milestone though this method could be possibly used for comparison of different materials. It is absolutely necessary to identify key degradation factors and establish a transfer function between *ex situ* and *in situ* testing, especially for commercially meaningful current densities. In addition, the duration of tests (100 hours) is clearly insufficient to identify the root causes of degradation. The demonstrated potential cost-competitiveness is based on not yet demonstrated current densities, so it is useful to monitor the current cost of SAFs using experimental performance and durability parameters. It is also unclear how the team is going to quantify technology risks.

- This is an important study looking into key factors that influence MEA degradation and performance during runs. To that end, the researchers have developed an *ex situ* carbon corrosion test relevant to their anodes. Unfortunately, significant mass loss and carbon corrosion were observed in only 24 hours. The project proposes testing lower voltages for longer periods of time. Although understanding the correlation between the demand on the cell and degradation is important, we need to be going up in voltage over time to achieve economic feasibility.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their time and feedback. We agree that increasing the durability of low-temperature CO_2 electrolysis systems is critical for moving this technology forward, and our close collaboration with TEA/LCA projects has highlighted the importance of achieving increased electrolyzer lifetime. Beyond lifetime, recent TEA/LCA (which has been incorporated into the strategic plan for the CO_2RUe) also shows that performance increases are needed, such as increasing current and single-pass conversion and decreasing voltage and electrolyzer cost. Regarding the carbon corrosion work, the high mass loss presented was collected at a high anode voltage of 2 V, which is an accelerated condition leading to higher corrosion rates. We have used higher voltages for the development of the *ex situ* carbon corrosion test and are currently exploring longer experiments (>1 month) at realistic anode voltages (~1 V). We also agree that it is likely that a metal-based anode (e.g., porous transport layer) will be needed to achieve sufficient lifetime in commercial electrolyzer devices; however, the majority of the field is currently using carbon-based GDEs on the anode. Our goal with the carbon corrosion work is to highlight that carbon corrosion is an issue under CO_2 electrolysis conditions and ultimately to provide recommendations on the types of experiments where carbon should be avoided on the anode. We hope that this work will encourage the community to switch to non-carbon materials on the anode, because moving toward commercially relevant MEA architectures sooner will accelerate the path toward commercialization. We also agree that the development of accelerated durability tests remains a large gap for CO_2 electrolysis. This will require a large, dedicated effort to be successful, and we agree that multiple degradation routes should be studied in parallel during longer-duration durability testing. Further, different routes to accelerating different degradation pathways (e.g., voltage cycling, increased molarity of solutions, increased temperature, increased voltage) will need to be probed to arrive at accelerated durability tests.

ELECTROLYZERS FOR CO_2 CONVERSION FROM BIOSOURCES

Dioxide Materials

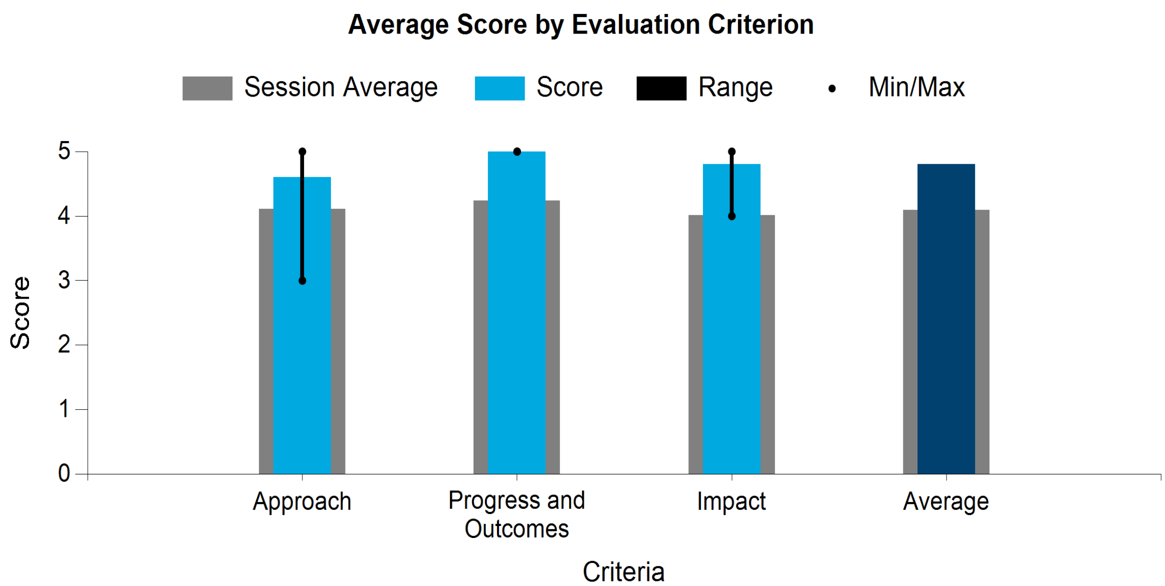
PROJECT DESCRIPTION

WBS:	2.3.1.418
Presenter(s):	Rich Masel
Project Start Date:	10/01/2020
Planned Project End Date:	02/28/2024
Total Funding:	$3,125,000

Dioxide Materials' anion exchange membrane electrolyzers for CO_2 reduction to CO have demonstrated the highest Faradaic efficiency and stability of any CO_2 electrolyzer reported in the literature. To interface with an industrial-scale biorefinery, the surface area must be increased to at least 1 m^2 and scaled to tens of megawatts. The performance is also reduced due to components in fermentation flue gas. In the proposed work, we will:

- Create electrolyzer designs that are scalable to the megawatt scale.
- Develop improved catalyst/ionomer layers that are robust to changes in flue gas composition.
- Integrate the improved electrolyzer with a CO fermenting microbe.

If successful, this project will create scalable electrolyzers that can be combined with bioreactors to convert biorefinery CO_2 into biofuels and products, thereby achieving BETO's goals of producing fuel.



COMMENTS

- Investigating the effects of scaling ECO_2R is as important as studying the individual processes, such as detailed catalyst degradation. The information they have gained from their approach of scaling a CO_2 electrolysis reactor and testing the performance and failure mechanisms in a larger system is valuable to the CO_2 utilization field. They are addressing effects such as humidity in the system, which will be able to be applied to other projects scaling ECO_2R.

  It would be great to see increased outreach and knowledge exchange of their investigations and results. Additionally, contributing to a facility where their system could be used by different groups to quickly gain initial insights into challenges associated with scaling may be helpful. Additional information/questions for further assessment:

Risk management:

- Additional information regarding the system; current and target flow rates of CO_2, mass balance calculations; additional information regarding CO_2 crossover, impurity management at scale, and analysis of the active catalyst (STY)
- Additional information regarding the target product—a performance comparison of when the system is optimized for production of CO versus a specific ratio of H_2:CO
- Additional information regarding experiments, the reproducibility of the system, and the duration and number of experiments with the 1,000-cm^2 electrolyzer
- Detailed plans for temperature management and further elaboration on the plans for redesigning flow and how it will scale.

Potential impact:

- Additional analysis regarding the use of specialized GDE in this system.

- The project aims to develop electrolyzers for CO_2 conversion to CO using bio-derived CO_2. Overall, very impressive progress in scaling up the electrolyzer has been achieved (stability of over 100 hours with 1,000-cm^2 electrolyzer). A critical challenge in scaling up this technology has been identified. The integration of the CO_2 electrolyzer with the biological reactor has been demonstrated. While most key performance metrics have been demonstrated, CO_2 crossover has not been quantified and addressed.
- This project focuses on scaling electrolyzer cells from the 250-cm^2 active area size commercially available today to a 1,000-cm^2 active area, which has been identified as the appropriate size for deployable cell stacks to convert CO_2 from biorefineries to CO for downstream bioconversion. A key part of the project approach is performing deconstructive tests in which failing components from the 1,000-cm^2 active area electrolyzers are removed and loaded into small test cells to determine failure mechanisms. The project makes use of the NREL process development unit for the large cell testing. The project team has designed eight 1,000-cm^2 cells and built three. All three met the milestone goals of >200-mA cm^2 for 100 hours with >90% selectivity. The project team observed failure at a longer time, however, and was able to identify several failure modes due to thermal hot spots in the membrane, mechanical failures of the cathode gas diffusion layer, and membrane ruptures. The project team has been able to address many of these failures with changes to the electrolyzer cell design or through modifications to the gas diffusion layer and membranes, including manufacturing stronger membranes. The project approach also examines which parameters influence product selectivity by running the electrolyzers with CO, CO_2, and H_2 gas mixtures from initial performance tests and tuning selectivity by modifying electrolyzer components such as humidity and catalysts. Through this process, the project team has identified that humidity plays a crucial role in catalyst utilization and electrolyzer performance. Immediate future goals of scaling to 1,000 hours of performance for the large cells are appropriate. This project has made excellent progress on an important topic of scaling electrolyzers, and it will have significant impact in practical CO_2 conversion and utilization.
- The team successfully built and tested a commercial-scale, 1,000-cm^2 cell in CO_2 reduction to CO with high Faradaic efficiency. An anion exchange membrane with increased strength has been developed. The durability milestone (100 hours at 200 mA/cm^2) has been met; however, the cell voltage was steadily growing, and the cell failed after 200 hours due to a cracked gas diffusion layer. This and other pathways of the electrochemical cell failure were established and studied, which is very important for commercial

deployment. Reaction selectivity was studied using a differential cell, and factors controlling the selectivity (e.g., relative humidity) were established. A major focus for future work should be on MEA quality control and durability (cell voltage and Faradaic efficiency).

- This was easily the most impactful presentation of those reviewed. It was refreshing to see a team invested in "breaking things and figuring out what went wrong." Top marks for progress and innovation. I was also very pleased to see open communication from an industry partner like this.

PI RESPONSE TO REVIEWER COMMENTS

- I want to thank the reviewers for taking the time to review our program and for their constructive comments. The reviewers raised valuable points, and I do not disagree with anything they said. We have taken the reviewers' suggestions. The major focus for future work will be on MEA quality control and durability (cell voltage and Faradaic efficiency). We are sending the system shown on slide 22 to NREL, as the first reviewer suggested.

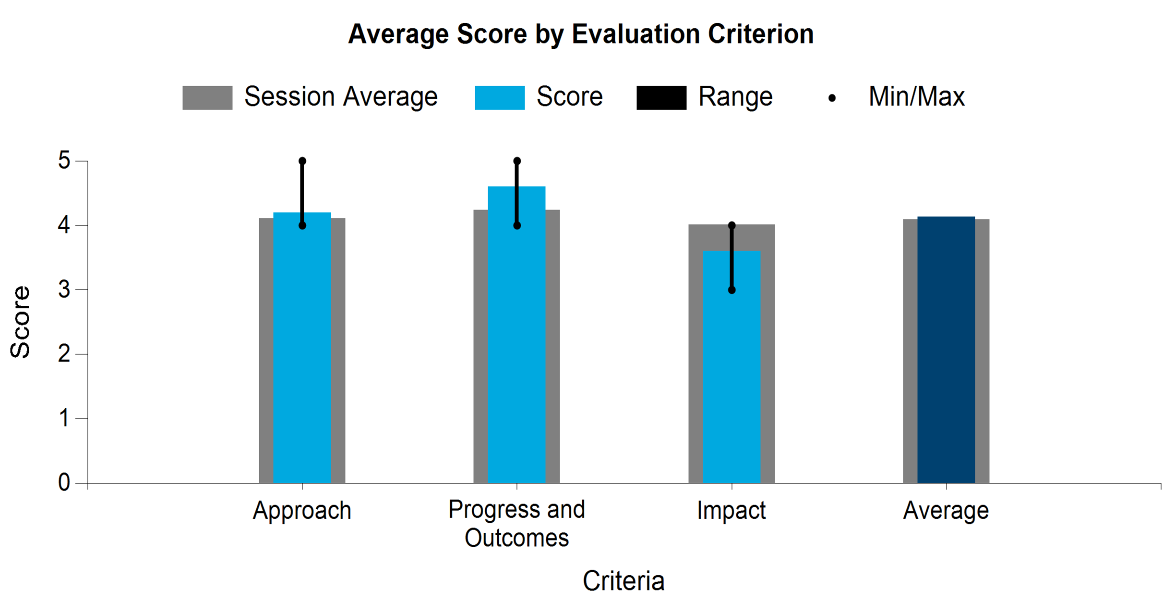
ELECTROCHEMICAL PRODUCTION OF FORMIC ACID FROM CARBON DIOXIDE IN SOLID ELECTROLYTES

University of Delaware

PROJECT DESCRIPTION

WBS:	2.3.1.421
Presenter(s):	Feng Jiao
Project Start Date:	10/01/2020
Planned Project End Date:	08/31/2024
Total Funding:	$3,135,186

The proposed work is divided into three distinct R&D phases, with clear milestones needed to progress the state of the art (SOA) for CO_2 electrolysis to formic acid. In particular, the work scope is directed at improving the activity, selectivity, and durability of individual components and a large-scale (>750-cm^2) electrolyzer. In Phase I, we will focus on the initial verification of the results from the team that stand out as the SOA in ECO$_2$R to formic acid. Here, we will use the bismuth catalysts, which have been able to show high selectivity (90% Faradaic efficiency to formic acid) at current densities of 100 mA/ cm^2 while also showing long-term stability (100 hours, continuous or noncontinuous interval operation) at an applied current density of 30 mA/cm^2. This phase is expected to be complete upon meeting the performance in a 5-cm^2 electrolyzer, as previously published. Phase II will focus on maintaining the high selectivity toward formic acid (90% Faradaic efficiency) while doubling the current density to 200 mA/cm^2 in a cell that is >100 cm^2. The stability of the system will also begin to be assessed at >200 hours (continuous or noncontinuous with interval system regeneration) to record potential degradation in terms of increased cell voltage and decreased Faradaic efficiency toward formic acid. The main goal is to achieve all these metrics in one cell, but individual performance metrics will be assessed to gain insights into which operating conditions lead to overall cell degradation (increasing voltage and decreasing selectivity to formic acid). The final phase of the project, Phase III, will translate the catalytic performance of the bismuth catalysts to an industrial electrolyzer. Here, the selectivity and activity (Faradaic efficiency and current density) of the previous phases will be maintained while focusing on translating this performance to a large (>750-cm^2) cell and operating for >1,000 hours (continuous or noncontinuous with interval system regeneration).



COMMENTS

- Approaching the design of a reactor that considers the energy intensity of electrolyte processing and greatly minimizes it is important to developing a commercial system. Testing has been done in larger electrodes (25 cm^2 and 100 cm^2), which increases the number of challenges; however, the information gained will help guide the R&D to investigate scaled systems. Additional information/questions for further assessment:

  Risk management:

  - More information regarding the amount and rate of formate oxidation in these systems compared to liquid electrolytes
  - More information regarding any other byproducts formed on the catalyst and their interaction with the solid electrolyte
  - More information regarding impurity management in the electrolyte and the interactions with the catalyst
  - More information regarding any temperature change within the catalyst/solid electrolyte.

  Potential impact:

  - Further information and analysis regarding the justification of using this approach over liquid electrolytes
  - Further details on the stability of the selectivity and carbon conversion percentage
  - Further details on the analysis of formate as an H_2 carrier.

- The proposed project focuses on producing formic acid from CO_2 reduction using solid electrolytes. Significant progress has been made in the area of catalyst development and TEA. Excellent publication outcome. The PIs have identified challenges with scaling up the solid-electrolyte layer. Several strategies have been tried and proposed. While impressive progress has been made, it is still unclear how the final milestone (demonstrate formic production with cell size >750 cm^2) can be achieved. A key challenge with using the solid-electrolyte layer is the high cell resistance. Together with current density, Faradaic efficiency, and stability, it is also important to set the target for cell voltage.

- The aim of this project is to scale electrolyzers using solid electrolytes for formic acid production to the >750-cm^2 sizes with stable 100-hour performance at >200 mA/cm^2 with 90% current density. This project approach builds from previous demonstrations of selective formic acid production by solid-electrolyte electrolyzers at the lab scale. The approach is well structured, with eight specific tasks divided into three phases: initial verification, catalyst and reactor scaling, and performance and durability testing at scale. The project team has made substantive progress, although they have run into significant technical challenges in the scale-up of solid-state interlayers and catalyst scale-up. The catalyst challenge has been overcome due to changes in synthesis routes, but challenges with scaling the solid-electrolyte interlayers have required a complete redesign of the interlayer structure. Still, the project team has managed to produce 100–250-cm^2 reactors with 15-hour stability for formate production at >90% initial Faradaic efficiency. Overall, the project has made good progress, especially given the low TRL level of the novel solid-electrolyte CO_2 electrolyzers compared to other electrolyzer technologies. If successful, this technology would have enormous impact. The solid-electrolyte CO_2 electrolyzers produce formic acid directly, which eliminates the need for downstream acidification and salt removal needed by the more conventional CO_2 electrolyzers that produce formate. It remains to be seen whether this technology can scale to the 750-cm^2 electrolyzer size with the necessary 100-hour performance stability, but the project has made promising initial progress in this direction.

- The team proposed a novel electrochemical cell structure with the incorporation of a porous layer, which allows for direct production of formic acid with high Faradaic efficiency at reasonable current density, albeit at high cell potential; however, this approach requires application of the IrO_2 anode catalyst, which may be an issue due to low iridium availability and competition with PEM water electrolyzers. The high variability of performance with time and the decrease of Faradaic efficiency should be greatly improved. The proposed novel operando diagnostic tool for overpotential breakdown is useful for electrolyzer development. The TEA shows some promise for this electrochemical method to be on par with conventional formic acid cost if all design parameters are achieved. Note that the prospective of using formic acid as a hydrogen carrier is overestimated, and the projected transportation cost is clearly wrong.

- This project is another example of an early-stage effort to explore novel electrolyzer technologies. As such, it is an important part of the consortia's portfolio as long as expectations are tempered around how much risk is baked into the proposal and the TRL of the technology being pursued. It was clear from the presentation that many challenges have been faced along the way but that measurable progress was being made despite those challenges.

PI RESPONSE TO REVIEWER COMMENTS

- Dear reviewers, thank you so much for your constructive comments. Below is a point-by-point response to all comments. We hope that your concerns are fully addressed.

  Comments: Approaching the design of a reactor that considers the energy intensity of electrolyte processing and greatly minimizes it is important to developing a commercial system. Testing has been done in larger electrodes (25 cm^2 and 100 cm^2), which increases the number of challenges; however, the information gained will help guide the R&D to investigate scaled systems. Additional information/questions for further assessment—risk management: more information regarding the amount and rate of formate oxidation in these systems compared to liquid electrolytes, more information regarding any other byproducts formed on the catalyst and their interaction with the solid electrolyte, more information regarding impurity management in the electrolyte and the interactions with the catalyst, more information regarding any temperature change within the catalyst/solid electrolyte; potential impact—further information and analysis regarding the justification of using this approach over liquid electrolytes, further details into the stability of the selectivity and carbon conversion percentage, and further details into the analysis of formate as an H_2 carrier.

  Reply: We appreciate the feedback provided by the reviewer. For clarity, we have separated and answered the concerns in the following list:

  - Formate oxidation has the potential to create significant losses in energetic efficiency. We plan to quantify this effect in future experiments by measuring CO_2 produced on the anode.

  - The only other possible byproducts formed are hydrogen and carbon monoxide. We quantify both products using gas chromatography. A typical working electrolyzer at the beginning of the test using bismuth catalyst will typically have <10% hydrogen Faradaic efficiency and <5% CO Faradaic efficiency. Both products are gaseous and do not cross over an intact polymer membrane; therefore, they cannot affect the solid electrolyte.

  - We have specific elemental characterization capabilities, such as X-ray fluorescence and inductively coupled plasma mass spectroscopy, to assay potential impurities in the product stream. Details regarding operating conditions and the performance stability of the system will become available as tests are completed.

- Temperature change is negligible at the laboratory-scale testing but will become more significant at the larger scales. The temperature increase is related to the overpotential, which can fluctuate during a long-term test. We find that the 100-cm^2 reactor can reach up to 35°C, but we have not yet tested the impacts. Further experimentation is needed. If detrimental, the interlayer deionized water flow can potentially also act as a cooling channel to keep temperatures homogenous.

- Our preliminary TEA shows a clear advantage in our novel design versus using a liquid electrolyte due to downstream separations cost. Further in-depth comparisons will be made in the comprehensive TEA and LCA.

- From our long-term testing at 25 cm^2, the Faradaic efficiency toward formate does decrease with respect to time. Further analysis will be performed to see if the stability of the selectivity can be improved or recovered through different methods. Because our current goal is to achieve high selectivity, we have not experimented with improving conversion. The current carbon conversion is ~2%. Analysis on an economically appropriate conversion will be performed in our comprehensive TEA.

- Thank you for the additional comments and feedback on using formic acid as a hydrogen carrier. This study was an interesting tangent our team analyzed. In relation to the project, note that our main project outcome is coupling formic acid to a bioreactor, not using it as a hydrogen carrier; thus, this project should only be judged based on the current market for formic acid and will be the focus of our comprehensive TEA in Task 8.

Comments: The proposed project focuses on producing formic acid from CO_2 reduction using solid electrolytes. Significant progress has been made in the area of catalyst development and TEA. Excellent publication outcome. The PIs have identified challenges with scaling up the solid-electrolyte layer. Several strategies have been tried and proposed. While impressive progress has been made, it is still unclear how the final milestone (demonstrate formic production with cell size of >750 cm^2) can be achieved. One key challenge with using the solid-electrolyte layer is the high cell resistance. Together with current density, Faradaic efficiency, and stability, it is also important to set the target for cell voltage.

Reply: We thank the reviewer for the comments. The identification of reliable methods to scale up the size of individual reactor components is critical for the success of this project in achieving large cell sizes, and therefore we have developed several different solid-electrolyte layer designs as a risk mitigation strategy. Activities in the upcoming quarters to reproduce the developed interlayer designs with suitable properties at the final cell size area will provide key information for the down-selection and optimization of the solid electrolyte. Further planned activities to refine the solid-electrolyte layer by manipulation of material properties—such as conductivity and porosity by choice of initial resin, binder, or substrates—will inform achievable cell resistances using a porous solid electrolyte.

Comments: The aim of this project is to scale electrolyzers using solid electrolytes for formic acid production to the >750-cm^2 sizes with stable 100-hour performance at >200 mA/cm^2 with 90% current density. This project approach builds from previous demonstrations of selective formic acid production by solid-electrolyte electrolyzers at lab scale. The approach is well structured, with eight specific tasks divided into three phases: initial verification, catalyst and reactor scaling, and performance and durability testing at scale. The project team has made substantive progress, although they have run into significant technical challenges in the scale-up of solid-state interlayers and catalyst scale-up. The catalyst challenge has been overcome due to changes in synthesis routes, but challenges with scaling the solid-electrolyte interlayers have required a complete redesign of the interlayer structure. Still, the project team has managed to produce 100–250-cm^2 reactors with 15-hour stability for formate production at >90% initial Faradaic efficiency. Overall, the project has made good progress, especially given the low TRL level of the novel solid-electrolyte CO_2 electrolyzers compared to other electrolyzer technologies. If successful, this technology would have enormous impact. The solid-electrolyte CO_2 electrolyzers produce formic acid directly, which eliminates the need for downstream acidification and salt removal needed by the more conventional CO_2 electrolyzers that produce formate. It remains to be seen whether this technology can scale to the 750-cm^2 electrolyzer size with the necessary 100-hour performance stability, but the project has made promising initial progress in this direction.

Reply: We thank the reviewer for your kind comments. Scaling up the porous solid-electrolyte layer is a new challenge being addressed by ongoing and proposed activities for this project. If successful, these activities will provide transferable knowledge regarding the design of materials for other electrochemical reactors and devices, such as electrodialysis cells, that use porous solid-electrolyte materials. To ensure the greatest chance of success, we have identified and explored multiple working solutions for preparing solid-electrolyte material that will be screened at the final electrolyzer size for the final deliverable.

Comments: The team proposed a novel electrochemical cell structure with the incorporation of a porous layer, which allows for direct production of formic acid with high Faradaic efficiency at reasonable current density, albeit at high cell potential; however, this approach requires application of the IrO_2 anode catalyst, which may be an issue due to low iridium availability and competition with PEM water electrolyzers. The high variability of performance with time and the decrease of Faradaic efficiency should be greatly improved. The proposed novel operando diagnostic tool for overpotential breakdown is useful for electrolyzer development. The TEA shows some promise for this electrochemical method to be on par with conventional formic acid cost if all design parameters are achieved. Note that the prospective of using formic acid as a hydrogen carrier is overestimated, and the projected transportation cost is clearly wrong.

Reply: We thank the reviewer for the comment. Note that comparing hydrogen carriers was an interesting tangent that our team explored and is not related to the outcome of this project. Our goal is to directly couple a bioreactor with a CO_2 electrolyzer for formic acid production. The comprehensive TEA in Task 8 will focus on analyzing a bioreactor coupled with a CO_2 electrolyzer for the current formic acid market.

Comments: This project is another example of an early-stage effort to explore novel electrolyzer technologies. As such, it is an important part of the consortia’s portfolio as long as expectations are tempered around how much risk is baked into the proposal and the TRL of the technology being pursued. It was clear from the presentation that many challenges have been faced along the way but that measurable progress was being made despite those challenges.

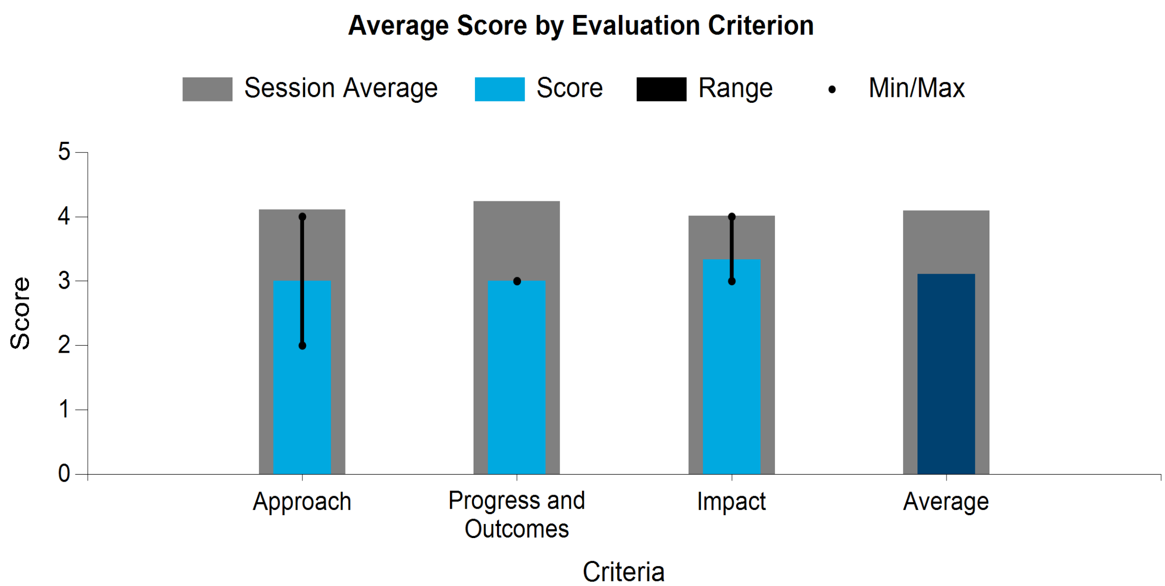
Reply: We thank the reviewer for acknowledging the progress made by the team.

PEM CO_2 ELECTROLYZER SCALE-UP TO ENABLE MEGAWATT-SCALE ELECTROCHEMICAL MODULES

Twelve

WBS:	2.3.1.423
Presenter(s):	Kendra Kuhl; Sadia Kabir
Project Start Date:	10/01/2020
Planned Project End Date:	02/28/2024
Total Funding:	$3,125,000

The objective of this project is to accelerate the development and deployment of our commercial-scale membrane electrode assemblies, which are the core component of our novel carbon dioxide electrolyzers. Specifically, this project seeks to validate the design, fabrication, electrochemical performance, and characterization processes for large-format membrane electrode assemblies. Key challenges include: optimizing across a complex parameter space and coordinating with partners from across the value chain (universities, national labs, vendors, etc.).



COMMENTS

- The project aims to develop electrolyzers for CO_2 conversion to CO. It appears that good progress has been made and some key milestones have been achieved; however, it is difficult to evaluate the overall progress of the project due to the lack of details. The level of collaboration is strong, with contribution from both academic and other industry partners. The final milestone seems attainable. Two key performance metrics in CO_2 conversion to CO are cell voltage and CO_2 crossover; however, they were not discussed in the presentation.

- The presentation mostly focused on the selling points, was overly sanitized, and lacked the experimental data. All reported parameters, including TEA, are vague or relative to an unknown baseline; therefore, although the milestone was met, it was very difficult to evaluate the team's progress toward the project and FOA goals without performance data.

- Threes for progress and impact here because the data were so sanitized that it was difficult to get a sense of how well the project was structured, how much progress they had actually made, and how impactful their results might be. I encourage BETO to push industry partners to agree to being more open about their progress and results in the future. This is a major concern because it is a publicly funded project. I gave this project a two for approach because I feel as though they did not appear to have any interest in collaboration or sharing their results with the group.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments and feedback. We particularly appreciate their recognition of our milestone progress and collaborative approach with academic and national laboratory partners. Collaboration is one of Twelve's core values, and BETO offers a facile platform for working with leading researchers and organizations. The reviewers' feedback largely focused on the availability of data, which made it difficult for them to evaluate the overall project progress. In general, Twelve defaults to not sharing business-sensitive information to avoid enabling competitors or complicating customer negotiations; however, we acknowledge the validity of the reviewers' criticism and the necessity of being transparent with taxpayer-funded work. As such, we have added an additional slide showing additional lifetime data (Slide 22). Further, we have added numbers to our cell performance plots as well as throughout the deck, and we have highlighted the differences between Twelve's performance targets and the targets of the FOA.

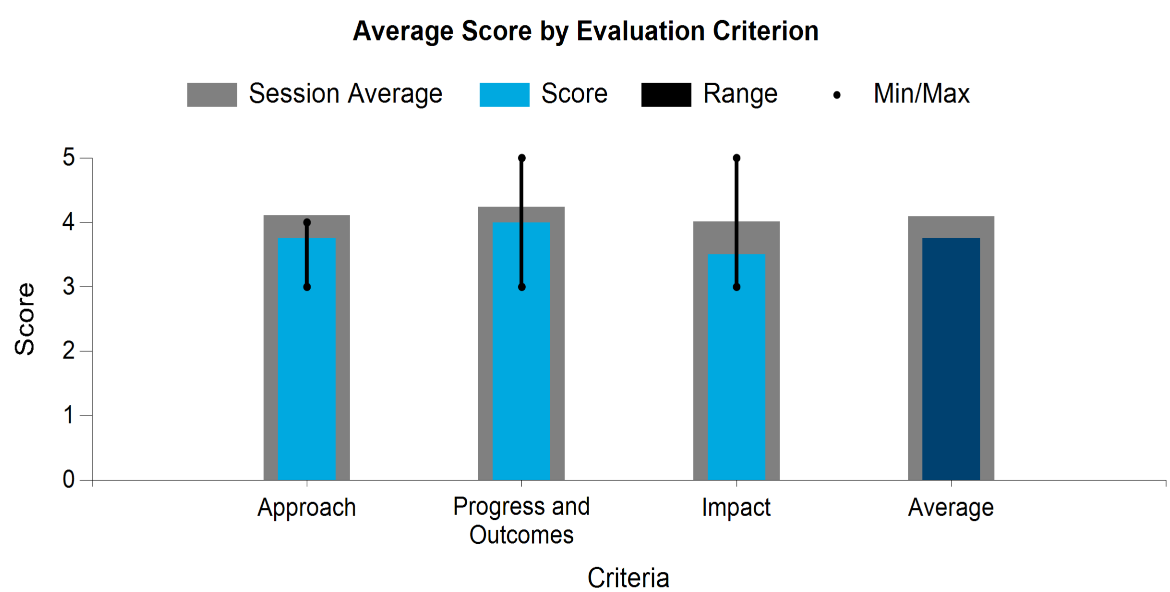
CO_2 VALORIZATION VIA REWIRING CARBON METABOLIC NETWORK

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.2.106
Presenter(s):	Wei Xiong
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$275,000

Energizing the world sustainably requires revolutionizing the way we harness natural resources. New renewable technologies include the microbiological upgrading of CO_2, the primary GHG that causes climate change. This project aims to develop a new bioeconomy by taking up CO_2 and converting it into high-value products using an autotrophic microbe. Specifically, the team constructed an acetogenic bacterium, *Clostridium ljungdahlii*, and developed gas fermentation processes that convert syngas (CO_2/H_2/CO) to the platform compound 3-hydroxybutyrate (3HB). The project has achieved several key successes, including the design and construction of 3HB genes in the gas-fermenting bacterium, the identification of a native 3HB pathway, the conversion of syngas to 3HB through strain engineering, and the improvement of the conversion through rational and iterative strain development. The optimized strain has achieved industry-relevant production rates (0.1 g/L/h) and titers (9.2 g/L), and it has sustained continuous gas fermentation for 3HB production for >50 days in a benchtop gas bioreactor. The project has both industry and scientific implications, including the exploitation of host microbes and processes to improve industrial-scale production of value-added compounds from CO_2 and the promotion of gas fermentation technology. The team is also strengthening R&D synergies with other teams and industry partners in the CO_2 consortium, developing cutting-edge approaches for the rapid and rational engineering of gas-fermenting hosts and dissecting the thermodynamics and kinetics of processes for biological syngas valorization. So far, one patent application and one research article have resulted from this work, and the team anticipates additional significant outcomes from this project.



COMMENTS

- Developing methods to rapidly engineer robust microorganisms to consume relevant intermediates to produce valuable products with high productivity is an important aspect of these integrated systems. This project seems to have a good method to achieve this and further test the system. Additional information, including the LCA and TEA regarding their target product 3HB, would be helpful in evaluating the potential impact of this project.

- The project aims to upgrade syngas to liquid fuels using metabolic engineering approaches. Progress has been made, but the carbon conversion efficiency for ethanol and 3HB seems quite low compared to that of acetate. It would be interesting to develop strains that are capable of converting acetate and ethanol to 3HB.

- This project aims to use strain engineering and adaptive laboratory evolution to modify acetogen anaerobes to convert syngas into 3HB, a useful chemical precursor to plastics and hydrocarbon fuels. As part of the project approach, the project team designed a lab-scale syngas fermenter, one of the few available in the United States that can safely handle syngas mixtures at this scale. This fermenter is a unique capability of the project. The project team has successfully engineered acetogens for 3HB production through genetic engineering that produce decent titers >9 g/L of 3HB and that can operate for up to 50 days of continuous 3HB production. Future work is focused on further engineering the microbes to achieve >12 g/L of 3HB titers. Overall, this project has made appropriate progress in its aims. The choice of acetophens as the host organisms for genetic modification instead of rewiring native strains that already produce 3HB remains an unanswered question for the project. The project has demonstrated good impact in the development of new gas fermentation technology and new strategies for the rapid genetic engineering of acetophen hosts. The project team has one publication and one patent, and it has engaged with key companies regarding integrating fermentation technology.

- This project presents a fairly straightforward approach for upcycling syngas to value-added compounds, specifically 3HB. That said, I have several concerns about the approach and presentation of the results that need to be addressed.

    1. Why were the same strains not tested on fructose and syngas on Slide 10? Each of the modifications made have the potential to affect both pathways to 3HB.

    2. Slide 10: 3-hydroxybutyryl-CoA dehydrogenase from *Clostridium ljungdahlii* and *Clostridium kluyveri* improved 3HB production, not *Clostridium ljungdahlii* alone, as stated.

    3. Slide 12: This is not a continuous run and should not be claimed as such. There were significant changes in the gas regime that resulted in changes in the optical density and therefore could impact production metrics. Also, it seems as though the feed rate was very influential for 3HB production, but this was never discussed. At 0.6 mL/min, 3HB production spikes and then falls off. Interestingly, a feed rate of 1.2 mL/min produced the same spike in optical density but not in 3HB. It would be useful to further explore the 70/20/10 $CO/CO_2/H_2$ gas regime with a 0.6-mL/min feed rate because the data in the first ~350 hours look very promising.

    4. Slide 15: “CRISPRi targeting the pta gene (encoding phosphate acetyltransferase) has increased 3HB titer as well as decreased acetate titer from a competing pathway.” It would have been useful to describe what “T0” and “Mid” are, because it is unclear to the reader. Also, some statistics would be helpful for the interpretation of the titer data. While 3HB might be slightly increased, I’m not sure how significant the decrease in acetate titer is.

    5. Downstream processing: This is a significant concern. The fermentation will yield acetate, EtOH, and 3HB, which are all largely miscible in water, and no explanation was given for how to deal with purifying the 3HB away from the other products.

    6. The project goals were not clearly covered. This should be included for those who are not intimately familiar with them.

7. ALE goals on Slide 13: The criteria are not very specific (“Isolate adapted acetogen strains.”). What are they adapted for? A numeric metric should be added to this goal.
8. The maximum 3HB titer is claimed to be 9.15g/L (Slide 11), but the data are not shown. Also, under what conditions was that titer achieved, and how long was it maintained? This should be included because it is an important data point linked to project milestones.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: Developing methods to rapidly engineer robust microorganisms to consume relevant intermediates to produce valuable products with high productivity is an important aspect of these integrated systems. This project seems to have a good method to achieve this and further test the system. Additional information, including the LCA and TEA regarding their target product 3HB, would be helpful in evaluating the potential impact of this project.

  Reply: We have indeed conducted preliminary TEA back in 2020. This preliminary work was instrumental in setting our industrial benchmarks and initial laboratory research objectives. This project has met the TEA metrics of 0.1 g/L/h for commercial viability. We absolutely concur with the reviewer that updated TEA along with additional LCA would enhance our evaluation process. We are currently in conversation with BETO to shape our next phase of research.

  Comments: The project aims to upgrade syngas to liquid fuels using metabolic engineering approaches. Progress has been made, but the carbon conversion efficiency for ethanol and 3HB seems quite low compared to that of acetate. It would be interesting to develop strains that are capable of converting acetate and ethanol to 3HB.

  Reply: The reviewer rightly pointed out the significance of acetate in the role of acetogenic hosts. Bioenergetics of acetogens indicate that acetate production is integral to adenosine triphosphate (ATP) generation, a critical factor that is particularly important in a syngas fermentation process where the thermodynamic driving force would be constrained. We are actively working on a metabolic engineering approach to reduce acetate production by modifying relevant genes and pathways. We are also interested in a potential strategy involving a helper microbe that can recycle acetate and redirect the carbon flux toward our target compounds. Our preliminary findings are promising, and we are optimistic about the potential benefits these strategies could bring to the syngas fermentation process.

  Comments: This project aims to use strain engineering and adaptive laboratory evolution to modify acetogen anaerobes to convert syngas into 3HB, a useful chemical precursor to plastics and hydrocarbon fuels. As part of the project approach, the project team designed a lab-scale syngas fermenter, one of the few available in the United States that can safely handle syngas mixtures at this scale. This fermenter is a unique capability of the project. The project team has successfully engineered acetogens for 3HB production through genetic engineering that produce decent titers >9 g/L of 3HB and that can operate for up to 50 days of continuous 3HB production. Future work is focused on further engineering the microbes to achieve >12 g/L of 3HB titers. Overall, this project has made appropriate progress in its aims. The choice of acetophens as the host organisms for genetic modification instead of rewiring native strains that already produce 3HB remains an unanswered question for the project. The project has demonstrated good impact in the development of new gas fermentation technology and new strategies for the rapid genetic engineering of acetophen hosts. The project team has one publication and one patent, and it has engaged with key companies regarding integrating fermentation technology.

  Reply: Thanks! Regarding the use of native strains for the production of 3HB, these strains, to our knowledge, typically generate the polymer form (polyhydroxybutyrate [PHB]), not the monomer. Extracting PHB requires breaking (kill) the cells and extracting the polymer from the cells, which we understand to be an inefficient process; hence, our focus is on producing the monomer, which can be excreted from the microbial hosts, thus facilitating downstream processing.

Comments: This project presents a fairly straightforward approach for upcycling syngas to value-added compounds, specifically 3HB. That said, I have several concerns about the approach and presentation of the results that need to be addressed.

1. Why were the same strains not tested on fructose and syngas on Slide 10? Each of the modifications made have the potential to affect both pathways to 3HB.

2. Slide 10: 3-hydroxybutyryl-CoA dehydrogenase from *Clostridium ljungdahlii* and *Clostridium kluyveri* improved 3HB production, not *Clostridium ljungdahlii* alone, as is stated.

3. Slide 12: This is not a continuous run and should not be claimed as such. There were significant changes in the gas regime that resulted in changes in the optical density and therefore could impact production metrics. Also, it seems as though the feed rate was very influential for 3HB production, but this was never discussed. At 0.6m L/min, 3HB production spikes and then falls off. Interestingly, a feed rate of 1.2 mL/min produced the same spike in optical density but not in 3HB. It would be useful to further explore the 70/20/10 CO/CO2/H_2 gas regime with a 0.6-mL/min feed rate because the data in the first ~350 hours look very promising.

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5. Downstream processing: This is a significant concern. The fermentation will yield acetate, EtOH, and 3HB, which are all largely miscible in water, and no explanation was given for how to deal with purifying the 3HB away from the other products.

6. The project goals were not clearly covered. This should be included for those who are not intimately familiar with them.

7. ALE goals on Slide 13: The criteria are not very specific ("Isolate adapted acetogen strains."). What are they adapted for? A numeric metric should be added to this goal.

8. The maximum 3HB titer is claimed to be 9.15g/L (Slide 11), but the data are not shown. Also, under what conditions was that titer achieved, and how long was it maintained? This should be included because it is an important data point linked to project milestones.

Reply: I appreciate the detailed feedback and constructive suggestions. Allow me to address them in order:

1. All our strains were indeed tested on fructose as a primary step. The best-performing strains under fructose conditions were subsequently tested on syngas. More details can be found in our publication (https://doi.org/10.3389/fmicb.2022.948369).

2. Yes, we concur that 3-hydroxybutyryl-CoA dehydrogenase plays a pivotal role, regardless of its origin.

3. The experiment was conducted under continuous-feed conditions. The objective was to assess the impact of different gas ratios on 3HB production. We are open to exploring other conditions to further optimize 3HB production.

4. In our experiment, “T0” represents the point when the inducer of Cas9, anhydrous tetracycline (aTc), was initially added, and “Mid” represents when aTc was added during growth.

5. We agree that downstream processing is a critical factor, and we aim to focus more on this aspect as we advance toward achieving viable titers.

6. The project’s main goal, as stated in Slide 2, is to “develop a carbon-negative biorefinery with gas-fermenting bacteria.” Our current focus is on developing an engineered *C. ljungdahlii* for 3HB production as a model system.

7. Our aim is to improve H_2 utilization in gas fermentation. Because H_2 is a cleaner electron source than carbon monoxide, which has to produce CO_2 as a byproduct when providing electrons, we are striving to enhance hydrogen usage in our fermentation process.

8. On Slide 11, we provided the maximum 3HB titer in millimolar (mM), which equates to 9.15 g/L. We apologize for any confusion caused by not presenting this directly in grams per liter. The conditions under which this titer was achieved involved a gas mix of 70% CO, 20% CO_2, and 10% H_2, at pH 5.2, grown in YT media. We thank you for pointing out this crucial data point’s relevance, and we will be sure to include such details for a more precise understanding in the future. All thoughtful feedback and suggestions are invaluable to us and will certainly guide us in our ongoing research endeavors. We will strive to address all these points and improve our project for better outcomes. We look forward to further discussions and insights from reviewers.

INTEGRATION OF CO_2 ELECTROLYSIS WITH MICROBIAL SYNGAS UPGRADING TO REWIRE THE CARBON ECONOMY—NREL

National Renewable Energy Laboratory

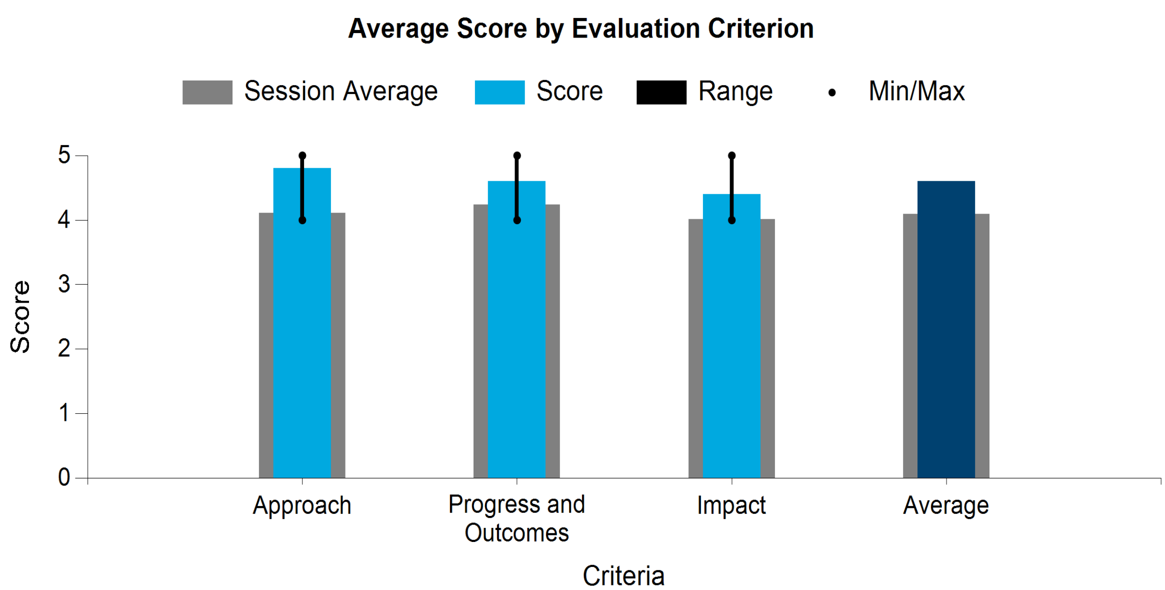
PROJECT DESCRIPTION

WBS:	2.3.2.116
Presenter(s):	Michael Resch
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$1,750,000

The production of valuable products from flue gas-derived CO_2 could incentivize conventional carbon capture technologies, leading to a more economically favorable and sustainable process. This project is a member of the CO_2RUe, focusing on integrating electrochemistry with gas fermentation, with ongoing unique modeling efforts. The production of valuable products from flue gas-derived CO_2 will reduce the net cost of conventional carbon capture technologies, leading to a more economically favorable and sustainable process, and it can increase the carbon conversion efficiencies of biorefineries.

We are actively working with our industry cost-share partners LanzaTech and Dioxide Materials to identify integration hurdles for the scale-up of the conversion of biorefinery flue gas mixtures. At scale, we envision that this type of system would be collocated at an industrial source for the direct conversion of concentrated or dilute sources of CO_2.

Presently, we are focusing on understanding the effects of sulfur on CO_2 electrolyzers' ability to reduce CO_2 into CO, to improve the carbon conversion efficiency of gas-fermenting microbes, and to develop transformation tools for *Clostridium autoethanogenum*. We are also analyzing renewable electricity requirements and cost implications in utilizing biorefinery CO_2 waste streams at scales of up to 14 T/h.



COMMENTS

- The approach is well thought out, and pulling together the expertise of industry players to tackle key aspects of these bio-integrated systems is advantageous. Their approach of utilizing the larger CO_2 electrolyzers from Dioxide Materials and the knowledge from LanzaTech has the potential of filling knowledge gaps, which some of the more detailed studies do not fill at this time. In addition, testing and optimizing the CO_2 electrolysis process with the contaminants from flue gas is an important challenge to tackle. Additional information/questions for further assessment:

Risk management:

- Additional information or tests regarding using the recycle loop with flue gas
- Additional information on potential methods to mitigate the contaminants on the catalyst or catalyst regeneration methods.

Potential impact:

- Additional information regarding the comparison of CO_2 to liquid intermediates versus CO_2 to gaseous intermediates
- Additional information on the TEA and cost drivers of these systems and the numbers they need to reach to make it cost-competitive
- Additional information on the baseline TEA calculations and how sustainable and saleable are the SOA numbers from Dioxide Materials
- Additional information regarding the TEA of storing the produced CO or using batteries to store electricity.

- The project focuses on combining CO_2 conversion to CO and microbial syngas upgrading. Overall, great progress on the stability of the CO_2 conversion system in the presence of H_2S. The integration of CO_2 conversion and the CSTR bioreactor has been demonstrated. One milestone of the project is to reduce CO_2 crossover, but this has not been discussed/demonstrated. It seems that the path toward this goal is also unclear. The LCA shows the significant effect of the single-pass conversion. It would be important to study the effect of the single-pass conversion on the durability of the CO_2 conversion system. While the CO_2 conversion system is not affected by low H_2S concentration, it would be impactful if strategies for addressing high H_2S concentration were discussed/studied.

- This project uses a multifaceted approach to explore the durability and carbon conversion efficiency of both electrochemical and biocatalytic CO_2 upgrading technologies using realistic feedstocks. The research directions are focused on closing technology gaps that address key cost drivers identified by the analysis teams of the CO_2RUe. The close collaboration between this project and the analysis teams at the CO_2RUe is a significant strength of the project. To date, much of the progress has focused on testing the effect of the flue gas contaminant H_2S on electrolyzer performance and adapting *C. autoethanogenum* to produce acetate from low- and high-CO gas outputs from electrolyzers. The project team has demonstrated 3,000 hours of operation of a 250-cm^2 CO_2 electrolyzer at 100 mA cm^2 with H_2S-contaminated CO_2 feedstocks, although they identified Ag and S accumulation in the membrane after operation. This is an important finding for eventual integration of electrolyzers using S-contaminated CO_2 streams from biorefineries, because such electrolyzers may need sulfur purging built in to prevent catalyst degradation and accumulation, especially if recycling is used to increase the carbon conversion efficiency. The project team has successfully integrated an electrolyzer with a gas fermenter for 120-hour operation. Overall, this project is an important part of the CO_2RUe, with significant impact in guiding future research directions by identifying integration challenges related to key cost drivers for CO_2 utilization technologies.

- The project has a clear technical path forward and has demonstrated progress toward the project goals. The integration of a 250-cm^2 CO_2 electrolyzer with the CSTR was demonstrated. Preliminary data on H_2S tolerance are encouraging but only for low current densities. Reasonable coordination between partners can be seen. Milestones have been met; however, one of the stated goals is the reduction of CO_2 membrane crossover by 20%, but no work has been started yet. The idea of using CO_2 feedstock from ethanol refineries is good but is not analyzed in depth. For example, requirements as to the source of renewable electricity (wind)—such as placement, capital investment, availability, and the business model—are not developed. The performed TEA points to the CO_2 single-pass conversion as a major cost factor. In other processes, its importance is very low, because the addition of an inexpensive CO_2 separation and recycling loop eliminates this issue.

- It's very exciting to see a project integrating electrolyzer technology with a proven, industrial microbe to produce SAF precursors. The approach here is solid, and the team has made good progress toward their goals. In regard to the mevalonate pathway introduction, the product is a good choice, provides a great deal of flexibility for further refinement, and has been proven out by industry (albeit in yeast). Generating some detectable level of mevalonate should be straightforward, but going beyond that might prove difficult as the team tries to shift flux away from acetate. Some flux balance modeling specifically looking at redox equivalents and energy consumption might help mitigate risks.

PI RESPONSE TO REVIEWER COMMENTS

- Risk management:

  - Additional information or tests regarding using the recycle loop with flue gas. We have examined recycling the CO_2 from the electrolyzer and fermenter to optimize carbon conversion efficiency. There are benefits to the overall system carbon conversion efficiency and considerations for removing contaminants such as sulfur compounds from the fermenter and oxygen from the electrolyzer. The process engineering of designing a recycle loop is of interest but outside the scope of our current project.

  - Additional information on potential methods to mitigate the contaminants on the catalyst or catalyst regeneration methods. The current results showed that H_2S induced the carbon corrosion in the anode. We proposed to use titanium-based substrate to replace carbon fiber paper used in the anode and to refresh anolyte every 200 hours. If these two strategies do not mitigate the effects of sulfur on the electrolyzer, we will know the maximum sulfur amounts allowable to the system and use a SulfaTrap to remove sulfur and other contaminants before introduction to the cell.

  Potential impact:

  - Additional information regarding the comparison of CO_2 to liquid intermediates versus CO_2 to gaseous intermediates. Work focusing on key trade-offs between liquid and gaseous intermediates has informed the project scope (https://doi.org/10.1039/C9EE02410G). We build on this work by focusing on CO_2 converted to gaseous CO via low-temperature electrolysis because it represents one of the more near-term pathways for electrochemical CO_2 conversion. We acknowledge that this is an extremely active research space, with the SOA subject to change in the future as the performance and cost of these electrolyzers progresses. We intend to continue TEA to inform and guide these research efforts.

  - Additional information into the TEA and cost drivers of these systems and the numbers they need to reach to make it cost-competitive. The identification and analysis of key process-level parameters is the subject of ongoing work in the TEA tasks in this project. We intend to publish an exhaustive report outlining these considerations prior to the end of this project. Initial results indicate that the levelized cost of carbon monoxide produced via low-temperature CO_2 electrolysis is primarily driven by the cost of supplying low-carbon electricity to the electrolyzer. As such, TEA activities have focused on relationships between the variable supply of low-carbon electricity and possible gas or energy storage to act as a buffer to manage temporal variability.

- Additional information on the baseline TEA calculations and how sustainable and saleable are the SOA numbers from Dioxide Materials. There are ongoing CO_2RUe analysis projects looking into the economics and life cycle of liquid versus gaseous intermediates.

- Additional information regarding the TEA of storing the produced CO or using batteries to store electricity. This is a topic of interest to us, and we hope to have a report or paper to compare these process parameters to take advantage of low-cost, low-carbon electricity and CO_2 feedstocks. In the case of either storing electrolysis feedstocks and products versus storing energy to supply the electrolyzer, the added capital cost of storage systems must be contrasted with the cost savings from supporting the variable operation of the electrolyzer. In other words, the cost of purchasing and operating a battery energy storage system must be less than the cost savings from the ability to selectively purchase surplus grid electricity. Ongoing TEA tasks are focusing on addressing these questions, and we intend to publish a document addressing the results of these analyses in the near term. The reduction of CO_2 crossover was scheduled to start on October 1, 2023, and meet the milestone by December 31, 2024. We propose to recapture CO_2 from anode exhaust. First, we will determine the acceptable oxygen level in the CO_2 stream, and then we will design a membrane separation system to separate CO_2 from the CO_2/O_2 mixture. We agree with the reviewer. We have demonstrated thousands of hours of stability of CO_2 electrolyzer with single pass at a stoichiometry of 3–4. We have investigated the effect of concentration of H_2S up to 25 ppm. The CO_2 electrolyzer was able to run over 1,000 hours at 25 ppm of H_2S. It seems that H_2S in CO_2 induced the corrosion of carbon substrate used in the anode, leading to the loss of IrO_2 and the increase in the cell voltage. We propose to use titanium-based substrate to replace carbon fiber paper or refresh anolyte every 200 hours or so. The detailed degradation mechanism is under investigation. We also proposed to use SulfaTrap to remove sulfur before the cell if these strategies do not work. We agree with the reviewer that questions regarding business models and risk management considerations for such conversion pathways are not proven at scale yet. We hope that ongoing TEA work within this project will help inform and support the community, identifying key R&D pathways as well as economic drivers to support de-risking and proving these technologies at scale.

The performed TEA points to the CO_2 single-pass conversion as a major cost factor. In other processes, its importance is very low, because the addition of an inexpensive CO_2 separation and recycling loop eliminates this issue. Initial results indicate that the levelized cost of carbon monoxide produced via low-temperature CO_2 electrolysis is primarily driven by the cost of supplying electricity to the electrolyzer. As such, TEA activities have focused on relationships between the variable supply of electricity and possible feedstock or energy storage to act as a buffer to manage temporal variability. These findings do vary from one case to another, depending on project location and process design. This is a very good point, and we will monitor the flux balance and redox requirements necessary to maintain energy for cellular metabolism and maximize product formation.

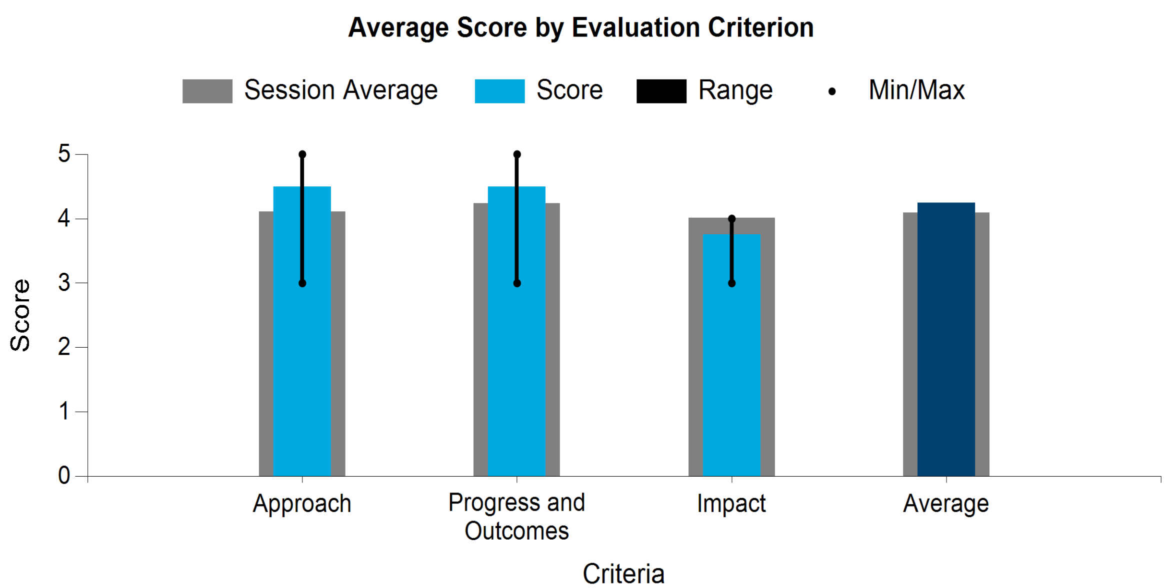
BIOCONVERSION OF SYNGAS FROM ELECTROCHEMICAL CO_2 REDUCTION TO SUSTAINABLE AVIATION FUELS—LBNL

Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	2.3.2.118
Presenter(s):	Eric Sundstrom
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$1,000,000

The economic conversion of CO_2 and renewable electricity to fuels and chemicals is a critical technological component of deep decarbonization. This project couples electrochemical syngas generation with aerobic carbon monoxide bioconversion to generate SAF directly from CO_2. Electrolyzer technology development focuses on efficient single-stage generation of tunable $CO:H_2$ blends from influent CO_2 and water, with an emphasis on computational modeling to drive quantitative improvements in the efficiency, longevity, and scalability of the electrolyzer assembly. Bioconversion technology development relies on metabolic engineering of the aerobic carboxydotroph *Hydrogenophaga pseudoflava* for heterologous expression of the isoprenoids epi-isozizaene and isoprenol, both promising intermediates for high-energy-density SAF. Experimental results to date have validated the tunability of syngas composition, and they have demonstrated high Faradaic efficiency over operating times exceeding 10 hours. In addition, we have developed inducible promoter and DNA methylation systems for *H. pseudoflava*, and we have commissioned a gas fermentation bioreactor system for high-density cultivation at dry cell weights exceeding 8 g/L. If successful, this project will develop an efficient and flexible platform for the direct synthesis of highly reduced and long-chain molecules from CO_2, overcoming a significant drawback associated with incumbent anaerobic syngas conversion technologies. The project team is well positioned to disseminate these learnings via inter-consortium collaboration, via collaborations with other BETO programs, and via new and existing connections to a variety of industry partners.



COMMENTS

- I believe their approach of combining modeling, system design, and experimental tests to guide research to enable scale-up is very valuable. Their specially designed electrochemical cells enable a high level of control of the conditions in the reactor, which increases our understanding of the ECO_2R process. Their use of modeling can further increase our understanding of these systems, help design optimal reactors, discover optimal conditions, and increase the chances of successful scaling of the technology. The approach of focusing on using microorganisms that can produce a diverse array of products is advantageous due to increasing the potential flexibility of these integrated systems. Additional information/questions for further assessment:

Risk management:

- Further information regarding the stability of the electrolyzer after longer durations and simulated scaled conditions or stress testing.

Potential impact:

- Additional information regarding the comparison of CO_2 to liquid intermediates versus CO_2 to gaseous intermediates
- Additional information regarding the system; TEA including various components, such as electrolyte and pH management, recycle-loop operations, carbon selectivity, CO_2 flow rate, CO_2 crossover, the effect of the ratio of $CO:H_2$, what is necessary to achieve to make this a cost-competitive technology, and how they plan to achieve their necessary targets
- Additional information regarding the higher-density fuels and how they will be used as SAF
- Additional information regarding how this method compares to other methods to make SAF.

- The project focuses on developing an electrolyzer for CO_2 conversion to syngas with a tunable $CO:H_2$ ratio. The syngas is then upgraded via biological process. Although progress has been made in electrochemical CO_2 conversion to CO, its performance is much lower compared to other projects focusing on electrolyzer development. It is unclear why the $CO:H_2$ ratio should be controlled with the CO_2 electrolyzer. It would be easier (and more economic) to achieve the goal by simply combining CO_2 and water electrolyzers. Stable operation of around 10 hours has been demonstrated, but it is unclear what would make the system unstable and how the target of 100 hours can be achieved.
- The team selected aerobic bioconversion of syngas to cyclic hydrocarbons with high energy density, which could be important for the implementation of this pathway for the production of mixed SAFs. The application of an adaptive oxygen supply allowed for optimizing isoprenoid formation. The team demonstrated that increasing the back pressure may be an effective tool for the reduction of the cell voltage and changing $H_2:CO$ ratio. The one-dimensional model showed good correlation with experimental data, but a model for the membrane crossovers was not as accurate. The electrochemical longevity tests (tens of hours) are clearly not sufficient. It is unclear if the benefits of the proposed pulsed-current approach outweigh the increased complexity. Unfortunately, TEA was not discussed, and the projected costs of cyclic SAFs (below Jet A) and fuel savings look unlikely.
- This is a very interesting and unique project in the CO_2 utilization portfolio. *H. pseudoflava* is an interesting organism that should provide a robust platform to build off of. I have given the impact section a score of three because I found little discussion or consideration of a few important risks with the proposed approach.

    1. One issue with producing more complex products is cellular toxicity. The project has a goal of bioreactor isoprenoid titers >1g/L over 24 hours, but it is unclear which isoprenoid compound(s) are being pursued. This is important because many isoprenoids are very toxic to microbial hosts, and achieving titers of 1g/L might be very challenging. I suggest the authors look at the toxicity of different isoprenoids to *H. pseudoflava*.

2. Related to the first point, defining a product (or a few products) now will save a great deal of time later.

3. There was no mention of what would be done with the excess CO_2 that will (assumedly) be produced in this aerobic fermentation. Most organisms produce vast quantities of CO_2 under aerobic growth conditions, and that risk should be incorporated into the vision for this project. You could likely recycle that gas stream into the electrolyzer.

4. I suggest switching everything from plasmids to chromosomal integrations as soon as possible. Several critical variables related to flux and performance will likely be significantly different, and working with plasmids is inherently prone to genetic escapees and is unscalable.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for their thoughtful comments and guidance. We share their enthusiasm for this product and the impact it can provide as a unique synthesis of electrochemical syngas generation and aerobic syngas conversion. We look forward to presenting our continued progress at the next BETO Project Peer Review. The two target molecules for our biological production system (isoprenol and epi-isozizaene) were chosen based on previous experience engineering expression in heterotrophic hosts and on commercialization interest from biofuel producers, industry end users, and the U.S. Navy. The production of these molecules is already characterized in heterotrophic host organisms, mitigating risk associated with pathway expression. Chemical and fuel properties are also well characterized, mitigating downstream risks, including purification, catalytic upgrading, and the suitability of the resulting fuels as SAF blendstocks. In-depth TEA of the integrated system is scheduled for FY 2024 within the CO_2RUe analysis and modeling working group. Key considerations for TEA and LCA include: (1) comparison of integrated versus separated CO_2 and water electrolysis and (2) comparison of direct aerobic synthesis of high-energy-density molecules with a higher-TRL alternative: anaerobic syngas fermentation coupled to catalytic upgrading. This work is planned for FY 2024 and will be heavily informed by our research results, projections of optimal system performance, and outcomes of related analysis efforts within the consortium.

  A dual system featuring both CO_2 and water electrolyzers would certainly exhibit preferable economics at the current SOT development; however, we believe that with further development, a single electrolyzer producing the desired ratios of syngas directly from CO_2 and H_2O could significantly simplify the system design, enabling the reductions in manufacturing cost and reductions in infrastructure required to support the process. While water electrolyzers are currently a much more mature technology with superior operating expenditures (OpEx) and energy efficiency, there are no thermodynamic barriers suggesting that a single electrolyzer could not reach the same energy efficiencies with equivalent investment in technology development. We note that the CO_2RUe is taking a portfolio approach by exploring both combined and integrated approaches for electrochemical syngas generation, and we emphasize that the single electrolyzer approach is a lower-TRL (2–3) R&D project that is less demonstration oriented. Within this portfolio approach, our research efforts will be heavily influenced by the CO_2RUe analysis and modeling working group, as they quantitatively compare the economics and emissions impacts of both system designs.

  We fully agree with the observation that 10 hours of electrolyzer operation is insufficient. Unfortunately, due to the timing and brief format of the presentation, we were unable to incorporate our most recent electrolyzer stability results into the official slides. With automated salt dosing and pulsed-current protocols, we have now been able to achieve >130 hours of stable operation, with voltage decay indicating potential for significantly longer operation barring a sudden failure, such as a membrane rupture. Given the lower TRL (2–3) of this project, we are currently focused on optimization at +100 hours of operation to provide stress-testing feedback to our component R&D efforts. The development of accelerated stress-testing protocols for CO_2 electrolysis and evaluation of system performance over longer timescales (+1,000 hours) would be compelling topics for follow-on research efforts at a higher TRL. Because our pulsed-current approach has relatively long time constants—on the order of tens of minutes to hours—we do not see any barriers to implementing a pulsed-current approach in an industrial setting. In fact, our industry partners are leveraging similar pulsed-current protocols to achieve thousands of hours of stability in their CO_2 electrolyzer stacks.

We agree that there is room to improve the agreement between the experimental and simulated CO_2 crossover measurements. We will continue incorporating relevant physics into the model by gathering additional polarization data to reduce parameter uncertainty and by modifying the model equations to correctly account for salting-out effects and the electroosmotic drag of water. Experiments will also be performed to track the pH of the electrolyte over time and validate boundary conditions used in the model. Note that there is little precedent for modeling CO_2 crossover in the literature, particularly at high current densities. The validated experimental model we are developing is therefore an important contribution to the overall development of CO_2 electrolyzers.

When comparing our electrochemical system performance to other efforts, we note that our single-cell performance indicators are comparable to those of similar geometric surface area units from Dioxide Materials, a CO_2RUe member. Because our project is at a lower TRL (2–3), we are still conducting R&D on components such as the catalyst layer and flow fields to further advance these metrics, particularly for tunable syngas production at low cell potentials. Product toxicity for our chosen molecules (isoprenol and epi-isozizaene) is absolutely a critical factor for project success. Our data indicate isoprenol tolerance above 5 g/L without prior adaptation, well above the 1-g/L productivity target and aligns with alternative hosts previously engineered for isoprenol. While epi-isozizaene standards are not available for toxicity evaluation, we plan to use an extractive fermentation approach for this hydrophobic molecule to mitigate toxicity at higher titers, aligning with current industry standards for large-scale sesquiterpene production. Single-pass consumption of CO_2 is a key factor in our process design; under optimal gas transfer conditions, we anticipate higher CO_2 emissions at high $CO:H_2$ ratios, with minimal CO_2 emitted at stoichiometric $CO:H_2$ ratios. The interplay between electrochemical $CO:H_2$ ratios, single-pass gas uptake in the bioreactor, and overall process economics will be a key focus of analysis efforts in the coming years. If higher CO concentrations are superior economically, excess CO_2 could indeed be purified and routed back to the electrolyzer. Concerning the use of plasmids versus chromosomal integration for genetic engineering of *H. pseudoflava*, we appreciate this comment, and we agree completely. Genetic tools for *H. pseudoflava* are currently rudimentary, and Oak Ridge National Laboratory is therefore developing a suite of easy-to-use tools for chromosomal engineering. While the plasmid-based system is providing critical early data, we anticipate transitioning to chromosomal-based engineering later this year.

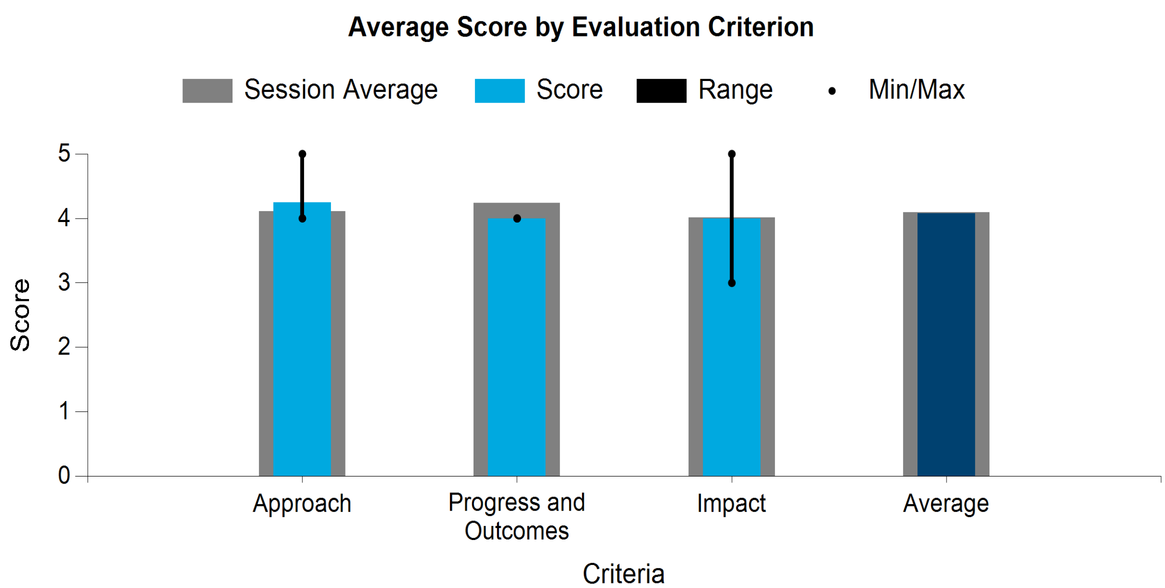
BIOLOGICAL CONVERSION OF FORMIC ACID FOR CO_2-TO-FUELS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.2.121
Presenter(s):	Christopher Johnson; Violeta Sanchez i Nogue
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$1,100,000

Increasing demand for energy and natural resources is causing a rise in the atmospheric concentration of GHG, including CO_2. The conversion of CO_2 to value-added products represents a key opportunity for the development of disruptive technologies to reduce GHG emissions and generate economic revenue. Formate/formic acid can be generated by electrocatalytic reduction of CO_2 and has been proposed as a soluble intermediate for the storage of carbon and energy. Biological systems capable of assimilating formic acid could enable the conversion of formic acid generated from low-cost renewable energy and waste CO_2 to myriad fuels and chemicals. To that end, the goal of this project is to develop the natural formatotroph *Cupriavidus necator* as a robust microbial chassis for the efficient conversion of formic acid to value-added products, in this case fatty acids, which can be readily converted to fuels using established methods. By introducing an acyl-CoA thioesterase to produce free fatty acids and attenuating the organism's ability to degrade them, we are engineering *C. necator* strains that produce fatty acids from formic acid in a pH-stat method of cultivation being concurrently developed. Toward an integrated process, we have also demonstrated the ability of this organism to convert a raw formic acid generated by electrocatalytic reduction of CO_2.



COMMENTS

- Engineering microorganisms to convert formic acid to fatty acids is important to the CO_2 utilization and SAF landscape. The approach of integrating these systems as they are being developed improves risk mitigation. I also appreciate the approach of both microbial engineering as well as developing scalable methods for the bioprocessing inoculation, feeding rate, and aeration. Further stress tests simulating real-world electrolyzer conditions and using the raw formic acid solution from these experiments could help determine if there are additional purification steps between feeding the raw formic acid to the bioreactor. Additional information/questions for further assessment:

Risk management:

- Additional information regarding the production of fatty acids; limits to the concentration of fatty acids in the system and separation costs and carbon intensity (of the fatty acid from the culture)
- Additional information regarding impurities in the electrolyte and the potential effect on microorganisms in real-word testing scenarios
- Additional analysis of how the concentration of the raw formic acid in the electrolyte will affect the system.

Potential impact:

- Analysis and comparison of integration projects using formic acid as an intermediate versus gaseous intermediates
- Additional information regarding how this method compares with other methods for producing SAF, such as reverse water-gas shift with Fischer-Tropsch and direct CO_2 to hydrocarbons
- Additional information and analysis regarding the type of SAF and blending requirements
- Additional information regarding the product production rate they need to reach to be cost-competitive with other methods
- More information about the bioreactor and culture, durability of the microorganisms, and sensitivity of the microbes to changes in the environment
- Additional information regarding carbon conversion to biomass versus product
- Additional information regarding the recycle loop, amount of CO_2 generated, and effect on recycling on the system and energy intensity.

- The project focuses on upgrading formic to fuels. CO_2-derived formic was used to demonstrate the potential of an integrated system. Good progress on biological growth on formic has been demonstrated. Does formic acid need to be concentrated for the integration? It seems that the concentration of formic in the bioreactor is not that high. It is unclear how the fatty acid can be effectively converted to SAF. Perhaps it is not a problem from a technical point of view, but TEA is needed to evaluate the economic aspect of the process.
- This project focuses on the bioconversion of formic acid to fatty acids that could then be converted to SAF via other downstream processes. *C. necator* was chosen as the microbial host organism due to its metabolic versatility, high cell density, and proven affinity for the production of polyhydroxyalkanoates (PHA). The main project approach focuses on using known genome modification methods to engineer *C. necator* to enhance free fatty acid formation and delete competing pathways for undesired products and on evolving *C. necator* to improve assimilation and the conversion of formic acid. To date, the project has met all performance milestones, and it has collaborated with WBS 2.3.2.121 to feed CO_2-derived formic acid from electrolysis directly to their bioreactor, leading to formic acid upgrading to 2-hydroxymucoante semialdehyde. The significant progress to date and close collaboration with other projects within the CO_2RUe are strengths of the project that highlight the impact of the project within the consortium; however, one significant limitation is the low relative yield of fatty acids from formic acid (~1.3%) compared to the maximum theoretical yield of ~20%. Also, the coproduction of biomass in the

bioreactors may lead to downstream separation challenges, depending on where the fatty acids accumulate. The initial results and the potential scalability of the process due to the high cell density of *C. necator* make this a promising direction with significant potential impact.

- This project is a great example of using an industrially relevant production strain with great potential for pushing a lot of flux toward value-added compounds. A couple of comments/risks worth mentioning:
    - The CoA synthetases are obviously a big concern. As discussed at the 2023 Project Peer Review, it could be just one, it could be two, or it could be any combination of 49 of the 50 that are required to knock out beta oxidation. Anything that can be done to expedite that workflow would be worthwhile to pursue immediately. Also, if the solution is indeed a combination of a few or more of these genes, it will be nearly impossible to determine the correct combination required within the timeline of this grant. It might also be worthwhile to do some sequence-based flux analysis or obtain omics data from the literature to determine which copies are functional and maybe even which are influential for flux to beta oxidation.
    - Longer term, CO_2 evolution during this fermentation will be significant and therefore will need to be addressed.

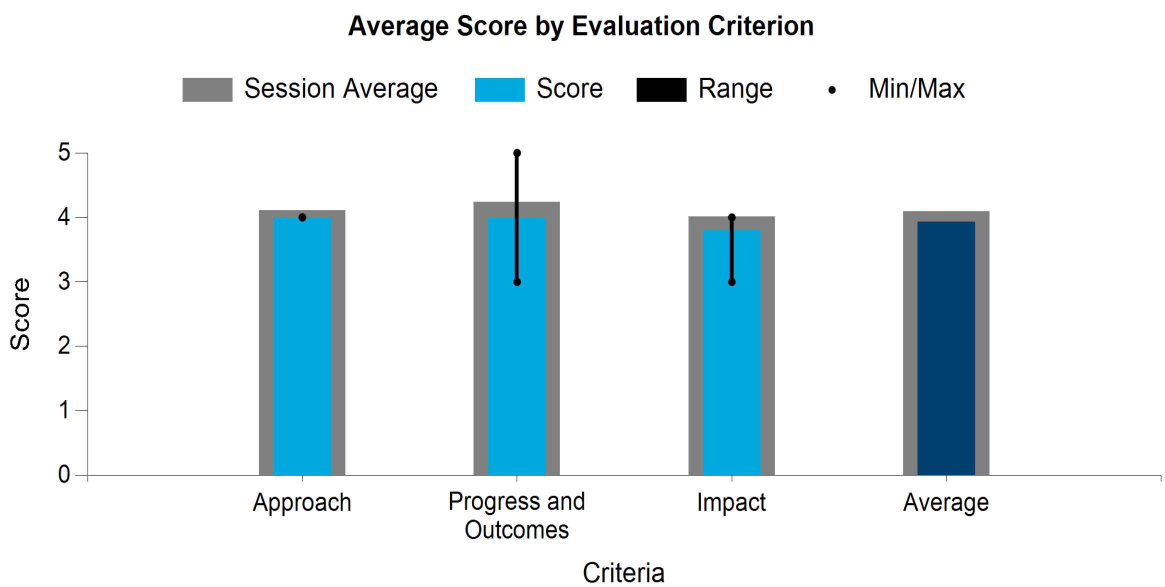
PI RESPONSE TO REVIEWER COMMENTS

- We are grateful to the reviewers for their careful evaluation of this project and thoughtful comments and suggestions. The goal of this project is to develop the soil bacterium *C. necator* as a host for the conversion of CO_2-dervied formic acid using fatty acids as an exemplary product. While it is outside the scope of this project, we recognize that the integration of our project with the upstream process of reducing CO_2 to formic acid, the downstream processing of fatty acids to fuels, and the TEA and LCA of the entire system will be critical to the development of this technology. These aspects are being addressed by other projects within the CO_2RUe (i.e., electrocatalytic reduction of CO_2 to generate formic acid, TEA, and LCA), outside the consortium (i.e., conversion of fatty acids to fuels), or will be incorporated into the project at a later stage (i.e., integration with upstream and downstream processes). With respect to what is within the scope of this project, we agree that a 1.3% carbon yield for the conversion of formic acid to fatty acids is low relative to the maximum theoretical yield of 20.5%, but we expect low yields at this point considering we have not yet deleted enough acyl-CoA synthetase genes to prevent these fatty acids from being degraded and re-assimilated. We presented the hypothesis that we may need to delete as many as 50 acyl-CoA synthetase genes, but it is very possible we may not need to delete all of them to prevent degradation of the C14–C18 fatty acids we are producing. And while we did not have the data at the time of the presentation, we are using omics to help prioritize these knockouts and could use tools being developed in other projects to further refine the list if necessary.

AN EFFICIENT, SCALABLE PROCESS FOR THE ELECTROCHEMICAL REDUCTION OF CO_2 TO FORMATE—NREL

National Renewable Energy Laboratory

WBS:	2.3.4.301
Presenter(s):	K. C. Neyerlin
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$1,400,000



COMMENTS

- The approach of developing a reactor with guidance from the TEA and using off-the-shelf components is mitigating risk and complications with scaling novel reactor materials. In addition, the information gained by investigating effects at a scale of 25-cm^2 and higher current densities also provides necessary information for scaling this technology and can be applied to other systems. Additional information/questions for further assessment:

  Risk management:

  - More information regarding the perforated membrane; durability, effects on the catalyst, and any effects on the integrated system
  - More information regarding key areas of failure in a scaled-up system and methods to mitigate them. For example, R&D plans regarding how they will mitigate the voltage increase over time.

  Potential impact:

  - More information regarding the sensitivity of the amount of formate oxidation and how it affects CapEx

   - More information regarding the specialized anode catalyst, durability, CapEx/OpEx, scalability, etc.
   - Additional information regarding the H_2 generation and how it affects the TEA in various scenarios.

- The project aims to develop a scalable electrolyzer for CO_2 conversion to formate/formic. Membrane development is the main strategy used in the project. A relatively stable system (over 100 hours) for formic production has been demonstrated using perforated membrane and hydrogen oxidation in the anode. One key question is whether hydrogen oxidation in the anode would be economically competitive compared to water oxidation. This is an important question because it governs the selection of anodic catalyst. With the current cell configuration, it would be expected that membrane delamination occurs due to the CO_2 bubble formation between the two layers of the membrane. It is unclear how the target of 500 hours will be achieved. Single-pass conversion of over 30% is a milestone, but strategies to achieve it are not clear.

- This project sets an ambitious goal of scaling CO_2 reduction to formic acid, an important feedstock for downstream bioconversion to SAF. It leverages existing capabilities developed at NREL for the roll-to-roll production of MEA components using automatic film applicators for catalyst loading. The key innovation of the project to date is the development of a perforated membrane MEA configuration, in which formate produced at an alkaline cathode is purposely allowed to migrate through perforation in a bipolar membrane (BPM) to the anode side, where it is pronated to formic acid from protons produced from hydrogen oxidation at the anode. Immediate future work will focus on suppressing formic acid oxidation at the anode by using encased Pt catalysts developed at ANL. This innovation directly addresses the need for product acidification of formate to formic acid for integration with bioconversion systems. From a fundamental science and engineering standpoint, using a perforated membrane is a clever strategy that leads to the production of the desired formic acid product; however, the project has not yet performed the crucial TEA and LCA to determine if the use of H_2 for proton production in the perforated membrane configuration is competitive with other conversion technologies using H_2, such as direct CO_2 hydrogenation or CO_2-to-CO electrolysis followed by CO hydrogenation. Such TEA and LCA are crucial to determine the practical viability of this otherwise interesting approach. Importantly, the project has successfully collaborated with project WBS 2.3.2.121 to feed their CO_2-derived formate directly into a bioconversion reactor for further upgrading, demonstrating the potential impact their approach to formic acid production may have on the process of CO_2 conversion to SAF pending TEA and LCA validation.

- The team showed a certain progress in scaling up electrodes to fit a 25-cm^2 cell. Faradaic efficiency is low, with substantial losses due to the crossover/back-diffusion that must be (but is hard) suppressed. The proposed increase of membrane thickness will reduce crossover but increase the cell resistivity (increase CapEx). This and high cell voltage led to low energy efficiency. The major reaction product in the conventional process is formate, which must be converted to formic acid. The proposed perforated BPM configuration allowed for the production of formic acid directly, which is encouraging, but the noticeable decrease (probably due to the catalyst ripening) in Faradaic efficiency with time is worrisome. It would be interesting to evaluate the pressure effect on the cell performance. In addition, for this method, it is necessary to use expensive hydrogen instead of inexpensive (but still costly) neutralization, and the effluent distillation of the diluted stream is still needed. A thorough TEA is necessary to compare these options.

- Formic acid oxidation seems to be a major limitation of this technology, and it should be recognized as a significant risk to mitigate against going forward. Second, the approach requires the electrolyzer to be split into two parts. This seems like an important variable considering that the electrolyzer CapEx is the top cost driver. Given that, is it worthwhile to invest in this approach given the other electrolyzer technologies available?

Are platinum catalysts an economically feasible option for this technology? No discussion was provided on this front, and I would caution against employing unscalable methods to meet a near-term goal.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The approach of developing a reactor with guidance from the TEA and using off-the-shelf components is mitigating risk and complications with scaling novel reactor materials. In addition, the information gained by investigating effects at a scale of 25-cm^2 and higher current densities also provides necessary information for scaling this technology and can be applied to other systems. Additional information/questions for further assessment:

1. Risk management—more information regarding the perforated membrane; durability, effects on the catalyst, and any effects on the integrated system.

   Reply: This is a newly developed system, and we are doing our best to provide more fundamental information while scaling.

2. More information regarding key areas of failure in a scaled-up system and methods to mitigate them. For example, R&D plans regarding how they will mitigate the voltage increase over time.

   Reply: First, we need to elucidate the mechanism of failure, which remains unclear at present. We have developed some studies to try to isolate the effect of increasing formic acid concentration on anode performance and also isolate catalyst degradation as a function of operating potential.

3. Potential impact—more information regarding the sensitivity of the amount of formate oxidation and how it affects CapEx.

   Reply: We are in the process of gathering initial TEA data to this point. In short, there is little sensitivity to formate oxidation and cell voltage relative to effluent formic acid concentration. The subsequent distillation costs dominate the process. We have identified that if we are able to produce 1.3M formic acid, then we can come close to the current market price of $0.66/kg formic acid using our approach.

4. More information regarding the specialized anode catalyst, durability, CapEx/OpEx, scalability, etc.

   Reply: This is ongoing, and a significant part of future work will be on durability (see above) and identifying solutions to mitigate formic acid oxidation and improve formic acid effluent concentration at scale.

5. Additional information regarding the H_2 generation and how it affects the TEA in various scenarios.

   Reply: With an intermediate estimate of $0.3.2/kWh electricity and $2.3/kg H_2, we are able to meet the current market price of 85 wt % formic acid if we produce 1.3M formic acid effluent. This is from a preliminary TEA that has just been completed.

6. The project aims to develop a scalable electrolyzer for CO2 conversion to formate/formic. Membrane development is the main strategy used in the project. A relatively stable system (over 100 hours) for formic production has been demonstrated using perforated membrane and hydrogen oxidation in the anode. One key question is whether hydrogen oxidation in the anode would be economically competitive compared to water oxidation. This is an important question because it governs the selection of anodic catalyst.

Reply: Currently, the most stable water oxidation catalyst is unsupported Ir or IrOx, which must be coated at a significantly higher loading (0.2 to 0.4 mg/cm^2) to obtain a uniform coating than the Pt-supported carbon catalyst, where we are currently using 0.05 mg Pt/cm^2 at the anode. Coupled with the fact that Ir is 4.5 times the cost of Pt and requires 4–8 times the loading, the Pt cost is a minimal contribution (approximately 1/16 to 1/32 of the Ir cost) to the overall device. This will be showcased in a TEA.

7. With the current cell configuration, it would be expected that membrane delamination occurs due to the CO_2 bubble formation between the two layers of the membrane. It is unclear how the target of 500 hours will be achieved.

   Reply: The approach using a perforated membrane prevents bubble formation within the membrane. The perforations allow CO_2 to escape from the anode. We showed a postmortem membrane cross-section image from an optical microscope for both the nonperforated and perforated BPMs. The nonperforated BPM had delamination, but the perforated BPM remained laminated and intact.

8. Single-pass conversion of over 30% is a milestone, but strategies to achieve it are not clear.

   Reply: This will come down to flow-field optimization during the scale-up process. Additionally, recent literature argues that single-pass conversion may not be relevant to reduce cost.

9. The team showed a certain progress in scaling up electrodes to fit a 25-cm^2 cell. Faradaic efficiency is low, with substantial losses due to the crossover/back-diffusion that must be (but is hard) suppressed. The proposed increase of membrane thickness will reduce crossover but increase the cell resistivity (increase CapEx). This and high cell voltage led to low energy efficiency. The major reaction product in conventional process is formate, which must be converted to formic acid. The proposed perforated BPM configuration allowed for the production of formic acid directly, which is encouraging, but the noticeable decrease (probably due to the catalyst ripening) in Faradaic efficiency with time is worrisome. It would be interesting to evaluate the pressure effect on the cell performance. In addition, for this method, it is necessary to use expensive hydrogen instead of inexpensive (but still costly) neutralization, and the effluent distillation of the diluted stream is still needed. A thorough TEA is necessary to compare these options.

   Reply: This is underway, and we have preliminary results (see responses to 3 and 5).

10. Formic acid oxidation seems to be a major limitation of this technology, and it should be recognized as a significant risk to mitigate against going forward.

    Reply: See responses to 3.

11. Second, the approach requires the electrolyzer to be split into two parts. This seems like an important variable considering that the electrolyzer CapEx is the top cost driver. Given that, is it worthwhile to invest in this approach given the other electrolyzer technologies available? Are platinum catalysts an economically feasible option for this technology? No discussion was provided on this front, and I would caution against employing unscalable methods to meet a near-term goal.

    Reply: Please see responses to 3, 5, and 6.

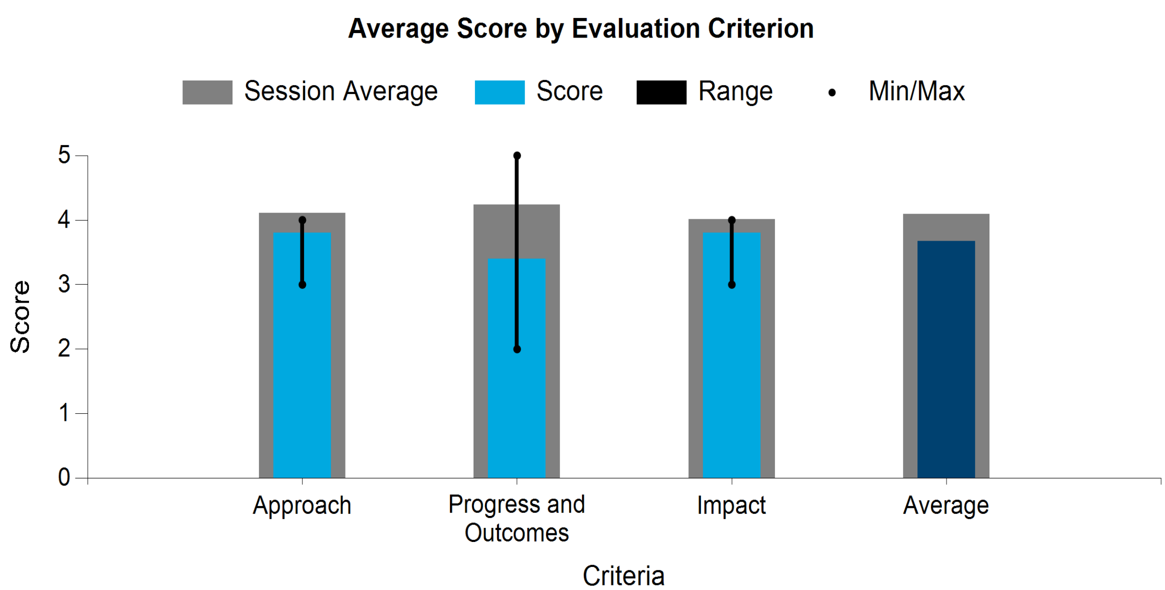
ELECTRODE AND MEMBRANE MATERIALS FOR CO_2 ELECTROLYZERS: A MOLECULAR APPROACH—ANL

Argonne National Laboratory

PROJECT DESCRIPTION

WBS:	2.3.4.304
Presenter(s):	Ksenija Glusac; Meltem Urgun Demirtas
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$800,000

Electrocatalytic CO_2 reduction to fuels and value-added chemicals is an important process in carbon recycling. A main challenge associated with CO_2 reduction is the product selectivity: Myriad reduced products—such as CO, H_2, formate, methanol, ethanol, and oxalate—are formed at similar thermodynamic driving forces, making it difficult to selectively generate the target product. Here, we investigate molecule/electrode hybrid materials for the selective and efficient electrochemical production of methanol from CO_2. Methanol was selected as a desired product because it can be used as a fuel to generate electricity (in methanol fuel cells) or heat (in methanol boilers) or in transportation (in road and marine engines). Further, methanol is an important chemical industry feedstock for the synthesis of formaldehyde, acetic acid, and other important products. Methanol is also a feedstock for the biosynthesis of amino acids and other products by methylotrophic microorganisms. Electrochemical methanol production is advantageous over the competing thermocatalytic CO_2 hydrogenation process because the energy input to drive the electrochemical process can, in principle, be powered using CO_2-free energy, leading to a net reduction of CO_2. Further, ECO_2R methods, unlike thermocatalytic CO_2 hydrogenation, can act as stabilizers of the electric grid by consuming the excess electricity generated by renewables.



COMMENTS

- Molecular catalysts for ECO_2R have the potential to be highly tailorable and efficient catalysts, which has potential to make an impact in the field of ECO_2R, despite currently being at a lower TRL. I appreciate their approach with using molecular catalysts immobilized on carbon nanotube. Focusing on converting CO_2 to MeOH, with high selectivity and in one step (eliminating the need for $H2_2$), could provide an efficient path for CO_2 utilization. I look forward to seeing more testing in real-word reactors and conditions as well as collaboration with industry partners as this project matures. It would be nice to see more communication/collaboration with the Betenbaugh group. Additional information/questions for further assessment:

Risk management:

- Address selectivity risk: Provide a road map for improving the MeOH selectivity in addition to pH effects.
- Address durability risk: Provide a road map for increasing durability.
- Assess the trade-offs in process stability and energy intensity between using a BPM versus pH control during continuous runs in a scaled-up system.
- Address the risk of the catalyst: Provide more information regarding the computational work on the catalysts, synthesis of the catalyst, and related experimental data.

Potential impact:

- Explain how your experimental targets (carbon selectivity, cell voltage, current density) relate to projected system performance (yield, product cost, energy efficiency).
- Demonstrate through analysis the advantage of using carbon nanotube supports over other supports with similar characteristics (e.g., why should carbon nanotubes be pursued?).
- Demonstrate through analysis the advantage of the one-step pathway: Compare the one-step pathway to pathways that leverage green H_2 using high/medium/low scenarios for the efficiency of the one-step pathway and high/medium/low scenarios for technology advancements involving green H_2.

- This project focuses on developing catalysts and electrochemical systems for CO_2 conversion to methanol. Molecular catalysts were selected and electrolyzers were developed based on BPM. A methanol Faradic efficiency of around 10% has been achieved. It is unclear how the target of 60% can be achieved by the end of the project. The catalysts are not so stable. It would be very challenging to achieve stability of over 100 hours at a current over 200 mA/cm^2. While the project focuses on CO_2 conversion, it would be interesting to see how the catalyst would perform if CO was used as the reactant. It is also important to compare e-methanol versus methanol produced via thermal catalysis. It is unclear how methanol produced directly from CO_2 electrolysis would be greener than the one produced from CO_2 and green H_2.

- The goal of this project is to enable the direct electrochemical conversion of CO_2 to methanol with high selectivity and energy efficiency. CO_2-generated methanol could be used directly as a fuel, a commodity chemical, or a feedstock for bioconversion to SAF, and thus the potential impact of this project is substantial; however, this project has the lowest TRL of all those in the CO_2RUe. The project's approach is to develop cobalt-based macrocycles, incorporate them onto carbon supports, and explore them for methanol production in a CO_2 electrolyzer. Progress to date has focused on exploring cobalt phthalocyanine (CoPc), a complex that has been previously shown to be effective for moderate methanol production in an electrochemical batch reactor. The project has confirmed low-single-pass Faradaic efficiencies.

- The team made some progress achieving a methanol Faradaic efficiency of 11% at the total current density of 100 mA/cm^2 and demonstrating a pH effect; however, substantial decline of Faradaic efficiency was observed at more practical higher current densities. The water dissociation BPM transmembrane potential (go/no-go milestone) was not even discussed during the presentation. The team clearly has a reproducibility issue, and more replicates are recommended. The selected catalyst, CoPc, demonstrated very low stability and, surprisingly, no methanol formation below 50 mA/cm^2. The methanol crossover through a BPM is noticeable. More mechanistic studies are required to understand the conditions and catalyst requirements for the preferential electrosynthesis of methanol.

- This project is at an earlier TRL stage than many of the other projects but provides important, foundational work on electrolyzer R&D. Projects like this are (in my opinion) an important part of BETO's investments as long as they are tethered to more mature parts of the consortia. One common challenge with this project and WBS 2.3.4.603 seems to be the specificity of methanol production by the electrolyzer. Significant investment will be needed to address this issue. One idea that was proposed was to increase the concentration of CO in the electrolyzer's microenvironment to promote the formation of methanol.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for taking the time to evaluate this project and provide useful feedback. We are quite excited to see that the reviewers recognized the significance of electrochemical methanol production and appreciated the challenges associated with the catalyst selectivity and stability. Addressing methanol selectivity is the main goal of this 3-year project. As the reviewers recognized, the methanol selectivity demonstrated so far by our team is 30% (in a three-electrode cell) and 10% (in an electrolyzer). Our synthetic and computational efforts are focused on increasing this value, and we look forward to reporting our progress in this direction next year. The reviewers' suggestion to use carbon monoxide as an initial feedstock for reduction is excellent, and we will follow up on this in the upcoming months. The reviewers' suggestion to perform the cost analysis of our one-step pathway for e-methanol and compare it to the existing two-step approaches is excellent. We are currently collaborating with Ling Tao on this project, and we anticipate that this analysis will provide us with information regarding the target performance characteristics of the one-step approach needed to ensure economic competitiveness relative to the two-step methods. While we recognize the catalyst durability challenge, our plan is to devote this initial 3-year funding period to the study of catalyst selectivity. Our catalysts are currently not tested for durability, and all our electrolyzers are evaluated during 1 hour of operation. The literature reports have shown that the durability of similar catalysts can be improved through molecular functionalization that prevents hydrogenation of the molecular macrocycle, and we anticipate that this approach will be applicable to our systems as well. Our plan is to address this issue in the next funding cycle. Our go/no-go work associated with BPMs has been terminated because we wanted to devote our full attention to the work associated with the catalyst design. We plan to redirect the resources planned for the BPM work toward the studies of selective methanol production with molecule/electrode hybrid catalysts. The reviewers' suggestion to increase communication with Dr. Michael Betenbaugh and their team (WBS 2.3.4.603) is excellent. We will follow up on this.

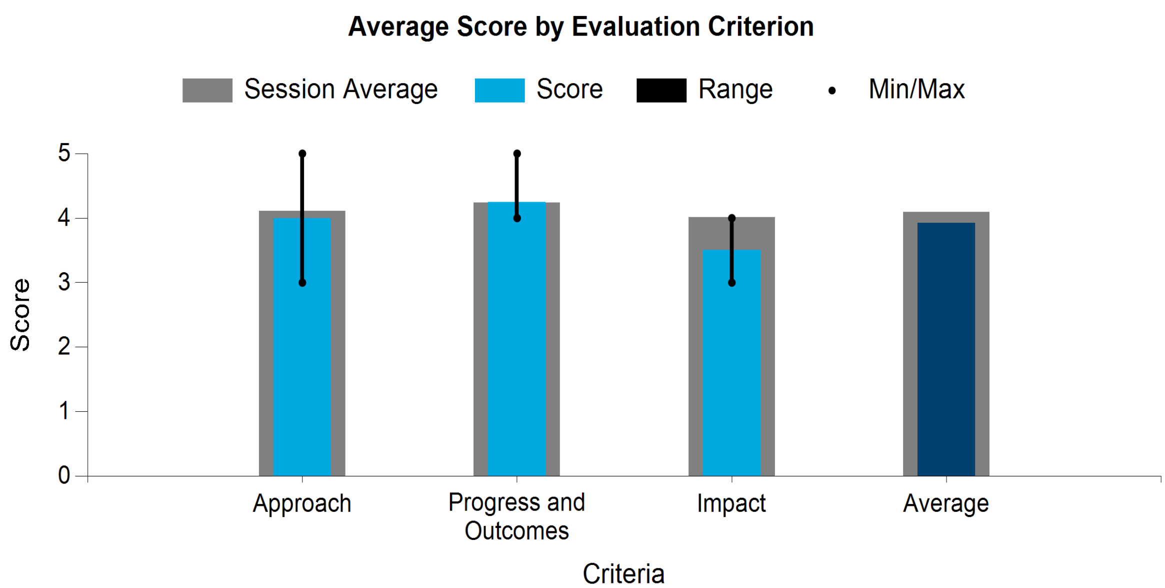
DEVELOPMENT OF A SCALABLE, ROBUST ELECTROCATALYTIC TECHNOLOGY FOR CONVERSION OF CO_2 TO FORMIC ACID VIA MICROSTRUCTURED MATERIALS

Montana State University

PROJECT DESCRIPTION

WBS:	2.3.4.600
Presenter(s):	Lee Spangler
Project Start Date:	10/01/2018
Planned Project End Date:	07/31/2022
Total Funding:	$1,862,958

The goal of this project is to develop an economically feasible pathway to convert CO_2 into higher-value chemical products. This project focusses on improving the efficiency of two key steps: (1) converting CO_2 to a formate salt intermediate by improving gas diffusion layers in a proven electrochemical reactor and (2) biologically upgrading the formate-to-ethylene glycol, a two-carbon compound using a new enzyme-catalyzed, carbon–carbon bond-forming reaction that uses single carbon inputs.



COMMENTS

- The project focuses on making ethylene glycol from CO_2 via a two-step pathway: ECO_2R to formate, followed by biological upgrading to ethylene glycol. The electrolyzer for formate production was developed based on a flow cell configuration where the flooding of the electrode is quite common. A relatively stable system (over 150 hours) has been demonstrated, with a formate Faradaic efficiency of over 85%. This was achieved by optimizing the composition of the gas diffusion layer. Self-supporting GDEs have been developed using a freeze tape casting (FTC) approach. Overall, good progress has been achieved in the part of electrochemical CO_2 conversion; however, it is unclear if the demonstrated system represents significant progress in the field. The operating cell voltage of 4.2–4.5 V at a current density of 125 mA/cm^2 is relatively high. With the flow cell configuration, it is unclear how the system will be scaled up. While the self-supporting electrode is interesting, it is unclear if it can be useful for a practical system. First, the cost of the electrode would be significantly increased. Second, its advantage over traditional carbon electrode is unclear.

- This project aims to enable CO_2 conversion to ethylene glycol by integrating CO_2 electrolyzers for formate production with a bioreactor for formate up-conversion. The overall project is divided into three distinct aims: (1) scaling CO_2 electrolyzers for formate production to >100-cm^2 sizes, (2) developing an FTC procedure for the preparation of gas diffusion membranes with lateral and vertical grading that will enhance electrolyzer stability and performance, and (3) engineering microbial systems to enhance formate conversion to ethylene glycol. The project team has made significant progress in each aim, but the research in each aim is siloed. While there is some evidence of communication between the different aims—such as testing the bioconversion process for compatibility with the potassium chloride electrolyte used in the electrolyzer—overall there has been almost no work on the integration of the work in the different aims. Some of this lack of integration may be due to travel and shipping difficulties during the COVID-19 pandemic. Another weakness of this project is the lack of a TEA-proposed CO_2 conversion process to ethylene glycol compared to conventional ethylene glycol production. The project has far-reaching potential scientific impact, especially the new FTC process for gas diffusion membranes and the biological up-conversion process.

- The team met most milestones, including relatively stable performance at 125 mA/cm^2 with an approximate 90% Faradaic efficiency for over 150 hours, but the cell voltage is higher than the target, and, more worrisome, a slight current increase to 150 mA/cm^2 resulted in fast performance decline. In addition, catholyte and anolyte have different pH values, which, without the appropriate membrane, would require some method of pH control and would increase material consumption. Unfortunately, there is no discussion of TEA and mass balance for bioconversion to support the selection of ethylene glycol as a target material. The cost of formate conversion to formaldehyde and the target product separation from the very dilute stream should be accounted for.

- This project seems to be progressing well. The electrolyzer work illustrates some very interesting and novel techniques for casting gas-permeable membranes. "Industrially relevant titer (>5 g/L), rate (>0.2 g/L/h), and yield (>90%), and remarkable scalability across different formats was demonstrated for the core condensation pathway, which can be further extended for formate-to-ethylene glycol conversion." I find the wording of this statement misleading. It would be more accurate to say that "work will now focus on integrating parts of the pathway and testing for complete conversion from formate-to-ethylene glycol." This is the most challenging aspect of the engineering portion of this project. Working with individual reactions is much simpler. Considering the confidence of the authors around the robustness of this system, I would suggest modifying Milestone 15.2 to include a metric around titer. The presenter mentioned that this is an aerobic process, and, as with other projects, this should be a concern for BETO because it undermines the vision of CO_2 utilization. *E. coli* grown under aerobic conditions produces *a lot* of CO_2. What is the plan for dealing with that?

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The project focuses on making ethylene glycol from CO_2 via a two-step pathway: ECO_2R to formate, followed by biological upgrading to ethylene glycol. The electrolyzer for formate production was developed based on a flow cell configuration where the flooding of the electrode is quite common. A relatively stable system (over 150 hours) has been demonstrated, with formate Faradaic efficiency over 85%. This was achieved by optimizing the composition of the gas diffusion layer. Self-supporting GDEs have been developed using an FTC approach. Overall, good progress has been achieved in the part of electrochemical CO_2 conversion; however, it is unclear if the demonstrated system represents significant progress in the field. The operating cell voltage of 4.2–4.5 V at a current density of 125 mA/cm^2 is relatively high. With the flow cell configuration, it is unclear how the system will be scaled up. While the self-supporting electrode is interesting, it is unclear if it can be useful for a practical system. First, the cost of the electrode would be significantly increased. Second, its advantage over a traditional carbon electrode is unclear.

Response: Effectively scaling CO_2-formate membranes is a confluence of fluid hydrodynamics and electrochemistry. Carbon papers are a common baseline given their usability across multiple electrochemical platforms, but they do not necessarily represent specific system optimums, particularly related to scale and degradation. The research of novel freeze-processed, porous tin-based membranes has numerous potential advantages over carbon paper; however, direct comparison with simple empirical tests is challenging given the multifunctionality of the FTC TiN, and it requires an iterative approach with real electrochemical testing. The TiN membranes have already been tested by the OCOchem company, demonstrating that they can be deployed in electrochemical systems. The MSU technology eliminates multiple layers because the FTC TiN serves as the GDE and catalyst support where the underlying TiN membrane is also selectively catalytic for CO_2 to formate. In this manner, multiple laminated planar layers are eliminated into a single multifunctional membrane, where interfaces always represent bottlenecks and degradation points in electrochemical systems. The electrical conductivity of the FTC TiN is shown to be nearly three orders of magnitude improved over the carbon paper, where current collection in larger-scaled systems can be particularly influenced when the length scales of the electron current pathways are expanded. Carbon can also catalyze the production of hydrogen, where TiN is selective to formate, also potentially improving yield. The cost of TiN has been in decline, and current prices of $25/kg represent a very low cost for metals. Further, the MSU processing is done at less than 200°C, requiring low-energy and low-cost ovens for processing in lieu of higher-performance furnaces.

Comments: This project aims to enable CO_2 conversion to ethylene glycol by integrating CO_2 electrolyzers for formate production with a bioreactor for formate up-conversion. The overall project is divided into three distinct aims: (1) scaling CO_2 electrolyzers for formate production to >100-cm^2 sizes, (2) developing an FTC procedure for the preparation of gas diffusion membranes with lateral and vertical grading that will enhance electrolyzer stability and performance, and (3) engineering microbial systems to enhance formate conversion to ethylene glycol. The project team has made significant progress in each aim, but the research in each aim is siloed. While there is some evidence of communication between the different aims—such as testing the bioconversion process for compatibility with the potassium chloride electrolyte used in the electrolyzer—overall there has been almost no work on the integration of the work in the different aims. Some of this lack of integration may be due to travel and shipping difficulties during the COVID-19 pandemic. Another weakness of this project is the lack of a TEA-proposed CO_2 conversion process to ethylene glycol compared to conventional ethylene glycol production. The project has far-reaching potential scientific impact, especially the new FTC process for gas diffusion membranes and the biological up-conversion process.

Response: The price of ethylene glycol made via conventional means is the basis for comparing the proposed process and TEA. Currently, mono-ethylene glycol is made from ethylene ($500/ton), with a higher CapEx, or ethylene oxide ($1,200/ton), with a lower CapEx. The mono-ethylene glycol market price has averaged $1,250/ton in the United States over the last year. Based on final experimental results, a TEA will determine the market price that is achievable based on the OpEx and CapEx cost profile of using the proposed process.

Comments: The team met most milestones, including relatively stable performance at 125 mA/cm^2 with an approximate 90% Faradaic efficiency for over 150 hours, but the cell voltage is higher than the target, and more worrisome, a slight current increase to 150 cm^2 resulted in fast performance decline. In addition, catholyte and anolyte have different pH values, which, without the appropriate membrane, would require some method of pH control and increase material consumption. Unfortunately, there is no discussion of TEA and mass balance for bioconversion to support the selection of ethylene glycol as a target material. The cost of formate conversion to formaldehyde and the target product separation from the very dilute stream should be accounted for.

Response: Yes, we agree that there is a few percentages higher voltage requirement in the demonstrated scale-up reactor performance. A further rigorous reactor design with optimization of the electrode-membrane gaps, which is out of the scope of the current project, will be needed, and it can be planned into the next project specifically looking at a scaled-up, industry-size reactor with optimal design to provide the desired electrochemical performance. The current density could be increased by further tuning the GDE, but was not done in this work because we were meeting our target current densities. The cation exchange membrane, under proper application of the voltage that then creates the electromigration impact opposite to the diffusive impact, should help maintain the reaction rate despite the different pH values on the two sides of the membrane, as evidenced by the >120-hour test performances demonstrated.

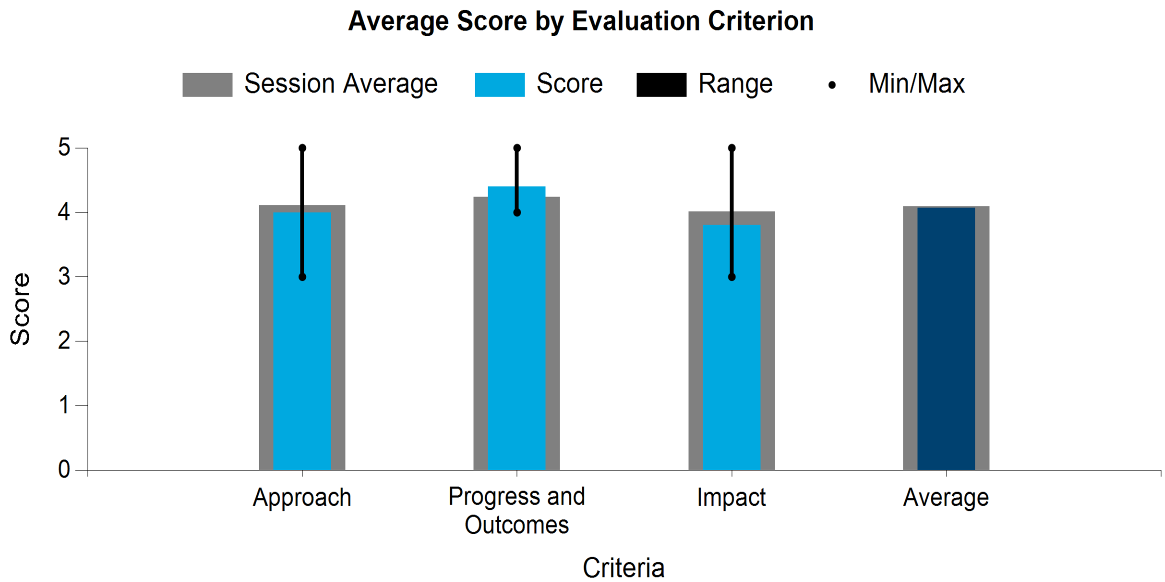
Comments: This project seems to be progressing well. The electrolyzer work illustrates some very interesting and novel techniques for casting gas-permeable membranes. "Industrially relevant titer (>5 g/L), rate (>0.2 g/L/h), and yield (>90%), and remarkable scalability across different formats was demonstrated for the core condensation pathway, which can be further extended for formate-to-ethylene glycol conversion." I find the wording of this statement misleading. It would be more accurate to say that "work will now focus on integrating parts of the pathway and testing for complete conversion from formate-to-ethylene glycol." This is the most challenging aspect of the engineering portion of this project. Working with individual reactions is much simpler. Considering the confidence of the authors around the robustness of this system, I would suggest modifying Milestone 15.2 to include a metric around titer. The presenter mentioned that this is an aerobic process, and, as with other projects, this should be a concern for BETO because it undermines the vision of CO_2 utilization. *E. coli* grown under aerobic conditions produces *a lot* of CO_2. What is the plan for dealing with that?

Response: The University of South Florida appreciates the comment and agrees that the statement should be reworded as suggested. The University of South Florida also agrees that Milestone 15.2 should be modified to include a metric around titer. With regard to CO_2 generation, we can distinguish CO_2 generation during the growth phase and bioconversion phase. For the growth phase, we solely focus on the biomass production with minimum time and resource input to obtain the required biomass and bioconversion rate. Our goal is to reduce the growth phase and extend the bioconversion phase to limit the resource input for biomass production (growth phase) below 10% (in carbon basis) of the amount of the substrate utilization in the bioconversion phase. While capturing CO_2 from this process would be challenging due to the presence of oxygen under aerobic conditions, as noted in the comment, we envision that the amount of CO_2 generation from the growth phase would be substantially smaller than the amount generated during the bioconversion phase, which we plan to capture and recycle. For the bioconversion phase, the generation of CO_2 is inevitable considering formate as the only source for the generation of ethylene glycol, a significantly more reduced product. We plan to use formate dehydrogenase to compensate the requirement for reducing power by oxidizing a fraction of formate to CO_2. The CO_2 generated from this process can be captured and recycled to the upstream CO_2 electrolyzer.

PRODUCTION OF BIOPRODUCTS FROM ELECTROCHEMICALLY GENERATED C1 INTERMEDIATES

LanzaTech, Inc.

WBS:	2.3.4.601
Presenter(s):	Jason Bromley
Project Start Date:	10/01/2018
Planned Project End Date:	07/31/2022
Total Funding:	$1,734,576



COMMENTS

- The information gained by their integration test setup can help advance the field of integrated bio-electrochemical systems. The recycle loop and other controls will provide valuable information regarding the integrated system and the mass balance. The test station setup (recycle loop, pressure control, gas chromatography analyzers, etc.) could be valuable to the other projects converting CO_2 to $CO:H_2$, so it may be beneficial to have more collaboration with the other projects. Additional information/questions for further assessment:

  Risk management:

  - I look forward to seeing the results when the recycle loop is continuously operational and a mass balance can be obtained, along with further insight into the efficiency losses.
  - Additional information regarding the potential toxicity of isopropyl alcohol (IPA), and how does this factor into operations and the energy intensity of the process?

  Potential impact:

- Additional information regarding the target product (IPA), what numbers their processes need to reach to be cost-competitive, and a road map as to how they aim to achieve their targets
- Additional information regarding the additional cost of generating hydrogen
- Additional information regarding the effect of the CO_2 conversion percentage on the TEA.

- The project focuses on integrating electrochemical CO_2 conversion and biological reactors at a relatively large scale. Great effort on demonstrating an integrated system, overcoming several obstacles. Carbon crossover in an MEA cell would limit the overall carbon conversion efficiency. It is important to evaluate the energy cost and carbon footprint for CO_2 separation (in the anode side) step. Combining the CO_2 electrolyzer and water electrolyzer to tune the CO_2:CO:H_2 ratio and achieve 100% carbon efficiency would have a significant impact.
- This project by LanzaTech focuses on integrating CO_2 electrolysis with gas fermentation to convert CO_2 to isopropanol with performance targets of 0.65 g/L/h isopropanol production with >37% carbon efficiency. The project uses a 250-cm^2 electrolyzer from Dioxide Materials for the CO_2 conversion to CO, followed by the integration of the output stream with their own biofermentation CSTR. All target performance metrics were achieved and exceeded, although circulation was required to achieve the carbon-efficiency targets. Recirculation did cause unforeseen issues in the system design due to the buildup of inert salts and sulfur impurities in the recycled CO_2 streams. The choice of the project to de-emphasize integration and focus on performance enhancement was well considered, as it is unclear that prioritizing integration is needed at such small production scales. This project achieved its stated objectives and is an important proof of concept that integrated electrolyzer and fermentation technologies can convert CO_2 to useful products.
- The team made substantial progress in the integration of Dioxide Materials' electrolyzer with the bioconversion of CO to IPA, including the energy consumption target. It would be interesting to evaluate the effect of temperature and back pressure on electrolyzer performance. The increase of the H_2:CO ratio may increase the CO_2 utilization, but this is not good for bacteria, so further microbial optimization is desirable; however, optimistic projections of IPA cost are based on the assumption of very low electricity and arginine prices that should be dropped five times. It is not clear what capacity factor for renewable electricity is used and how the arginine price could be reduced so much (unfortunately, attempts to replace it with inexpensive ammonia were unsuccessful). Based on experimental data, the separation of IPA from biomass and ethanol should be included in the cost structure (so far not included in the flow diagram). The IPA market is noticeably smaller than that of ethanol, so it is desirable to add the market analysis to the project scope to estimate commercialization prospectives in this approach.
- This project seems to be progressing well, and I have little concern about the overall approach, results, or impact. The goals involving arginine should be modified, as it appears that despite the modeling, no benefit was seen when using arginine instead of ammonia.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate all the reviewers' comments and suggestions, including the acknowledgement of the progress made in integrating biologic and electrochemical systems and understanding the reasons for shifting the project focus to performance once initial integration data were generated. Some additional points to address questions and comments raised:
    - The test station setup has already been used to provide a sample of potable alcohol from biogenic CO_2.
    - We have reached the end of the project budget, and one main conclusion is to recommend larger piloting reactors (10–100 times this size) to make more accurate assessments of performance,

including the closure of mass and carbon and energy balances, which is a big challenge at this stage when including a recycle loop.

- IPA has similar physical properties to ethanol, whose toxicity is known to a greater degree on similar acetogens, but detailed toxicity data of IPA on the LanzaTech strain are unable to be shared publicly.
- TEA is part of the project, but unfortunately most details are unable to be shared publicly. The TEA model relies on data generated from lab experiments and are updated at each billing period.
- Additional hydrogen will consume CO_2 to the following stoichiometric ratio to produce IPA: $9H_2 + 3CO_2 \rightarrow C_3H_8O + 5H_2O$. The cost of green hydrogen is steadily decreasing based on improvements to sustainable electricity generation and water electrolysis.
- While this project has completed operations, the reviewer feedback on back pressure and temperature will be considered as avenues for future work involving electrolyzer integration.
- The project successfully demonstrated the production of IPA using an engineered strain from gases. The use of arginine as a nitrogen source to boost production was muted.

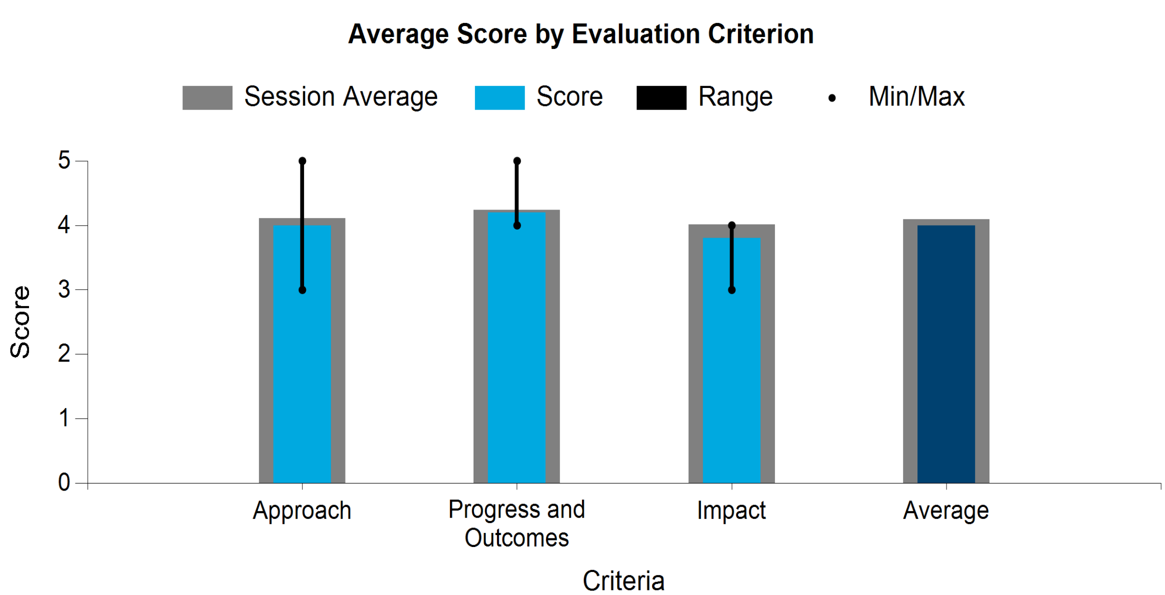
INTEGRATING CHEMICAL CATALYSIS AND BIOLOGICAL CONVERSION OF CARBON INTERMEDIATES FOR DERIVING VALUE-ADDED PRODUCTS FROM CARBON DIOXIDE

Johns Hopkins University

PROJECT DESCRIPTION

WBS:	2.3.4.603
Presenter(s):	Michael Betenbaugh
Project Start Date:	10/01/2018
Planned Project End Date:	07/31/2022
Total Funding:	$1,951,339

Capturing and upgrading point-source CO_2 represents a desirable technological goal to achieve sustainability targets. Electrocatalytic processes excel at reducing CO_2 into simple carbon compounds. Conversely, biocatalysts excel at upgrading reduced carbon compounds. In this project, we are developing a two-stage integrated platform that leverages the advantages of both electrocatalytic and biocatalytic systems: CO_2 is converted into methanol and hydrogen via electrocatalysis and is subsequently valorized using a methanotrophic bacteria. The electrocatalytic reduction of CO_2 uses an advanced catalyst that achieves a high carbon conversion efficiency into methanol. Cell line development to optimize the bioconversion of methanol by *Methylotuvimicrobium alcaliphilum* 20ZR incorporates metabolic engineering to channel the electrocatalytic product into PHA and biomass. Cell line adaptation is used to adjust to the high-saline electrocatalytic conditions entering the bioreactor, and transcriptomics analysis is applied to determine regulatory mechanisms for optimal cell line performance. A TEA and LCA of the complete process further investigate commercial feasibility and opportunities for future process development. In total, this technology represents a potentially transformative platform combining electrocatalytic and biological conversion steps into an integrated approach for the bioproduction of commercial products.



COMMENTS

- This approach to this project is novel, both in catalyst and biological upgrading, and well thought through. I appreciate the adjustments of the intermediate products made to determine an efficient path forward demonstrating continued communication, analysis, and risk mitigation. Targeting MeOH as an intermediate is an important path to explore regarding CO_2 utilization. I suggest more communication with other groups researching similar pathways, such as Glusac. I felt that the information shared regarding their electrolyzer was insufficient to make a good judgment; however, I understand there was not enough time to address everything during this review. Additional information/questions for further assessment:

Risk management:

- Additional information regarding the statement stable electrocatalysts for continuous operation. Details regarding the conditions, stability, and scalability (including pH, temperature, current density, voltage, etc.)
- Additional information regarding the covalent organic framework (COF)-CoPc catalyst; stability and scalability
- Additional information regarding the gas and liquid recycle loops; accuracy of the mass balance calculations, conditions in the liquid recycle loops, further analysis of the scaled-up version, TEA sensitivity regarding per-pass conversion of CO_2 and operation of the recycle loop, production of trace byproducts
- Additional information regarding their high conversion rate: stability and scalability.

Impact

- Additional information regarding the current and future target of the space time yield of MeOH/formate.

- This project focuses on converting CO_2 to bioproducts via methanol. The team has diverse and complementary expertise. Some progress on CO_2-to-methanol conversion has been achieved, especially the carbon efficiency; however, the selectivity of the process (Faradaic efficiency) has not been discussed. There seems to be some overlap with other projects (converting CO_2 to CO using molecular catalysts). It is unclear what the requirement for CO_2 to methanol would be based on TEA. In addition, CO_2 conversion to methanol via thermal catalysis has been quite advanced. It is unclear if the electrocatalysis process would have advantages compared to thermal catalysis. Comparisons of the two pathways using TEA/LCA would be helpful.
- This project aims to integrate a CO_2-to-methanol electrolyzer with engineered biocatalysts to convert methanol to PHA. The project is divided into three main tasks: electrocatalysis, biosynthesis, and integration. Each task has made significant progress during the project period. In electrocatalysis, the project team uses CoPc to convert CO_2 to methanol. CoPc is one of the few catalysts previously reported to produce methanol with up to 44% Faradaic efficiency in highly optimized batch reactors through a cascade catalysis process in which CoPc first converts CO_2 to CO and then CO to methanol; however, single-pass flow electrolyzers incorporating CoPc typically produce CO, not methanol, likely because the local concentration of CO is not allowed to build up in these traditional electrolyzer setups. The project team uses a recirculating electrolysis system and a COF support for the CoPc that has enabled them to achieve 90% carbon conversion efficiency with 40% Faradaic efficiency for methanol production. This is an important achievement and validation of CoPc as a CO_2-to-methanol catalyst; however, more comprehensive TEA and LCA are required to determine whether this approach could be economically viable due to the relatively low Faradaic efficiency for methanol. In the biosynthesis task, the project team has engineered microbes to convert methanol to PHA and biomass with a high carbon conversion efficiency, >50%, and good yields. In both the electrolyzer and biosynthesis tasks, the project team has met or exceeded milestone goals. In integration, the project team has also made progress, but

perhaps less than the other tasks. They are able to perform 50-mL-scale bioconversions using mock electrocatalysis products and meet their carbon conversion efficiency and process yield target milestones, but they have not yet scaled the process to the target 1-L scale or used real electrocatalysis projects. Still, there is evidence of close communication between the scientists in each task and clear demonstration of how integration challenges have led to new optimizations in the electrocatalysis and biosynthesis tasks. This is a well-executed project that has already made significant impact in electrocatalysis and biosynthesis, and it has a good chance of meeting its final integration milestone goal. This project would likely benefit from increased discussion and collaboration with members of the CO_2RUe, especially WBS 2.3.4.304, which aims to design new catalysts for electrochemical CO_2-to-methanol conversion.

- The project pivot from formate to methanol looks justified, and the team demonstrated noticeable progress in the conversion of CO_2 to methanol. Carbon conversion efficiency was close to the target (32% versus 37%); however, it was not quite clear what changes have been made (in addition to recirculation of the gas stream) to switch the reaction mechanism from CO to MeOH as a major product with the same catalyst. The methanol current density and Faradaic efficiency (~27%) are still too low to be practical. The stability of the single-atom cobalt catalyst was not presented. There are some questions about the performed TEA. The cost baseline was not defined, and the proposed credit for the hydrogen sell (\$5–\$6/kg) seems to be high in light of the current DOE target (\$1–\$2/kg). The energy balance for the two-step process (CO_2-MeOH-PHA) was not presented, and the process of PHA separation (6%) from biomass was not discussed.

- The project seems to be going well and is supported by a talented group of investigators. The strain engineering side seems particularly strong with the support of Dr. Marina Kalyuzhnaya. In regard to communication, I was surprised to hear that this team had not (apparently) heard of the work being conducted by Dr. Glusac in WBS 2.3.4.304 (hence the three on approach). I would encourage the two teams to meet and discuss their findings because that would likely benefit both groups.

PI RESPONSE TO REVIEWER COMMENTS

- In our study, we achieved a Faradaic efficiency of 40% for the conversion of CO_2 to methanol using our CoPc-COF electrocatalysts. This high efficiency was made possible by the CoPc active center, which has been established as a leading catalyst for methanol production, as reported in https://doi.org/10.1038/s41586-019-1760-8. Note that the byproducts of this conversion process were hydrogen and CO. Additionally, we observed a slightly lower Faradaic efficiency of 20%–25% for the conversion of CO to methanol on the CoPc-COF catalyst, without the presence of other carbon byproducts. Consequently, the overall carbon conversion efficiency in our electrocatalysis system exceeds 90%; therefore, our findings demonstrate the feasibility of achieving high methanol production rates while maintaining a significant carbon conversion efficiency. In terms of scalability, we used a 5-cm^2 flow cell electrolyzer, which has proven capable of producing approximately 1 gram of methanol/day. This was achieved by operating at a current density of 100 mA/cm^2 with a 40% Faradaic efficiency. Further, it is worth clarifying that our CO_2-to-methanol conversion process does not involve an intermediate step through formate. We have distinct electrocatalytic processes for CO_2-to-methanol and CO_2-to-formate conversions, each utilizing different catalysts. The CO_2-to-methanol conversion is facilitated by our synthesized CoPc-COF catalysts, while commercially available TiN oxide powder serves as the catalyst for CO_2-to-formate conversion. Regarding the stability of our system, we have identified catalyst deactivation as the primary failure mechanism for CO_2-to-methanol conversion. The reduction potential applied during the electrocatalysis process chemically reduces the CoPc catalyst, leading to deactivation; however, based on the findings presented in the aforementioned paper, the stability of CoPc can be enhanced by introducing amine groups to the aromatic rings. Our CoPc-COF catalyst incorporates tetraamine-substituted CoPc, which has demonstrated stability over 100 hours of continuous operation. While the failure mechanisms related to COF formation require further investigation, our current study focuses on the stability and efficiency of the electrocatalytic process for CO_2-to-methanol conversion.

There are two groups of PHAs according to the number of carbon atoms in the monomer units: short-chain-length PHAs (scl-PHAs) with 3–5 carbon monomers (most common, polylhydroxybutyrate, PHB), and medium-chain-length PHAs (mcl-PHAs) with 6–14 carbon monomers. While most bacteria produce PHB, the polymer is not "ready-to-go" plastic because it has low thermal stability and is brittle (not elastic). Contrary to PHB, mcl-PHAs are thermoplastic with attractive properties for biomedical applications (according to https://doi.org/10.1002/app.34772). As a result, mcl-PHAs have a higher price. We used two standard protocols for PHA separation at the lab scale: (1) chloroform extractions followed by cold acetone precipitation. The chloroform solubilization/precipitation step was repeated two to three times to achieve high purity of preparations for nuclear magnetic resonance studies (https://doi.org/10.1007/BF00500854). (2) Bleach extractions were used for quick culture screens (adapted from protocol provided by Dr. Averesch, Stanford University). Briefly, cell cultures (25–50-mg dry cell weight) were harvested by centrifugation and lyophilized overnight. Freeze-dried pellets are weighed for dry cell weight. PHA is released with 10% NaClO (0.2-mL/mg dry cell weight). Vortex vigorously until all biomass is dispersed. After no more than 1 hour, dH_2O is added 2:1 to allow precipitation of PHA by centrifugation (10 min, 4,800 g). The raw polymer is washed twice with dH_2O, washed once with methanol (or ethanol, or not at all), and freeze-dried. Dry PHA samples were weighed to determine the yield. If needed, the samples were further purified using the chloroform extraction method. Assessment of the scaled-up, integrated system is currently underway and is a primary focus for the remainder of the project. Previous experiments have shown that the mock electrocatalysis products used are comparable to the real electrocatalysis products produced in this project, although these data were not presented during the presentation due to time constraints. We intend to use the actual electrocatalysis products in the next tests of the integrated system. Preliminary testing has also shown comparable performance at larger (>1-L) scales, although final testing is still in progress.

As this project nears completion, we look forward to the opportunity to potentially collaborate with the other groups (Dr. Glusac, CO_2RUe) mentioned by the reviewers in the future. The previous TEA performed as part of this project confirmed that a formate product is preferred to methanol for the electrolyzer due to superior Faradaic efficiency and economic incentives. The production of methanol required a distillation column to separate the produced methanol from the electrolyte, resulting in significant operating costs; however, the production of methanol is found to achieve higher carbon conversion efficiency, and experimental work has been done to adapt the bioreactor system to higher concentrations of sodium bicarbonate electrolyte. This allows us to possibly bypass the distillation column, prevent significant utility costs, and achieve more favorable economics.

Regarding electrolyzer performance, the single-pass and overall conversion of CO_2 is 98% and 96%, respectively, according to the current technological benchmarks. In comparing between the choice to recycle CO_2 or not, there are slight differences in the net present value due to the reduced amount of mcl-PHA produced. Recycling CO_2 is preferred, and the implementation of a recycle stream is also important for preventing CO_2 emissions from the plant. A possible comparison of the use of thermal catalysts instead of electrocatalysis can be performed using reference data from other sources of literature. https://doi.org/10.3389/fenrg.2020.621119 provides a detailed analysis of thermocatalytic methanol synthesis and can be used for comparison in terms of both TEA and LCA. For the downstream processing of biomass and mcl-PHA, the process is based on work developed by from the patent "Process for the solvent-based extraction of polyhydroxyalkanoates from biomass" by Narasimhan et al. and from https://doi.org/10.1016/j.jece.2016.07.033, with guidance from industry experts. Bioreactor effluent is sent to a gravity belt thickener where the liquid is thickened to 8 wt % solids content. The thickened sludge is fed to a decanter centrifuge, where it is further dewatered to 35 wt % solids. The wet solids are then sent to a horizontal belt dryer to be dried further to 90 wt % solids. A pressurized solvent extraction vessel is used to extract the mcl-PHA from the biomass where acetone is used as the solvent.

The mcl-PHA is dissolved in the acetone phase using a mixer and heater. A disk stack centrifuge is used to separate the biomass from the hot liquid to 20 wt % solids. Any mcl-PHA lost in the wet biomass effluent needs to be recovered using a rotary drum pressure filter. This produces a solid biomass product for sale. The mcl-PHA liquid stream is cooled and sent to a stirrer where it is combined with water at a predetermined ratio to precipitate the mcl-PHA. A gravity belt thickener and a rotary vacuum drum filter is used to dewater the mcl-PHA to 65 wt % solids. It is then washed with acetone to remove extra lipids and then sent to a final horizontal belt dryer to evaporate off solvents and produce a dried mcl-PHA product at 99.5 wt % solids. For the improved technological scenario without the use of a distillation column, we currently have calculated a cost baseline of $968.61 million for total capital costs and operating expenses of $748 million/year. Note, however, that this baseline assumes an H_2 sale price of $5.75/kg. This estimate was originally chosen based on a 2020 report from NREL; however, it is understandable that this baseline sale cost is still considered high and can be reduced to the target sale price of $1–$2/kg for the final analysis.

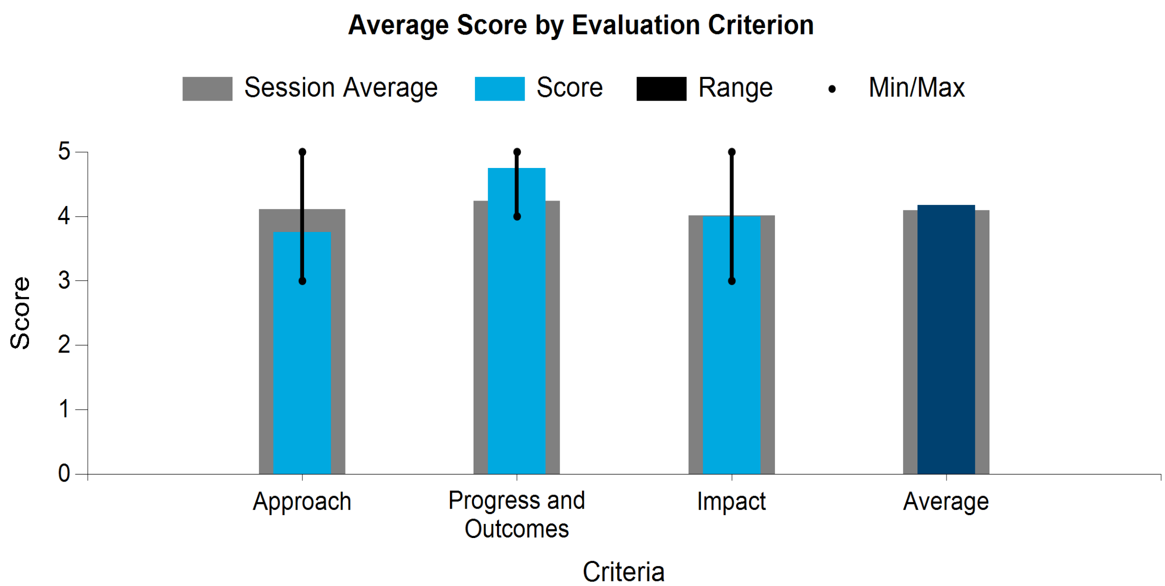
MULTIPHYSICS CFD FOR DESIGN AND SCALE-UP OF GAS BIOREACTORS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.4.1.102
Presenter(s):	Hari Sitaraman
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024
Total Funding:	$250,000

Gas fermentation technology offers sustainable and high-carbon-efficiency routes to fuels and chemicals; however, efficiently delivering low-solubility substrate gases to production-scale bioreactors is a significant technical challenge that could limit productivity. We perform fundamental and applied multiphysics computational fluid dynamics (CFD) research targeting specific challenges of gas delivery in fermentation systems that used varied gas compositions—e.g., CO_2/CO/CH_4/H_2 substrates: bubble dynamics, coupled mass transfer and reaction—that can lead to optimal reactor designs at scale. This work will support BETO goals toward GHG reduction, de-risking technologies toward commercialization/deployment and SAF synthesis targets.



COMMENTS

- The knowledge gained from this project has the potential to improve the efficiency of bioreactors across the field. It is not clear to me how much of an impact this project can have without further information regarding the range of improvements in TEA, LCA, productivity, etc., that can come from the findings of this project.
- The project focuses on modeling bioreactors for scaling up. There are several experimental projects on biological upgrading that could be beneficial from this project. Progress has been made on the effect of gas mixture (H_2:CO_2:CO) on the mass transport in the bioreactor; however, experimental design to validate the model is needed. I am not sure if mass transport is the limitation factor in this type of reaction or the rate of the bioreaction. Also, products from biological reaction (e.g., fatty acid) can act as bubble stabilizing agents and affect bubble size and the mass transport.

- This project plays an important role in the CO_2RUe by modeling the performance of different bioreactors as they translate from the lab scale to the industrial scale. Understanding the challenges and limitations to scaling bioreactors to relevant industrial production scales is crucial for the eventual implementation of CO_2 utilization technologies for SAF, so this project has high potential impact. The project has mostly focused on bubble reactor designs for the current funded work, but the project team has previously considered other reactor designs. A key strength of this project is the close interactions with stakeholders, including industry partners who provide experimental data and advice on scale-up. Much of the future immediate work will focus on simulation validation and expanding the simulations to new reactor designs. The project would be strengthened through closer interactions with the consortium analysis teams who could provide TEA and LCA to help down-select reactor designs. Overall, this is an impactful project that should continue to make important contributions to scaling biofermentation processes.

- Developing and validating novel reactor designs is critical to the success of gas utilization platforms, and this project provides excellent insight into how different reactors influence performance metrics. The only concern I have regarding this project is really a hope that this work will translate into tangible improvements in reactors that can be validated in the real world. I understand that is out of scope for this project.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their comments and constructive feedback that will strengthen the impact of this project. Our efforts in the past year (during early stages of the project) have been working toward developing a validated and predictive computational model for bioreactors that use CO_2. The real impact on TEA/LCA improvements will be achieved through the final phase of our project on novel reactor designs at scale that can improve CO_2/syngas conversion. Our models can predict theoretically possible bioreactor yields and efficiencies through more accurate, three-dimensional, multiphase simulations compared to zero- and one-dimensional models used in current TEA software. As improvements in microbial bioreactions are being pushed to the limits, mass transfer and mixing limitations at scale are going to drive the overall productivity, thus emphasizing the need for accurate and predictive multiphase flow models for reactor optimization and scale-up. We agree with the reviewers regarding the effect of surfactants on bubble size distributions, which is being added to our model for the validation work planned in our second year. Our current efforts on model validation have been through experiments from literature that are idealized (pure CO_2, constant bubble size), which will be improved for achieving the go/no-go milestone in September 2023. We agree with the reviewer on tightening collaborations with analysis efforts within the consortium, which is planned in the final phase of this project where we simulate large-scale reactors. We are also working closely with industry partners such as LanzaTech to enable the widespread usage of our modeling tools and provide tangible improvements in reactor designs.

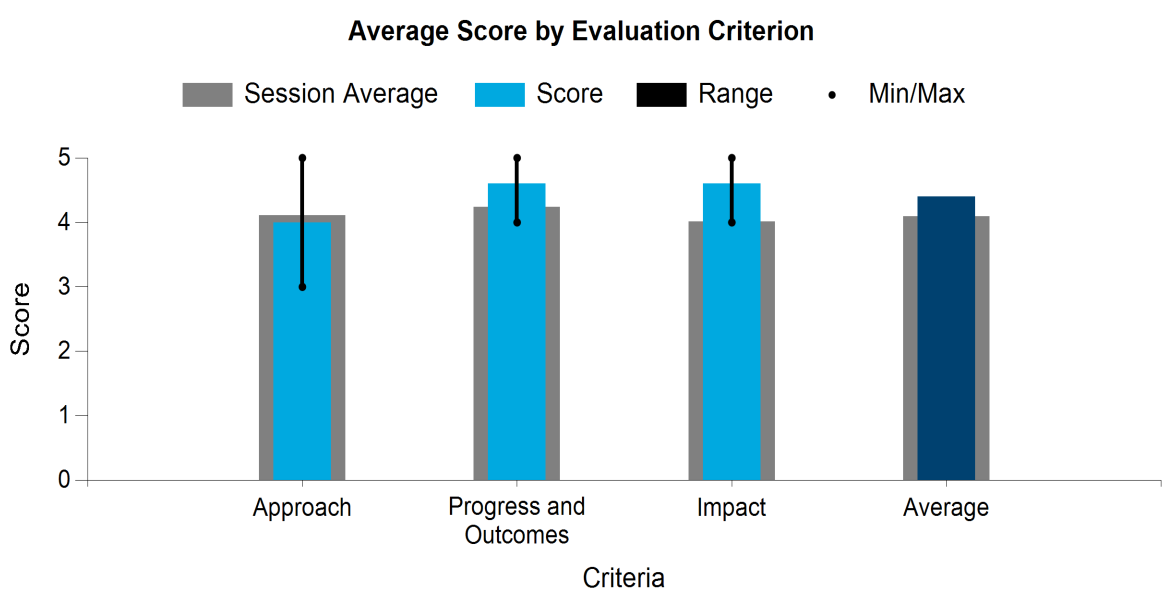
CO_2 CONSORTIUM PROJECT MANAGEMENT

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.6.3.502
Presenter(s):	Michael Resch
Project Start Date:	01/01/2022
Planned Project End Date:	12/31/2024

This project funds the management activities of the CO_2RUe. The PI and project manager coordinate the analysis, electrolysis, and biological working groups focusing on the integration process to convert CO_2 into SAF and high-value products supporting BETO's goal of decarbonizing energy-intensive industries. This project will directly support BETO's CO_2 Utilization program goals under "Decarbonizing energy-intensive industries" by providing project management support and oversight to BETO's CO_2RUe and ensuring that BETO has a robust plan and well-run consortium to develop technologies to upgrade CO_2 to fuels and chemicals to reduce GHG emissions, decrease land and water use, and incentivize decarbonization. The project will support the PI and project manager at NREL. The PI will provide scientific direction and leadership, assist BETO with technical management and organization of all consortium projects, integrate the scope and effort of individual projects into a cohesive consortium, promote the consortium to external stakeholders, and maintain a positive relationship with internal and external advisory boards, BETO, and the PIs of individual projects. The project manager will maintain documentation and outreach materials; curate information management; manage communication; develop and revise processes; launch the consortium website; and craft and implement a diversity, equity, and inclusion (DEI) plan. This project directly supports BETO's DEI goals by making resources available on the consortium website for students and teachers to learn about BETO technologies in a free and accessible environment.



COMMENTS

- The CO_2 utilization consortium has done an amazing job with overviewing and managing complex interconnected projects. The CO_2 utilization consortium project leaders have the potential to guide the direction of the consortium as well as the individual research projects in a unique way with a broad perspective.

Risk management:

- Increased communication between the groups and further collaboration and synchronization between each research effort
- More connection between the LCA/TEA groups and the experimental research projects would guide research efforts and synchronize target outcomes.
- More information and effort on outreach to industry and widespread knowledge exchange
- Plans to prioritize DEI. As leaders of the CO_2 consortium, there is an opportunity to make an impact regarding DEI.

Approaching the complex challenge of scaling ECO_2R from multiple angles is key to determining the most viable route to scaling this technology; however, more clarity and focus on which topics to address may help limit R&D overlap between the groups, e.g., designing and testing larger electrodes. Increased synchronization between the groups focusing on scaling the reactor and system setup (recycle loop, humidity control, pressure regulation, etc.) could prove to be more efficient. Some of these experiments get hampered by operability and equipment, and with further collaboration, more real-world testing could be done faster from an equipment, analysis, and operability standpoint.

Another example is with the research on bio-electrochemical systems. There is emphasis on proving that the integrated system can work, and this can lead the integrated systems to function for a short amount of time in an unsustainable way. The separate systems need to reach a higher level of maturity, particularly electrochemical CO_2 reduction, before focusing on their integration; however, I believe the information gained from integrating the systems is critical. Perhaps having fewer groups focusing on designing test stations to integrate the system could help improve efficiency while not losing the valuable information gained from the integration early on in R&D.

- This is a great initiative with combined expertise and technical capability. There seem to be multiple TEA and LCA projects looking at the integration of different processes. Many projects focus on the conversion of CO_2 to CO and formic as intermediates for further fermentation. Each project seems to focus on different parts or performance metrics for CO_2 conversion; perhaps it would be more impactful if there was a unified effort on advancing the electrolysis part that can be combined with subsequent upgrading processes.
- The focus of the CO_2RUe is to facilitate collaboration between research groups working on the CO_2 conversion to SAF. The CO_2RUe divides its projects into three working groups: CO_2 electrolysis, biological upgrading, and analysis and modeling. To foster collaboration, CO_2RUe members participate in regular working group meetings and larger consortium meetings and have collaborative milestones built into their individual projects. This collaborative approach is well considered and effective, and it has led to substantive collaborations between the individual CO_2RUe projects. The consortium structure is reasonable and consists of a central lead advised by internal and external advisory boards. The consortium lead's role is to help coordinate project goals, facilitate collaborations, set overarching research directions, and meet biweekly with BETO program managers. The consortium uses a bottom-up leadership approach rather than top-down mandates, so the project lead has no direct control over project funding or research directions. This is a strength in terms of engagement and project buy-in, but it may provide future complications if a project is underperforming or not effectively engaging within the consortium portfolio. A strength of the CO_2RUe is that it magnifies the impact of the individual consortium projects. For instance, the CO_2RUe hopes to set near-term technical targets for the entire community in terms of electrochemical and biological CO_2 upgrading and help de-risk technologies by evaluating location-specific feedstock and output markets. These efforts require communication between several projects in each working group, and they can only be achieved through a coordinated

multiproject effort. The CO_2RUe appears to be a well-run consortium with a reasonable management structure that has the potential to have appreciable impacts on CO_2 upgrading to SAF.

- The project has a clear technical path forward and has demonstrated progress toward the project goals. The integration of a 250-cm^2 CO_2 electrolyzer with CSTR was demonstrated. Preliminary data on H_2S tolerance are encouraging, but only for low current densities. Reasonable coordination between partners can be seen. Milestones have been met; however, one stated goal is the reduction of the CO_2 membrane crossover by 20%, but no work has been started yet. The idea of using CO_2 feedstock from ethanol refineries is good but is not analyzed in depth. For example, requirements to the source of renewable electricity (wind)—such as placement, capital investment, and availability—as well as the business model are not developed. The performed TEA points to the CO_2 single-pass conversion as a major cost factor. In other processes, its importance is very low because the addition of an inexpensive CO_2 separation and recycling loop eliminates this issue.

- The organization around the CO_2 Utilization consortium is clearly adding a lot of value. The project seems well integrated with BETO's higher-level strategy and is generally managed effectively. Some feedback worth considering for future iterations of this consortium:

    - Improve communication between research groups. It was clear during the review that many of the groups had not interacted with each other that much or at all. This is a clear area for improvement that should be led by the group's leadership.

    - Balance lower- and higher-TRL projects. There is a need to continue investment in lower-TRL projects, but that obviously comes with some risk. BETO is encouraged to ensure that these projects are anchored to well-established aspects of the consortium to promote engagement and success. I would also encourage BETO to calibrate their investment for these projects based on the balance between risk and reward.

    - Continue engagement with industry, with some prerequisites. Industry partners have a unique opportunity to add value to this program and should be included in future iterations. That said, BETO is encouraged to set some expectations regarding communication around results to ensure that there is a sufficient level of openness around these data.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the supportive comments, and we will address the listed concerns.

  To increase communication between the groups and further collaboration and synchronization between each research effort, we will have our second annual all-hands meeting in June 2023. The intent of this consortium meeting is to discuss progress and plan for future work. The majority of the participants will be able to attend in person, and we believe this will be an important opportunity to build relationships and collaborations between projects and working groups. Additionally, this will be an opportunity to identify research gaps and identify ways to improve our collaborations as a consortium. To enable more connections between the LCA/TEA groups and the experimental research projects to guide research efforts and synchronize target outcomes, the all-hands meeting will be an opportunity for cross collaborations between working groups with a focus on future planning. There has been expressed interest in more collaborations between the analysis group and the other two working groups, so this is something that will be explored further. Our project management effort on outreach to industry and widespread knowledge exchange will be expanded. We are in the process of communicating with other CO_2 upgrading research consortia in Europe to collaborate and exchange ideas and find ways our projects synergize. Our external advisory board was selected from industry and academic members with backgrounds across the value chain. We are also attending international scientific meetings to present the ongoing work in the consortium.

We agree that DEI is an important priority for the consortium. We recently hired a project manager with experience in DEI and community development, and she will work with the consortium to improve DEI and community benefit plans in current and future projects. We are also employing GEM fellows on two research projects. The mission of The National GEM Consortium is to enhance the value of the nation's human capital by increasing the participation of underrepresented groups (African Americans, American Indians, and Hispanic Americans) at the master's and doctoral levels in engineering and science.

At NREL, we have been working with the recently formed design-build team, who have experience in building CO_2 electrolyzer test stands in coordination with industry and environment, safety, health, and quality. We hope that these efforts can be standardized to safely build and install test stands across the national labs.

To synergize the electrolyzer efforts, we have the electrolyzer CO_2 working group (e-COWG). This group collectively focuses on key aspects of electrolyzer conversion efficiency, durability, and cell hardware designs.

Although we prioritize a bottom-up leadership approach, the leaders of the consortium work to find solutions with projects that are underperforming or not engaging. We have bimonthly individual meetings with each project team to discuss project progress and any challenges the PI or project may be facing.

CATALYTIC UPGRADING

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Catalytic Upgrading Technology Area is one of 12 technology areas reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 19 presentations were reviewed in the Catalytic Upgrading session by five external reviewers. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer the corresponding Program and Technology Area Overview presentation slide decks, which can be accessed at the Peer Review website: www.energy.gov/eere/bioenergy/2023-project-peer-review.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $16 million, which represents approximately 3% of the BETO portfolio reviewed during the 2023 Peer Review. During the Project Peer Review meeting, the presenter for each project was given 20–90 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored based on their approach, impact, progress, and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Sonia Hammache as the Catalytic Upgrading Technology Area review lead, with contractor support from Umakanta Jena of Boston Government Services. In this capacity, Sonia Hammache was responsible for all aspects of review planning and implementation.

CATALYTIC UPGRADING REVIEW PANEL

Name	Title and Affiliation
Dr. Cory Phillips*	Director of Engineering Development, Air Company
Dr. Qing Shao	Assistant Professor, University of Kentucky
Dr. Chris Bradley	Program Manager, Catalysis Science Program, DOE
Dr. Xunhua Mo	Catalyst Development Scientist and Laboratory Supervisor, Johnson Matthey
Dr. Andrea Strzelec	Director for the Master of Engineering: Engine Systems, University of Wisconsin-Madison

* Lead Reviewer

CATALYTIC UPGRADING REVIEW PANEL SUMMARY REPORT

Prepared by the Catalytic Upgrading Review Panel

INTRODUCTION

For the 2023 cycle in the Catalytic Upgrading Technology Area, the review panel evaluated a portfolio of 16 projects. Most (15) of these were housed within the national-laboratory-led (National Renewable Energy Laboratory [NREL], Pacific Northwest National Laboratory [PNNL], Los Alamos National Laboratory [LANL], Oak Ridge National Laboratory [ORNL], and Argonne National Laboratory), annual operating plan (AOP)-based Chemical Catalysis for Bioenergy Consortium (ChemCatBio). The remaining project was a funding opportunity announcement (FOA)-based project led by the University of South Florida. The overall quality of the presentations was excellent, and the session was completed in just 2 days, remaining on schedule, with adequate Q&A following each talk. Frequently, there was ample time for the audience to offer some technical inquiry as well. The high-level themes remained the same: (1) core technology—catalytic upgrading of C1, C2, and biochemical intermediates and catalytic fast pyrolysis (CFP)—and (2) crosscutting and enabling tools—catalyst synthesis, characterization, deactivation, multiscale, computational modeling, and data hub. However, in this cycle, the conceptual process designs and objectives pivoted and focused mainly on sustainable aviation fuels (SAFs) and chemicals as key products to align with the overall BETO objectives.

Because ChemCatBio was already focused on pathways to produce bio-derived hydrocarbons and oxygenates as fuels for internal combustion applications over the last few review cycles, the switch to SAFs and chemicals seemed like a natural progression. For the *core technology* thrust, the C1 team successfully converted CO_2-rich syngas into precursors for SAF using the syngas-to-hydrocarbons (STH) method developed through insights gained from high-octane gasoline (HOG) production over copper (Cu)/beta zeolite (BEA). The team also initiated a proof of concept for isoalkane dehydrocoupling. The C2 team focused on directly converting ethanol to mixed C4 olefins in one step, bypassing the dehydration step over a tunable dealuminated beta zeolite and M/SiO_2 (M = Ag/Zr) materials, followed by oligomerization to SAF-range material. The CFP team developed a regenerative fluidized-bed system capable of CFP followed by upgrading to SAF using traditional hydrotreating approaches. The Catalytic Upgrading of Biochemical Intermediates (CUBI) team worked on four approaches to SAF based on catalytically upgrading biomass-derived feedstocks such as organic acids (volatile fatty acids [VFAs], butyric acid), furan, and butanediol (BDO). The upgrading was achieved by incorporating a variety of catalyst-driven synthesis steps to accomplish C-C bond formation and deoxygenation, such as condensation, ketonization, hydrodeoxygenation (HDO), dehydration, and methyl ethyl ketone (MEK) deoxygenation. From the *enabling tools* thrust, the Advanced Catalyst Synthesis and Characterization (ACSC) team accelerated the development of next-generation M/BEA zeolites and collaborated with the deactivation team to understand the degradation in activity for the Pt/TiO_2 system during CFP. The Consortium for Computational Physics and Chemistry (CCPC) team showed good agreement between density functional theory (DFT) predictions and characterization experiments for the VFA upgrading work, as well as a number of studies in support of the C2 upgrading work on Cu/BEA and M/SiO_2 systems covering deactivation and regeneration mechanisms. Further advanced material characterization tools and analysis were provided in the biogas conversion project, where the team did an excellent job of understanding the surface and bulk behavior of Zinc using isotopic transient kinetic analysis, *in situ* X-ray photoelectron spectroscopy, diffuse reflectance infrared Fourier-transform spectroscopy, extended X-ray absorption fine structure, and X-ray absorption near edge structure.

The principal investigators (PIs) provided copies of the presentations prior to the in-person session. This allowed each peer reviewer to make preliminary comments and compile a short list of key urgent questions. Most of the presenters were able to answer any concerns and provide additional context. There seemed to be an adequate number of breaks throughout the day, and presenters were able to engage with the review panel easily for any additional knowledge exchange. The organization of the sessions allowed for seamless transitions between speakers. For example, the CUBI team presented an overview talk on Day 1, along with several subtopic presentations related to each of the biochemical intermediate upgrading pathways, that was well received by the review panel. An informal debriefing between the Catalytic Upgrading program leadership and the review panel occurred at the end of each day to share thoughts and comments on the presentations.

The review panel was asked to evaluate each project using straightforward criteria based on the three elements of (1) research approach, (2) impact, and (3) results and progress, providing scores from 1 (unsatisfactory) to 5 (outstanding). The entire session scored well on the research approach element. Projects that received high scores tended to have early feasibility and techno-economic analysis (TEA) guidance, a clear understanding of the current state-of-the-art competing catalyst/process technology, a variety of strong collaborations across ChemCatBio, results with real feeds and engineered formed catalysts, inclusion of experiments and multiscale modeling, strong project management organization, effective external collaborations that included industry, a track record of publishing articles and patents on similar topics, tools to accelerate R&D, use of bifunctional catalysis to invoke process intensity, effective use of advanced catalyst characterization tools, significant time-on-stream (TOS) testing to understand catalyst deactivation, realistic and clear risk management, demonstrated ability to pivot and be flexible based on unforeseen bottlenecks, use of high-throughput synthesis and screening methods, and an effective ongoing diversity, equity, and inclusion (DEI) plan. Projects that that scored well in the impact category had features such as effective and actionable go/no-go stage gates, publicly available tools and knowledge, a significant number of articles in high-impact catalysis journals (impact factor >10), technology licensors, viable new pathways for underutilized bio-feedstocks to hydrocarbon fuels, conference presentations, webinars, analytical method development, enablement of other projects, direct connections to DOE/Office of Energy Efficiency and Renewable Energy (EERE)/BETO goals and metrics (e.g., greenhouse gas [GHG], minimum fuel selling price [MFSP], carbon utilization, carbon efficiency), reduction of capital expenditure (CapEx) and operating expenditure (OpEx) relative to the state of the art, commercial analogs, reduction of catalyst synthesis cost, improvements to catalyst lifetime (mitigating deactivation), a considerable amount of close industry collaboration at the business unit level, and experience with novel tools and techniques. Finally, the projects that scored above average in the results category had the following qualities: technical breadth and SAF pathway diversity; attainment of key milestones; experimental and modeling/simulation results with excellent agreement; TEA optimization via experimental work; molecular class level understanding; elucidation of structure-property relationships for catalysts, intermediates, and fuels; multiscale data and analysis from active site to engineered formed catalysts; tangible and clear evidence of catalyst development acceleration; examples that demonstrate the elucidation of selectivity, stability, and deactivation mechanisms; introduction of novel tools and methods for catalyst synthesis and characterization; and tangible, actionable DEI outcomes.

STRATEGY

Goal Alignment

The mission and goals of the Catalytic Upgrading portfolio are well aligned with those set at the BETO, EERE, and DOE level. Specifically, two of the three proposed 2030 BETO goals were clearly targeted in this cycle:

- Support scale-up of SAFs and other biofuels with >70% GHG emissions reduction.
- Enable 10+ renewable chemicals and materials with >70% GHG emissions reduction.

There was also clear alignment and support for other initiatives and goals as outlined in the SAF Grand Challenge, U.S. Blueprint for Decarbonization, Inflation Reduction Act, and Multi-Year Program Plan (MYPP). The mission is highly aligned with the MYPP decarbonization objectives, where there is a clear shift away from specific biofuel molecules, blend compositions, and corresponding pathways. There is a focus on climate process technology that can reduce carbon emissions. The Catalytic Upgrading thrust toward using more engineered catalysts across the portfolio aligns with the MYPP goal to demonstrate four integrated biorefineries by 2030 with SAF capability. Several of the Catalytic Upgrading projects address the goals of decarbonizing the chemical industry and using waste streams to further decarbonization efforts. In terms of the latter, the benefits to disadvantaged communities must be realized and measured. With respect to the Catalytic Upgrading portfolio, this objective commences with the DEI activities, which were available to most projects. A high degree of R&D acceleration will be required to meet many of these aforementioned goals and objectives, which have deadlines less than a decade away. The Catalytic Upgrading portfolio goals are well defined, with a flexible mission and clear technical targets that are being implemented through a very successful consortium-based research program. This is why the goals of the program focus on acceleration of the catalyst design cycle, improvement of catalyst performance, process intensification via catalyst surface engineering, and production of high-value chemical byproducts through selective catalytic processes. These activities support future commercialization and technology transfer milestones. It should be noted that all of the goals, objectives, and targets were covered by the Catalytic Upgrading portfolio management using a variety of methods: peer reviewer training presentation, plenary lecture, and the session introduction/background presentation.

Stakeholder Impact

Most of the projects reviewed in this cycle adequately addressed the 2021 peer reviewer commentary and recommendations, which also seemed to have impacted the goal development for the session—in particular, (1) the need for high-value coproducts and chemicals, (2) bolstered effort on catalyst deactivation, and (3) the use of engineered forms of catalysts (e.g., extrudates, pellets). The 2030 BETO goals of developing processes to produce renewable chemicals and scale up align well with this stakeholder input. In particular, ChemCatBio has shown considerable success with industry stakeholder engagement via industry advisory board (IAB) meetings, work within cooperative research and development agreements (CRADAs), and support across multiple directed funding awards (DFAs). These industry interactions continue to influence the language and objectives within FOAs and national lab calls. The technology licensing activities in collaboration with key industrial partners demonstrate that the work done in ChemCatBio is being noticed and leveraged appropriately. Due to the tight presentation schedule and agenda during the Peer Review, it is difficult to see how the Catalytic Upgrading program participants interact with other BETO programs. For example, the Catalytic Upgrading team should consider including an update on these kinds of activities as part of the introduction presentation given on the first day of the session. Topics like the collaboration between ChemCatBio (CUBI) and the Bioprocessing Separations Consortium (SepCon) would be an example of the cross-consortia interactions that could be highlighted in such a discussion. BETO also has an opportunity to engage airline original equipment manufacturers (OEMs) at a deeper level, as well as wholesale fuel blenders and manufacturers for SAF. The IAB composition should reflect this new strategic direction.

Funding for Major Gaps

Overall, the review panel was in consensus that no major, unfunded technical gaps were identified across the Catalytic Upgrading portfolio. The program supports the most critical technologies using various funding mechanisms properly. Certain projects remain below desired carbon efficiencies and GHG reduction levels, but these projects are tied to other factors (renewable hydrogen) and have strong research trajectories within the budgeting limits to close these gaps. The gaps in the technologies available to achieve the MYPP objectives must be identified further and built out to pivot the technology area quickly. For instance, ChemCatBio has done an excellent job of isolating the key mechanistic events contributing to deactivation on several classes of catalysts. There is still more research to be conducted in the area of active site stability and selectivity, as well as liquid-phase catalysis. Although these aren’t major technical gaps, there is an opportunity to bolster the funding resources on these topics. Many of these same gaps exist for the new SAF-focused pathways as well. From a nontechnical standpoint, there was a lack of consistency in DEI reporting and efforts across the projects. The review panel understands that this initiative is still new and evolving. The deliberate high-level planning and recent hiring of DEI professionals in this area is a positive step forward. The review panel looks forward to seeing the results of the implementation phase by the next review with the expectation of being on par with ChemCatBio technical efforts in terms of focus and quality. The technology area managers and coordinators are actively involved in managing the projects and are keenly aware of the limiting factors, gaps, and de-bottlenecking efforts that need to be resolved in order to achieve success.

Funding Relevance

In this review cycle, there were 16 projects funded: 15 from ChemCatBio and one from a university awardee. The ChemCatBio projects were awarded through the AOP funding vehicle, which is appropriate given the high degree of interlaboratory collaboration and support across the consortium. Obviously, the Catalytic Upgrading program managers will continue to attempt to balance the funding sources across the portfolio in the future, but this cycle happened to be more heavily skewed toward ChemCatBio work. The one university-led project came from a Fiscal Year (FY) 2018 FOA: BioEnergy Engineering for Products Synthesis, which seemed to be appropriate and adequate funding based on the solid results presented. The data hub and catalyst deactivation projects have the potential to contribute even more to the Catalytic Upgrading program if they receive more funding. However, it is understandable that the program must be very careful to distribute the funds across a variety of projects in the most effective way. The management team has indeed done an impressive job of trying to keep this financial balance. With the push toward SAF, there may be an opportunity to partner with ASTM International and provide support through the DFA funding vehicle for novel pathways. As the project portfolio evolves to the next cycle, the review panel would like the Catalytic Upgrading team to consider including projects that address other chemical driving forces beyond thermochemical, such as electrochemical, photochemical, and hybrid approaches. For example, organic electrosynthesis has made significant strides in technology readiness over the past decade. The Catalytic Upgrading team should monitor and leverage opportunities to connect these advances to the catalysis and engineering expertise across the portfolio. DFA projects might provide one such outlet to pursue these topics without significant risk to the core areas. It is recommended that the DFA funding vehicle be continued. This funding strategy successfully connected industry projects to the enabling technologies across ChemCatBio.

STRATEGY IMPLEMENTATION AND PROGRESS

Support for Catalytic Upgrading Strategy

The overall aligned BETO and Catalytic Upgrading strategy centers on catalyst development, specifically (1) improvements in selectivity, (2) determination of impurity impact, (3) elucidation of deactivation mechanisms, and (4) early use of engineered catalyst forms in the material development cycle. The program is funding an excellent range of projects that are very closely tied to the BETO and program strategic direction mentioned above, especially across ChemCatBio. For instance, all of the enabling projects (e.g., ACSC, CCPC, Deactivation) have tasks that tie into one or more of the catalyst development strategic elements mentioned above. ChemCatBio is central to the catalytic upgrading component of the BETO portfolio. The effort melds catalysis and applied engineering in a unique way, allowing for intermediate technology readiness level (TRL) process technology integration to happen. It is clear that ChemCatBio plays a critical role in accelerating catalyst and process development associated with bioenergy-derived conversions. The continued push toward the study of engineered and more industrially relevant catalyst formulations is justified given the evolving nature of ChemCatBio along the catalyst development cycle. This strategic direction helps to accelerate catalytic process technology development and deployment, especially the experimental testing component required to scale up design. There also appears to be significant collaboration between the national labs and universities across the portfolio, which could be critical in fulfilling DOE’s commitment to workforce development and DEI.

Leading-Edge Industrial Catalysis

As far as decarbonization is concerned, many of the projects have found themselves on the leading edge by developing industrially relevant catalytic materials capable of converting oxygenates, such as alcohols, to jet-range hydrocarbons for SAF blending. Additionally, at the leading edge appear liquid-phase catalytic transformations for key intermediates, such as the promising work of the CUBI team, as well as electrochemical transformations, like the work in collaboration with a leading carbon transformation startup company. Other notable work with industrial partners can be considered leading edge because their deliverables could have a significant impact on the first-generation bioethanol industry. These projects show their potential to be scaled up and commercialized into industrial-scale processes. The catalyst and process technologies used in these projects are on the leading edge considering their potential to be industrialized. If successful, these projects will most likely meet the BETO goals concerning SAFs and GHG emission reduction. Other evidence of many projects in the Catalytic Upgrading portfolio being on the leading edge relates to the quality of the partnerships and the level of industrial participation. Collaboration across ChemCatBio consortia with industrial partners—such as the data hub project's engagement of a leading multinational computing corporation along with the numerous projects that enlist catalyst OEMs as scale-up partners—drives technology development and transition. It is clear that many of the projects in this area are indeed leading the field, creating benchmarks and serving as repositories for relevant process technology. The DFA projects are great examples of how the ChemCatBio teams are adapting and maturing their research for industry applications by quickly incorporating new results into their business partners' workflows. The general record of publications and intellectual property (IP) generated across the portfolio of projects is strong (140 papers and 29 patents), with a significant percentage appearing in high-impact, high-visibility journals that ensure dissemination of new knowledge to the broader catalysis community. This level of scientific productivity as an aggregate metric is just another indicator of the leading-edge contributions from the Catalytic Upgrading program. For example, ChemCatBio continues to shed light on the research premise that C-C bond formation via oligomerization in the vapor phase or carbonyl coupling chemistry in the vapor and/or liquid phase will be increasingly important in order to upgrade the biogenic carbon routes sponsored through BETO. One DFA project clearly demonstrated how additive manufacturing can offer a novel and unique set of potential opportunities within the areas of reactor design, process intensity, and material synthesis. The Catalytic Upgrading team is encouraged to look for new ways to leverage these advances, particularly in the areas of catalyst synthesis and performance testing. For example, the strong additive manufacturing expertise at ORNL could be leveraged and partnered with the strong material synthesis and characterization acumen of the ACSC and funded under ChemCatBio.

Catalytic Upgrading Portfolio Viability

The targets in the Catalytic Upgrading program seem quite achievable and fit well within previous MYPP elements. The BioEnergy Engineering for Products Synthesis FOA responded to the final strategic goal related to decarbonization by using waste streams. In general, projects tend to be near or exceed GHG targets at or before go/no-go deadlines. The Catalytic Upgrading Technology Area has been very deliberate on the strategy to enable higher TRL and focus on decarbonization with a product emphasis on SAF. This appears to be very aligned with the overall DOE/EERE/BETO direction. In general, this review cycle dealt with all pathways to SAF focused on understanding catalyst stability, deactivation, and progressing the TRL (>2 or 3). In previous cycles, there was ample discussion dedicated to MFSP estimates for every project. Here, the TEA project consolidated all of this information, and more emphasis was placed on catalyst development activities. The state-of-technology (SOT) TEA estimate for the CFP route had the modeled SAF MFSP at less than $3 per gallon gasoline equivalent (GGE), which is well on par with petroleum-based commercial Jet A. In the same way, single-step syngas conversion to SAF also gave a preliminary MFSP of $2.61/GGE. These were significant results, because many novel SAF routes can be as much as 2–3 times higher in MFSP than the commercial baseline. The Catalytic Upgrading portfolio's focus on accelerating catalyst development was apparent, as less emphasis was placed on formulation discovery and more was placed on the art of engineering robust, stable industrial materials with respect to process synthesis and product design. This was exemplified in the meso- and reactor-scale work of the CCPC on (1) engineering catalyst modeling using X-ray reconstruction tools, (2) coking kinetic modeling for CFP regeneration cycles, and (3) reaction network modeling for the ethanol to jet route. It should be noted that most presentations included backup materials that included "responses to previous reviewer comments" and addressed any previous concerns of relevance.

Catalytic Upgrading Portfolio Management

The review panel was given an opportunity to discuss the Catalytic Upgrading portfolio management approach in more detail during the debriefing sessions after each day of presentations. The Catalytic Upgrading program's overall success is a reflection of the active, engaged management style of leadership, who have stayed fully committed to the critical success factors and use their expertise across the portfolio to assist in closing technical gaps where possible. Effective industry engagement, along with continuous, actionable program cycle-to-cycle improvement based on recommendations and feedback, have proven to be credible success factors in many projects. Both the Catalytic Upgrading and ChemCatBio management teams have made a concerted effort to respond to the concerns raised in prior review cycles, and the consortium continues to evolve based on changing BETO directives. The consortium has continued to foster industry collaborations, the majority of which are successful endeavors that have positively impacted all the companies involved as well as the ChemCatBio. There are other examples of successful projects linked to the Catalytic Upgrading/ChemCatBio management style and oversight: (1) the three DFA projects completed in 2022, (2) the industry-led CRADAs, and (3) the C2 upgrading work.

RECOMMENDATIONS

Based on the comments and conclusions discussed above in this summary report, the 2023 review panel submits the following recommendations:

1. ***Portfolio Balance and Budget:*** For the next program cycle, the Catalytic Upgrading team should consider diversifying and rebalancing the project portfolio funding among AOP, FOA, and DFA, but not from a budget neutrality standpoint. It is recommended that additional funding be pursued in parallel with this endeavor. The current $32-million budget should be increased by a factor of two to deal with the acceleration needed for decarbonization, especially when most climate technology development starts with catalyst and material development. A strategic cross-office partnership with the Office of Clean Energy Demonstrations—maybe even publishing joint AOP calls and FOAs—could be effective here.

2. ***Renewable Chemicals and Coproducts:*** Prioritization on high-margin chemicals continues to be a promising and refreshing direction for the office from both a scale feasibility and de-risking standpoint. This trajectory should be sustained with additional TEA optimization iterations guiding the process feasibility options. Furthermore, coproduct development continues to be a space where the Catalytic Upgrading team has even more opportunity. One approach could be to look at higher-risk feedstocks and/or investigate alternative energy inputs to drive selectivity to new products. The goal is not to place too much risk on the portfolio, so just a single project investigating this at a lower TRL could suffice here.

3. ***DEI Reporting:*** There appears to be a lack of consistency in how DEI and environmental justice (EJ) efforts are reported across the projects. It is recommended that a common reporting format with a more prescribed granularity be considered here. This will be critical for evaluating the impact in this area. The leadership on DEI and EJ has been genuine, deliberate, and tangible. Although dedicated professionals have been hired as resources to help guide the cohort in DEI, it is increasingly important that each scientist, engineer, technician, operator, and manager can connect their work to some type of benefit to the community.

4. ***Artificial Intelligence (AI):*** At this point, it is unclear how AI technology will impact the catalyst manufacturing, bioenergy, chemical processing, hydrocarbon processing, and biochemical industries of the future, but its presence as a tool utilized daily by professional scientists and engineers around the globe is imminent. It is highly recommended that the Catalytic Upgrading team make room in the portfolio for this disruptive technology by coordinating, monitoring, and partnering with other programs across DOE that are already positioned to take advantage of these next-level algorithms. The development of technologies such as digital twins; fully automated, large-scale, high-throughput catalyst discovery processes; and detailed, machine-learning (ML)-based process design and development may eventually factor into the scale-up activities required for bioenergy processes. The Catalytic Upgrading team should be prepared for this seismic shift in workstreams, as most process design activities begin with catalyst development. This work could be led by the CCPC, and it is strongly recommended that funding levels increase for that consortium within ChemCatBio.

CATALYTIC UPGRADING PROGRAMMATIC RESPONSE

INTRODUCTION

The Conversion R&D Program would like to thank the five Catalytic Upgrading session reviewers for their time and effort in reviewing the 16 projects presented in this session. The time and effort contributed by each reviewer to review the projects before the meeting, attend the meeting, provide their insight, and prepare their review is greatly appreciated. Their substantial contribution made this Peer Review meeting a success.

The review panel recognized the high quality of the presentations and was largely impressed with the ability of the presenters to answer their concerns with added context. The panel was particularly impressed with the research approach of the projects, scoring this criterion highly in every project. The high-scoring projects were noted to have strong collaborations across ChemCatBio and with industry, to involve real feeds and engineered catalysts, and to have flexibility in the face of unforeseen bottlenecks. In addition to direct improvements in process performance, projects with high scores for the impact criterion displayed effective and actionable go/no-go gates and released knowledge and tools to the public through scientific articles, presentations, and patents. The final formal criterion, results and progress, was found in high-scoring projects with wide technical breadth that attained their key milestones. Special mention was made of aspects that demonstrated good understanding of the factors that affect process performance, including agreement between experimental work and modeling and elucidation of catalyst structure-property relationships. Tangible and actionable outcomes were characteristic of high impact in this year's new criterion, DEI.

BETO was gratified to see that the reviewers noted that the Catalytic Upgrading mission is well aligned with BETO's 2023 goals to support scale-up of biofuels with greater than 70% GHG emissions reduction, and to enable 10+ renewable chemicals and materials with greater than 70% GHG emissions reduction. The use of engineered catalysts was also identified as a strength of the Catalytic Upgrading activity, specifically of ChemCatBio.

The reviewers suggested that BETO consider projects that use electrochemical, photochemical, and hybrid approaches in addition to the existing portfolio of thermochemical processes, noting that these technologies have made strides in recent years. BETO has an interest in these technologies and is currently supporting the electrochemical process by creating a $10-million CO_2 utilization consortium that focuses mainly on CO_2 conversion through electrocatalysis. BETO has been following the advances in the field of organic electrosynthesis closely and is poised to support this technology when its maturity allows it to support BETO's goals and mission.

Recommendation 1: Portfolio Balance and Budget

The role catalysis can play in the effort toward decarbonization is well understood by BETO. Catalytic Upgrading of bio-based feedstocks can provide sustainable, economically viable sources of biofuels and other valuable bio-based chemicals. In the last 2 years, the BETO portfolio has included several projects focused on catalytic upgrading and is continuing to develop in this area. Communication with other offices, including the Office of Clean Energy Demonstrations, remains strong, although the difference in the TRL of the portfolio of each program creates barriers to increased cooperation.

BETO's strategy includes utilizing a variety of funding strategies, including AOPs, FOAs, and DFAs. In the last 2 years, the BETO portfolio has included several projects focused on catalytic upgrading and is continuing to develop in this area.

Although the session included 16 catalysis projects, other projects involving catalysis were assigned for review to other sessions and were therefore not reviewed in this session. As an example, many of the electrocatalysis and renewable natural gas catalytic upgrading projects from the FY 2021 FOA were presented/reviewed in the CO_2 Utilization and Organic Waste Conversion sessions, respectively.

Recommendation 2: Renewable Chemicals and Coproducts

BETO continues to pursue multiple pathways to the upgrading of biomass to fuel and chemicals. Our main emphasis remains upgrading biomass to fuel. This includes the major focus of the Catalytic Upgrading portfolio, generation of SAF. However—and as noted in the recently published MYPP—chemicals/products can also make significant contributions to decarbonization goals, and BETO has goals to contribute to a minimum of 10 molecules and at least 1 million metric tons per year of carbon-dioxide-equivalent reductions. BETO recognizes that several conversion and feedstock processes can be de-risked by recognizing the economic potential of valuable chemical coproducts or intermediates that can be upgraded to fuel or higher-value chemicals. Favorable routes will be shaped by TEA and life cycle analysis (LCA) results. The Catalytic Upgrading portfolio includes two recently completed directed funding opportunity (DFO) projects (Sironix and Visolis), which are continuing to develop processes to produce bio-based chemicals, and we expect that the formation of high-value chemicals will remain a project de-risking strategy for future BETO projects.

Recommendation 3: DEI Reporting

DEI and EJ efforts are a priority in the BETO portfolio. Although DEI reporting has only been recently implemented and is still developing, it is expected that with experience in reporting, it will become more expressive and more effective in its goal of improving the BETO portfolio. As projects include more diversity, BETO expects that reporting of DEI will naturally improve. Although assistance from DEI and EJ experts continues to be important, project officers are becoming increasingly adept at both developing DEI and EJ plans and reporting on their performance. To aid in this, BETO has distributed new guidance ahead of this year's lab call with suggestions on milestones and activities that can support these DEI and EJ priorities. These include suggestions that can be incorporated into research plans at any TRL and opportunities to collaborate with broader DEI initiatives.

Recommendation 4: AI

BETO agrees that AI can be a very powerful tool in designing catalysts. However, AI is still in its infancy for catalysis design. It can be a strong tool for determining reaction mechanisms and predicting and tweaking the best catalysts. This type of work is currently facilitated by the Office of Science. Even so, BETO is always looking for opportunities to improve catalyst design using new techniques, including AI and related computational techniques, that can provide a clear and reasonable path to serve office goals. At present, BETO's major focus is scaling up the catalysts developed in the last 3+ years. Consequently, most of the work will be on developing the engineered form of the catalysts.

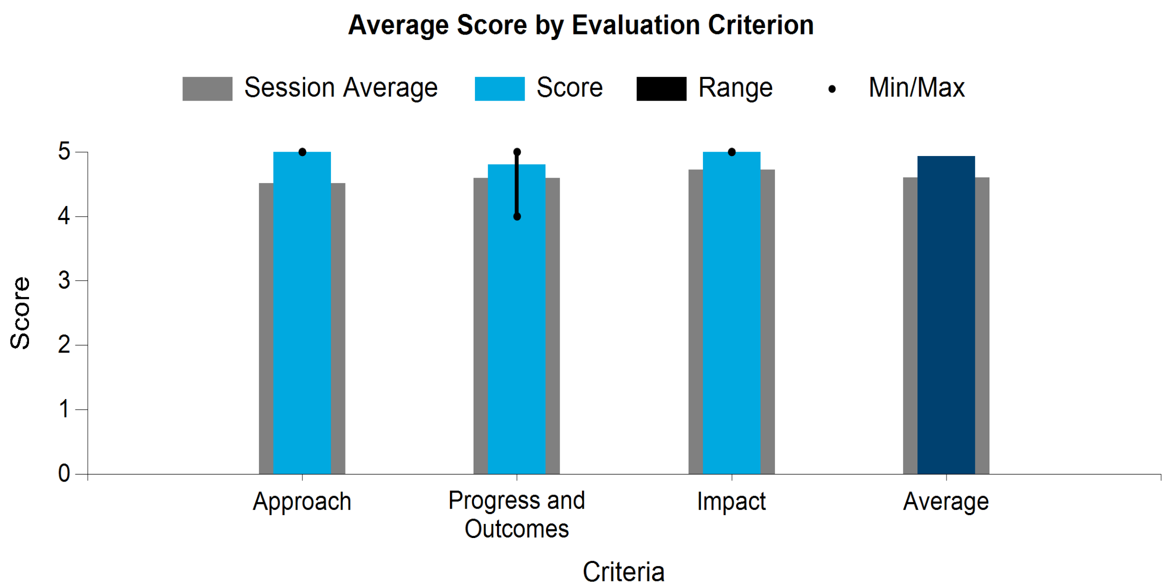
CHEMCATBIO LEAD TEAM SUPPORT

National Renewable Energy Laboratory

PROJECT DESCRIPTION

Work Breakdown Structure (WBS):	2.6.3.500
Presenter(s):	Dan Ruddy
Project Start Date:	10/01/2017
Planned Project End Date:	09/30/2025
Total Funding:	$96,000.00

The goal of this project is to enable ChemCatBio to achieve its mission by providing leadership for the consortium, managing the R&D portfolio and DEI activities, serving as single point of contact for potential partners, pursuing action items identified from the IAB, and developing strategic initiatives to position the consortium for the future. In addition to the director, deputy director, and steering committee, the consortium structure includes an IAB, DEI lead team, and all contributing researchers. To facilitate internal coordination, this project organizes recurring ChemCatBio all-hands meetings (every 2 weeks) and biannual face-to-face meetings, coordinates quarterly IAB meetings, and engages with other consortia. Further, to enable effective management of ChemCatBio and to facilitate engagement from all national labs, critical steering committee roles were enacted in FY 2018 that included face-to-face meeting coordinators, conference outreach, industry outreach, website point of contact, capabilities point of contact, consortia liaisons (Feedstock-Conversion Interface Consortium [FCIC], SepCon), data hub point of contact, and media development. By the end of FY 2025, this project will support ChemCatBio as a central hub of knowledge, methods, and tools for catalytic bioenergy applications by (1) supporting the development of the Catalyst Design Engine; (2) publishing our biannual newsletter, *The Accelerator*; (3) maintaining and expanding the capabilities of the CatCost™ and Catalyst Property Database (CPD) tools; (4) developing and sharing content on our website about mitigation of catalyst deactivation and advancements in state-of-the-art technology for conversion pathways; and (5) leading consortium-level DEI activities.



COMMENTS

- I am extremely impressed with the dual-cycle approach for the catalyst and process development cycle. This research team has very cleverly designed a process that allows for the concurrent development of novel catalytic materials (synthesis/computational modeling) and processes (TEA and LCA/process scaling), with bench testing being the link between them. This scheme allows for concurrent work, tied by validation, and no doubt considerably accelerates the overall catalyst and process development timeline. Additionally, the approach to considering both fuel and chemical products that can be produced by the various feedstock and process combinations allows for the creation of a wealth of data that can be leveraged as market factors change. The management plan is being well implemented, with more than 130 researchers participating in the projects across eight national labs. This plan has resulted in an impressive amount of scientific impact, demonstrated by the number of publications/citations, patents, follow-on projects, and community resources it has spawned. This could only have been accomplished if there was substantial communication between the researchers and the 14 members of the IAB. In addition, this project is clearly a leader in the DEI space, having established the diversity, equity, inclusion, and accessibility (DEIA) lead team, along with an impressive collection of resources and trainings.

- First, I have to give kudos to the DEIA efforts of this project, which have already created a wealth of resources. Ditto for community engagement, which is a closely tied effort. I really appreciate the effort to lead on best practices in heterogeneous catalysis to improve the rigor and reproducibility of the work published in the literature. Next, the demonstration of a fourfold time reduction for the development of a next-generation catalyst while substantially improving its performance is an unprecedented feat that demonstrates the advantage of leveraging the work across this exceptional, collaborative research team. The work with Pyran and Catalyxx exemplifies this process. It is clear that risk mitigation strategies have been successfully implemented to address the issue of catalyst deactivation.

- This project has demonstrated significant impact at a bargain price—in the development time of next-generation catalysts, in the development of the chemical property database, in the work with Pyran and Catalyxx, in the DEIA efforts and community engagement, and in addressing critical challenges to the production of SAF.

- ChemCatBio is central to the catalytic upgrading component of the BETO portfolio. The intro presentation did an excellent job of framing and justifying the role of ChemCatBio in accelerating the catalyst and process development associated with bioenergy-derived conversions. The effort melds catalysis and applied engineering in a very suitable way to connect intermediate-TRL technologies to a transition phase to industrial adoption. The continued push toward study of engineered and more industrially relevant catalyst formulations is justified given the evolving nature of ChemCatBio. The current focus areas align with the BETO goals laid out in the SAF Grand Challenge and also represent an effort to evolve, as a multicycle center should, by building on the most impactful portions of prior work while also incorporating new elements with an opportunity to enhance the effort. The shift to carbon efficiency and GHG reduction metrics is appropriate given the cross-agency mandate to focus primarily on decarbonization efforts. The consortium has the difficult task of threading the needle of having suitable diversity in approaches and inputs while not being spread too thin across exploratory topics. By and large, the effort succeeds. There is diversity in the inputs considered across the portfolio—ranging from biogas to syngas to ethanol and others—but there is still a general focus on pathways and intermediates to SAF that link the efforts. Collaboration across BETO consortia and with industrial partners is important for an effort that sits in this technology development and transition arena. The ChemCatBio partnerships with IBM and other catalyst partners is a highlight in this space, along with many individual examples in the specific projects. Cross-consortia interactions exist—such as CUBI with SepCon—but these could be highlighted more effectively in future cycles. Project management is strong, with well-established mechanisms at this point for in-person and virtual meetings. The established synergies of the enabling capabilities continue to allow the individual projects to thrive. This reviewer sees no major gaps across the ChemCatBio portfolio. One could perhaps note that certain projects remain below desired carbon efficiencies and GHG reduction levels, but these projects are tied to other factors (renewable hydrogen) and do have potential trajectories to achieve the desired metrics. Some points for consideration as ChemCatBio evolves in the next cycle:

- ChemCatBio should begin to consider how nonthermal inputs (electro, photo) may begin to impact the conversion landscape. For example, organic electrosynthesis has made significant strides in the past decade, which will begin to transition to the technology space. The consortium should monitor these advances and leverage opportunities to connect these advances to the catalysis and engineering expertise in ChemCatBio. DFA projects may provide one such outlet to pursue these or related areas outside of core AOPs, expanding expertise without significant risk to core areas.
- The additive manufacturing space also offers some similar, evolving opportunities; consortium members are aware of many of these. I would encourage the group to continue to look for opportunities to exploit advances in this space to enhance catalyst synthesis and performance testing when possible.
- Although coproduct integration was included in strategic instances, I believe this is a space where ChemCatBio can continue to look for ways to be more ambitious. This may result from examining higher-risk feedstocks in a single project, alternative energy inputs to drive selectivity to new products, etc. I do not see this as a theme that must be incorporated in the majority of projects, but ChemCatBio should look to take advantage of opportunities when they present themselves in this space.
- In general, there was a lack of consistency in DEI reporting and efforts across the projects. The reviewer understands that this space is evolving and does note that the high-level planning and recent hiring in this space is a positive. I look forward to seeing the plans for this area and the activities implemented by the next review, with the expectation that they will be on par with all other ChemCatBio efforts. I do feel strongly that establishing a common reporting format for the presentations and regular reporting for individual projects will be critical to assessing the impact in this area in subsequent review cycles.

- Progress: BETO directions. Particular highlights from this reviewer's perspective include the CCPC multiscale modeling efforts, the general transition of the portfolio to robust and non-platinum-group-metal (non-PGM) catalysts, and the ability of all projects to access alkane fractions suitable for fuel testing. In general, projects tend to be near or exceeding GHG targets at or before go/no-go dates. It is clear that ChemCatBio has made a concerted effort to respond to concerns raised in prior review cycles, and that the consortium continues to evolve based on BETO directives. The consortium has continued to foster industry collaborations, the majority of which are successful endeavors that have impact for the company and ChemCatBio. The consortium-wide accelerator generates strategic ChemCatBio-wide partnerships in the areas of computing, catalyst evolution, and benchmarking, which have the potential to make a significant impact on the effort. For general management, the nine presentations at national and international venues are a good mechanism to spread the word about the activities and impact of ChemCatBio. The technical briefs are another vehicle to interact with the community in a separate but important way. I do appreciate the attempt to engage the catalysis community across all levels—from students (with the American Chemical Society travel award) all the way to the researcher level. One additional comment: Given the strong connection to industry partners, ChemCatBio could consider expanding its outreach efforts by having panels/webinars on career development topics that involve both ChemCatBio PIs and the partners. One could imagine a range of topics (general experiences and tips for startups, large industry, etc.; how to prepare for pursuing jobs in those areas; how technology transfer really works) that a spectrum of researchers would be interested in. I recognize that this isn't a highest-priority activity, but it is one that could have an outsized impact on increasing awareness about ChemCatBio.
- The ChemCatBio project continues to be the hub for catalysis research in BETO by serving as an umbrella resource provider and setting the vision for the entire consortium. The approach to accelerating bioenergy catalysis that can also assist in decarbonization is quite timely and relevant. The team should

continue to work out the decarbonization emphasis and harmonize it into the overall strategy, so it doesn't appear to be a parallel effort. The partnerships, collaborations, and industrial advisors are strong and are enabling the consortium to make an impressive impact in both peer-reviewed literature and published IP.

- The revised ChemCatBio mission, which is focused on rapid decarbonization, is a very timely and appropriate R&D direction that is responsive to public, private, and governmental interests. At the core of this mission is advanced catalytic material development for utilization pathways in support of the sustainable circular economy. There is an opportunity for the existing petroleum-rich carbon inventory to be addressed to a certain extent with new projects similar to hydrotreating coprocessing to assist the energy transition for existing refineries. ChemCatBio really tries to reduce the threshold of technical barriers throughout the project. It seems like there could be an opportunity to accelerate the process synthesis step in the applied process model. ChemCatBio has put together a DEI team to deal with the issues across the entire consortium, and they bring up a DEI conversation at every meeting. This is quite progressive. ChemCatBio should be benchmarked quantitatively in comparison to other consortia within BETO and DOE, using a set of metrics to evaluate the state of the art in scientific consortia.

- The ChemCatBio team has clearly shown how the project can accelerate catalyst development to the point of technology licensing. The team has learned from the C1 catalyst development cycle and has applied those learnings to the ethanol conversion development cycle. This is a successful technical story. The progress with modifying the effectiveness factor was a great contribution. The team developed an understanding of the effect of trace inorganic salts on the environment and the intrinsic activity of the active site for several catalyst systems to the level of publishing several articles. More insight should be provided into understanding inorganic precursor type and various synthesis methods. Several tools are available for public use, including the CPD and Catalyst Cost Model. The Option 3 approach to developing engineered forms for catalysts will benefit the entire catalyst community. The IAB should be leveraged even further to assist in this work. Any preliminary look at the effectiveness of the predictive ML methods being considered for the data hub catalyst development initiatives would be interesting. The team is working with a large, respected information/data science OEM to develop in-house tools with ML and AI. This is very promising.

- The impact that ChemCatBio has on the bioenergy community is undeniable; this impact includes several open-source web-based catalysis tools, webinars, technology licenses, patents, awards, and papers. The consortium has been very successful. The team should continue to educate the broader community about their contributions and resources.

- ChemCatBio provides a general framework for accelerating catalyst design, synthesis, understanding, and deployment. The team is focusing on the SAF Grand Challenge and provides versatile toolkits to accelerate the catalyst development and deployment for this challenge.

- The team focuses on developing tools to lower the barriers between the different development stages of catalysts. They integrate synthesis, computation, and testing to accelerate the research on catalyst science. They also integrate TEA/LCA, scaling, and testing for applying developed catalysts in real applications. These two integrations provide a unique way to connect foundational research and applied engineering. The team also conducted efforts in developing databases and tools to embrace new technologies such as ML and AI. It would be more beneficial if the team could leverage the potential of ML, AI, data-driven discovery, and high-throughput experiments.

- The team has achieved significant progress in catalyst development and deployment to help address DOE's SAF Grand Challenge. The related research has resulted in >100 publications, three technology licenses, six software packages, 29 patents, and 12 awards with industrial partners. These numbers illustrate the progress of the team. Meanwhile, the team also provides three tools, 11 webinars, and two technical briefs. These materials show the commitment of the team to engaging the community. It would be more beneficial if the team would work more actively to reach out to the communities that are not likely involved in BETO research, like some underserved communities. The team also shows a commitment to DEI efforts.

- The ChemCatBio lead team illustrates its impact by integrating a wide variety of efforts that aim to accelerate the development and deployment of catalysts for the SAF Grand Challenge. They build a robust mechanism to connect foundational catalyst research with applied engineering of catalysts to scale up processes. This connection will be critical to enhancing the commercialization of the catalysts developed under the Catalytic Upgrading program.

- ChemCatBio's platform is driving the advancement of catalytic processes to convert biomass into sustainable fuel and other value-added products, utilizing effective accelerating and prioritizing strategies. Collaborations among national laboratories, academia, and industry have led to impressive accomplishments in fundamental science, computation, economics, and engineering. These high-quality works not only promote sustainable energy, but also benefit the community by expanding knowledge and education and upholding high ethical standards. ChemCatBio's approach is outstanding, as it integrates aspects from both the micro level (atomic-level fundamental understanding) and macro level (market), which is not easily achieved by academia or industry alone. Such an approach requires significant project management skills. The ChemCatBio management team and PIs have done an excellent job ensuring that almost all projects progress on track at a fast pace, achieving a fourfold reduction in catalyst development time. The focus on deactivation, catalyst engineering, TEA, and kinetics, in addition to fundamental understanding, is a step in the right direction for scaling up. The successful approach has resulted in impressive outcomes, including high-quality publications, licenses, patents, and tools (e.g., CatCost), with numerous potential opportunities for industry to explore. The inclusion of DEI in project plans is also impressive. BETO sets a standard for others to follow to create a more equitable society, fostering innovation and creativity. It is encouraging to see that DEI is incorporated into every project, and I look forward to seeing its implementation. Overall, the impact of these projects will last for generations, as renewable energy utilization and decarbonization are essential for our only home, the Earth. The contributions from these projects also promote DEI and community engagement, which are equally important.

- Some suggestions for most projects under this program:

    - Providing a more detailed breakdown of budget allocation and timelines would enhance the reviewer's/reader's understanding of the project management. Many projects lack a breakdown of budget over the years, and some do not have clearly defined milestones or timelines.

    - To garner more support from the catalysis society, consider implementing additional promotional efforts, such as exhibiting booths, sending group emails, putting on webinars, and encouraging PIs to include promotional slides during their conference presentations.

    - To generate greater interest from industry stakeholders and increase their investment intentions, various uncertainties should be considered in TEA, instead of just presenting the best-case scenario.

    - To broaden the DEI efforts, consider creating visually appealing promotional materials with scientific content related to SAF. These materials can be developed for younger audiences, including middle and high school students, to promote and support STEM education.

PI RESPONSE TO REVIEWER COMMENTS

- The lead team appreciates the many positive comments about our consortium-level goals, approach, DEIA strategy, progress to date, and future plan. We appreciate the note on highlighting cross-consortia interactions in this overview presentation. We will take this action through FY 2025, especially highlighting existing partnerships with SepCon, FCIC, and the CO_2 Reduction and Upgrading for e-Fuels Consortium, as well as partnerships currently in development with other BETO consortia. Related, we appreciate the comment to stay abreast of advancements in electrochemical and photochemical conversion technologies, as they relate to both fuels and value-added chemical production that could intersect with the catalytic technologies being developed in ChemCatBio. Our collaboration with the CO_2 consortium is one way we currently do this. Participation at conferences is another way our PIs engage with emerging technologies. We will consider a consortium-level milestone by FY 2025 that assesses these topics and how they could integrate with ChemCatBio research. Similarly, advancements in additive manufacturing have been integrated into the ChemCatBio R&D portfolio through our newly added engineered catalyst development effort within the ACSC project. This effort builds on the preliminary success highlighted in one of our DFO presentations, where millifluidic reactors were designed and printed to enable high-throughput nanoparticle catalyst synthesis. We are seeking to expand additive manufacturing to access improved catalyst architectures in the ACSC project, but this effort may require additional funding support. Related to the engineered catalyst effort, our IAB has been instrumental in guiding our initial efforts. One of our IAB members from a major catalyst production company worked with our team to prepare and present an overview of industry standard practices for us. This presentation will be the basis of our next webinar, expected in the summer of 2023. We appreciate the note to standardize the reporting structure from our DEIA activities. As noted, this is a new effort for us, and it is still evolving, but the note is well taken and will be put into our immediate consortium-level plan that will be finalized by the end of this FY. The comment to participate in career development efforts is an excellent suggestion. Although noted as a lower priority within our consortium, it is an excellent complementary effort that will be implemented in our workforce development plan.

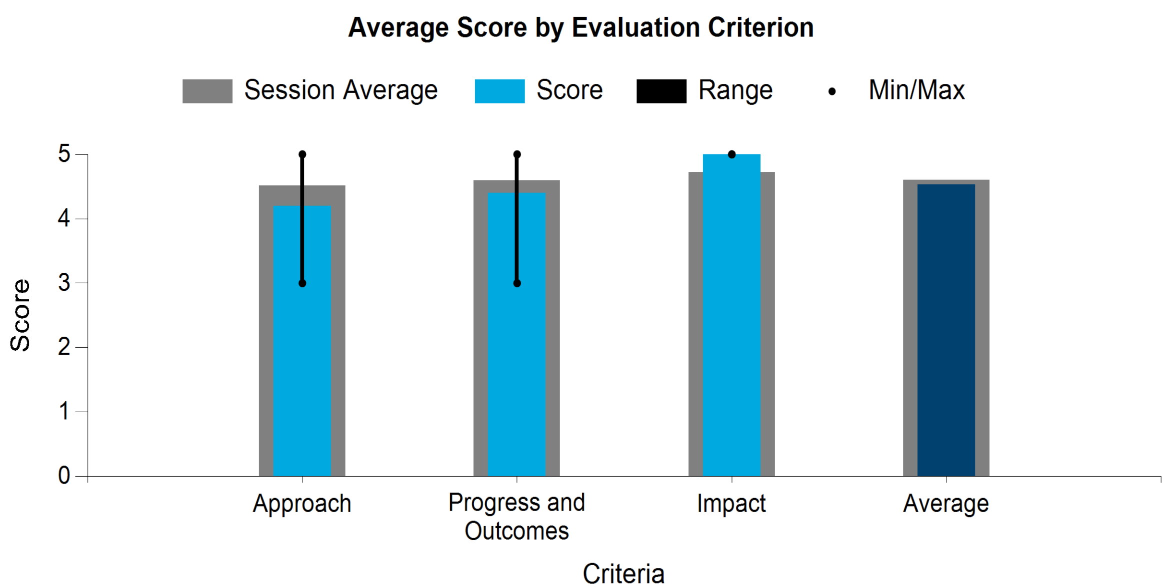
THERMOCHEMICAL PLATFORM ANALYSIS

National Renewable Energy Laboratory

WBS:	2.1.0.302
Presenter(s):	Abhijit Dutta
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$784,128.00

PROJECT DESCRIPTION

This Thermochemical Platform Analysis project serves to guide biomass thermocatalytic conversion research for significant-volume feedstocks toward higher-impact outcomes through TEA. Outputs include the quantification of associated sustainability metrics and environmental benefits. The key contribution of this project is to analyze ongoing and new research, as well as to explore new and hybrid conversion pathways for biomass and wastes, thus playing a key role in providing actionable metrics for BETO-funded research efforts. Our analyses have shown that thermocatalytic biofuels pathways, with associated coproducts (providing significant sustainability and cost benefits), have the potential to enable the achievement of BETO's ambitious SAF production goals while meeting GHG and cost reduction targets. Although the analysis of new conversion approaches will continue to be a primary thrust of this project, our efforts also emphasize industrial engagement and support partnership projects toward the successful deployment of biorefineries by leveraging our analysis knowledge and tools. Another key area of analysis under this project is facilitating integration with existing facilities and infrastructure, including at petroleum refineries, to enable lower production costs of liquid transportation fuels.



COMMENTS

- This project is focused on TEA and evaluation of process sustainability. It ties to the other projects in this area through experimental results from the other projects. The feedback loop from this project to the experimental work is through information on industrial context and risk. This process seems well poised to make sure that the laboratory developments stay relevant to things that can be industrially scaled. There is strong evidence of interlaboratory collaboration. The new approach, focused more on TEA and LCA, is the next logical step after the SOT report created in previous years. The focus on SAFs makes sense in light of the administration's goals; however, I believe that it would be a misstep to completely stop work on sustainable gasoline- and diesel-type fuels. The diversity, equity, and inclusion plan (DEIP) includes publication with a minority-serving institution (MSI), which seems like a reasonable goal, but I would like to see more substantive involvement—perhaps summer internships for the MSI students.

- The progress since the last review is significant. Although the 2022 CFP pilot scale did not proceed, that is actually a resounding success for the project based on the risk assessment. I can only imagine how much money and effort was saved by this analysis. The resultant analysis provides a framework for future consideration of the process as factors and technology change. Additionally, this analysis identifies the sources of risk, GHG emissions, production costs, etc.

- The project demonstrates clear impact—saving resources (money and time) by not scaling up the CFP process—and is able to narrow the expansive parameter space for investigation, as well as quantify the influence of various aspects of the project on risk, emissions, production costs, and other factors. In addition, this work and the learnings from it can be leveraged across multiple projects and processes.

- This project enables TEA and modeling across projects. It is critical to have this type of effort integrated with consortium projects to have any hope of transitioning technology as desired to the appropriate scale for industrial implementation and to ensure that the right perspectives on cost and other target metrics are represented accurately. It is clear that the project collaborators cover the needed areas and tap the spectrum of approaches necessary for success. At the same time, the presentation provided nice context for the entire analysis portfolio and where this piece fits within the broader national lab complex. The feedback loop established with experts in feedstocks, catalyst formulation, and fuels is absolutely essential to ensure that the right parameters and assumptions go into the modeling efforts. The use of modeling tools (Aspen Plus for process models; Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies [GREET] for LCA) is appropriate and standard practice for the field. The organization regarding the tiering of analyses performed is logical and prioritized to ensure that time-consuming, highest-level analyses are only performed as needed. The priorities of the modeling group are important to understand. In particular, the goals of SAF/heavy fuels and repurposing of existing refinery infrastructure are logical and aligned with current BETO directions. Moreover, the shift away from SOT reports and the focus on SAF, de-risking elements of technology, etc. seem to further align with current BETO priorities. The DEI plans are manageable and contain a quantifiable metric that seems potentially achievable and a realistic goal to work toward. As an enabling project, specific metrics are less critical than the examples presented in how the interaction with other upgrading activities has been influenced by the modeling analysis. It is clear that thermochemical platform analysis helps inform milestones and whether technologies should move forward as is or have some type of remaining barrier. The examples presented in the presentation highlighted the flexibility in the group in the types of analysis performed on a diverse range of systems. The ability to incorporate SAF specs into process models seems very important. Examples that both support changes in systems—from multistep to single-step processes, reactor engineering modifications, etc.—and flag critical issues were presented. Both types of scenarios highlight the key role thermochemical platform analysis plays. Moreover, the group consistently demonstrated the need for holistic considerations of system design and the need for this to occur with a group of experts outside those performing the upgrading technology directly. In general, I was also impressed with the diversity of feedback provided to the modeling team and how it was integrated into the effort. Broadly, the mechanisms—engaged experts, consultants, or advisors, as topics warrant—seem appropriate to ensure that expert opinions on rapidly changing areas are incorporated to develop the best analyses possible. The shift in this year and subsequent years to focus on SAF seems clearly aligned with ChemCatBio and broader BETO directions. Two broader comments:
    - In general, sensitivity/error analyses could be better represented to a larger degree in most project presentations. I have no doubt about the technical capabilities of the team; it was just a consistent issue that arose.

  - Some deeper general discussion of the differences/challenges in analysis involving powder versus scaled/engineered catalysts would be desirable, as this matches the direction of BETO and most of the projects. Specifically, I am thinking of ways to integrate transition into these formulations in early-stage analysis to serve as a tool to flag potential issues as early in the development process as possible.

- Impact: The pervasive impact thermochemical platform analysis has within the broader upgrading portfolio is clear. When projects attempt to radically change processing (moving to different reactors, different catalysts, etc.), risk assessments, emissions reduction estimates, coproduct values, etc. are needed to evaluate viability. Thermochemical platform analysis is a vital part of these efforts given the metric-driven nature of the projects—identifying the key choke points/bottlenecks beyond the science limitations is absolutely essential. Additionally, thermochemical platform analysis has broader impacts for the community, demonstrating the power of economic modeling to drive potential demonstration and ultimate deployment. The group has been productive in terms of outputs to the community, with several publications in a variety of field-relevant journals. I have no doubt that these reports will be viewed and picked up by the community. However, the group could look to expand presentations or perhaps participate in combined webinars with the projects they support to further articulate the value of the integrated approach and the critical need for this type of modeling within projects. Recording these presentations could provide a living reference for the community to access.

- Overall, the thermochemical platform analysis project team has made good progress since the last Peer Review, publishing several peer-reviewed articles and running meaningful targeted simulation cases, including GHG and cost/gallon impacts. The team avoided advancing pathways that were too risky and continued to drive the focus toward SAF pathways. This is a good pivot for the team, with research efforts adapting and moving forward in this new direction. The continued interest in working with existing refinery partners is a solid strategy, and the team should continue to drive those relationships.

- The current state of the art is to first compile experimental lab-scale and/or pilot-scale data from the published literature and/or in-house-run campaigns, then build process simulation models. The team should clarify which process scale is being used in these calculations, as well as the quality of the data. The two routes being considered are (1) catalytic pyrolysis product upgrading to SAF and (2) syngas to SAF via C4 oligomerization. Here, a simple statement of the design basis being considered should be provided for both routes. Any process design feasibility endeavor requires input from key stakeholders, in particular experimentalists. This approach appears to be no different, but incorporates additional LCA constraints and feedback from Argonne National Laboratory, as well as feedstock cost/specs from Idaho National Laboratory, which provides an opportunity for innovative solutions to optimize the TEA for SAF production. The risks were not clearly identified as compiled by the industry expert panels. It appears that hydrotreating coprocessing is one de-risking strategy. The beneficial cyclic and isoalkane components in CFP to SAF should be separated before any coprocessing step. The schedule and plan were not adequately addressed. The DEIP needs measurable goals and an action plan to track progress, as well as a community impact assessment from an EJ perspective.

- The team demonstrated the importance of TEA for making multiscale go/no-go decisions by placing the CFP on the shelf. The key specific risks associated with hydrogen introduction that halted the progress of the work should be highlighted here as a lesson learned for the BETO community; these can serve as a seed for future R&D efforts. It appears that downstream processing of coproducts was challenging and that finding a commercial partner for the coprocessing option was a hindrance.

- The thermal analysis team deploys developed tools such as Aspen Plus, Excel, and GREET to provide TEA/LCA to the other projects. This is an enabling project. They calculate TEA/LCA based on the data provided by the other projects and provide feedback about the projects based on their calculations. It would be more beneficial if the calculations involved uncertainty quantification because some data used in the TEA/LCA are based on estimation or present certain variations. It could provide more guidance if the TEA/LCA showed the confidence level in some way.

- The team provides three types of analysis: quick-turnaround analysis, more detailed analysis, and detailed design report. The three types of analysis cover the wide spectrum of needs of different projects well.

- The team also shows a commitment to DEI. They plan to develop work with identified MSI(s) to help develop the capacity of TEA/LCA. It is not very clear which MSIs the team is referring to or what stage the plan is at now. It would also be more beneficial if they could work with DOE/BETO to develop a plan for how to involve these MSIs in the project after they develop such capacity.

- The project presented impressive progress since the 2021 review. They conducted TEA for fixed-bed *ex situ* CFP and concluded the key closeout. This example indeed shows the importance of TEA/LCA in guiding the direction of an applied R&D project. They also presented progress in refinery integration and SAF.

- The impact of this enabling project is illustrated in driving the transition to a one-step hydrocarbon process. Because of its impactful role, it would be beneficial to evaluate how the uncertainty in the data may influence the TEA/LCA outcomes.

- The TEA project plays a critical role in assessing and guiding all projects toward commercialization. The outcomes generated from this project are of great interest to industry stakeholders and the general public. The project management approach, which allocates more resources to core projects and promotes close collaboration, is in the right direction, and a great effort has been put into this project.

- The TEA has covered almost all aspects of scaling up, including modeling, economic calculations, and LCA, showing good project management. It is impressive to see that almost all projects under this program have undergone TEA, and transparent data sharing among different projects has made the process more efficient, avoiding duplicated efforts. Partnerships with KBR and collecting feedback from industry reviewers have helped improve accuracy and reliability.

- The impact of this work is significant, as the estimations generated by the TEA work have not only been used by BETO to accelerate processes, but also serve as trustworthy references for researchers worldwide. However, carrying out TEA at a relatively early stage of the development cycle for a catalytic process is still challenging. In many cases, TOS longer than 1,000 hours is still considered short term for the industry, not to mention that most of these processes used model feedstocks.

- To avoid misleading information, TEA should consider adding uncertainties and should have a confidence factor or risk factor. This way, when comparing the likelihood of commercialization, entities can consider not only the projected cost, but also the challenges. For instance, TEA carried out at an earlier stage should have a lower confidence factor. If a process requires any modification of the current setup, the risk should be much more significant, regardless of the magnitude of the modification. Recent challenges facing the industry, including supply chain issues, labor shortages, and uncertainties in policy, should be part of the risk factor.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for your review highlighting the strengths of this project, as well as the constructive feedback regarding areas where changes can be made. Our responses below focus on how we plan to address or may already have considered addressing the suggestions made by the reviewers.

- Comment: I believe that it would be a misstep to completely stop work on sustainable gasoline- and diesel-type fuels.

- Response: While SAF will be our focus based on BETO priorities, we cannot achieve 100% selectivity to SAF in most processes. In our analysis, the remainder of the products will continue to be evaluated for use as blendstocks for other fuels, including gasoline and diesel.
- Comment: The DEIP includes publication with an MSI, which seems like a reasonable goal, but I would like to see more substantive involvement—perhaps summer internships for the MSI students.
- Response: Our plan, as shown in the diagram on Slides 14 and 24, includes internships. We did not present further specifics within the presentation because we are still in discussions with faculty to finalize the process.
- Comment: In general, sensitivity/error analyses could be better represented to a larger degree in most project presentations. I have no doubt about the technical capabilities of the team; it was just a consistent issue that arose.
- Response: We prominently highlight sensitivity analysis presented in tornado plots with most of our analysis. However, an example of a tornado plot was not included in this year's presentation. We will include an example with a tornado plot/sensitivity analysis in future Peer Review presentations to convey this emphasis in our work.
- Comment: Some deeper general discussion of the differences/challenges in analysis involving powder versus scaled/engineered catalysts would be desirable, as this matches the direction of BETO and most of the projects.
- Response: Thank you for this comment. We will work with the experimental research teams to incorporate this aspect in the future.
- Comment: The group could look to expand presentations or perhaps participate in combined webinars with the projects they support to further articulate the value of the integrated approach and the critical need for this type of modeling within projects. Recording these presentations could provide a living reference for the community to access.
- Response: Thank you for this comment. We will organize webinars/presentations with corresponding experimental teams in the future to address this.
- Comment: The current state of the art is to first compile experimental lab-scale and/or pilot-scale data from the published literature and/or in-house-run campaigns, then build process simulation models. The team should clarify which process scale is being used in these calculations, as well as the quality of the data.
- Response: We do highlight the source of our data (usually bench scale) in our analysis and highlight the assumption that we are scaling up bench-scale performance to a 2,000-dry-metric-tonne/day (typical) biomass conversion plant in our conceptual process models. The consistent plant scale helps to compare different conversion pathways on the basis of economic and carbon intensity performance. We will continue to highlight this aspect and assumption in our future work.
- Comment: The two routes being considered are (1) catalytic pyrolysis product upgrading to SAF and (2) syngas to SAF via C4 oligomerization. Here, a simple statement of the design basis being considered should be provided for both routes.
- Response: We tried to convey the design basis for (1) CFP oil upgrading to SAF on Slide 19, and (2) syngas to SAF with the simple diagram on the bottom left of Slide 23. In addition, process basis details are provided for each pathway in the "Additional Slides" section. We will continue to convey this via statements, tabulated summaries, and associated graphics in future presentations.

- Comment: The risks were not clearly identified as compiled by the industry expert panels. It appears that hydrotreating coprocessing is one de-risking strategy. The beneficial cyclic and isoalkane components in CFP to SAF should be separated before any coprocessing step. The schedule and plan were not adequately addressed.
- Response: This aspect is covered under the experimental research project and its associated milestones (linked to this project). Multiple experimental approaches are being assessed within the constraints of available resources. This analysis project uses experimental data (and engineering judgement, where appropriate) to assess the feasibility and impact of the various approaches. We have two joint milestones during this FY (in Q3 and Q4) documented in our AOP to explore various hydroprocessing strategies, and we will continue to include milestones in future years.
- Comment: The entire status of the current SAF material's ability to meet the entire spec should be provided, so the gaps are understood.
- Response: We will continue to emphasize this aspect, building on current efforts described on Slide 20 (right-hand side). The experimental team has included multiple property measurements covering major properties associated with SAF specifications. This TEA project is working with experimental projects to include property prediction capabilities within our process models.
- Comment: It would be more beneficial if the calculations involved uncertainty quantification because some data used in the TEA/LCA are based on estimation or present certain variations. It could provide more guidance if the TEA/LCAs showed the confidence level in some way.
- Response: We will continue to include and highlight uncertainties in our analysis and include this aspect wherever appropriate. For example, we highlighted key uncertainties/sensitivity analysis in the Executive Summary (page viii) of the 2020 *ex situ* catalytic fast pyrolysis SOT report (www.nrel.gov/docs/fy21osti/80291.pdf).
- Comment: It is not very clear which MSIs the team is referring to or what stage the plan is at now. It would also be more beneficial if they could work with DOE/BETO to develop a plan for how to involve these MSIs in the project after they develop such capacity.
- Response: We started our 3-year project cycle in October 2022, with a plan to execute the DEIP presented within the 3-year period. We did not publicly disclose the names of the MSIs with whom we are in ongoing discussions. Because our plans have not been finalized, mentioning names of MSIs would be premature. We plan to have deep and ongoing relationships that will include continued involvement of MSI partners in the future. We will publicly disclose the MSI(s) once we have agreements in place.
- Comment: The impact of this enabling project is illustrated in driving the transition to a one-step hydrocarbon process. Because of its impactful role, it would be beneficial to evaluate how the uncertainty in the data may influence the TEA/LCA outcomes.
- Response: Thank you for the comment. We will include sensitivity to uncertainties in forthcoming work and associated publications.
- Comment: In many cases, TOS >1,000 hours is still considered short term for the industry, not to mention that most of these processes used model feedstocks. To avoid misleading information, TEA should consider adding uncertainties and have a confidence factor or risk factor. This way, when comparing the likelihood of commercialization, entities can consider not only the projected cost, but also the challenges. For instance, TEA carried out at an earlier stage should have a lower confidence factor.
- Response: As mentioned above (in response to another comment), we will continue to include uncertainties, risks, and associated sensitivity analysis in our work.

- Comment: Recent challenges facing the industry, including supply chain issues, labor shortages, and uncertainties in policy, should be part of the risk factor.
- Response: While some of the cost escalations associated with the problems mentioned above get captured through our cost indices, we will include additional associated risk factors if these problems persist and require further highlighting beyond the cost escalations estimated by the indices.

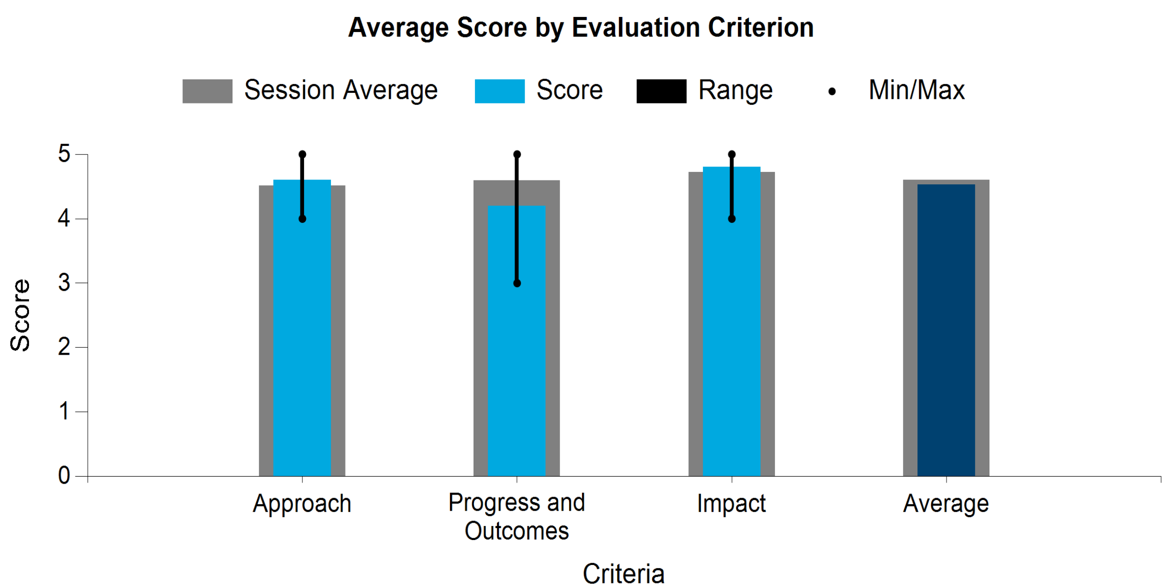
UPGRADING OF C1 BUILDING BLOCKS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.1.305
Presenter(s):	Dan Ruddy
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$2,190,407.00

This project is developing the centerpiece technology for an integrated biorefinery concept based on the conversion of renewable and waste sources of C1 intermediates (e.g., syngas, CO_2, methanol) to produce SAF with improved carbon efficiency and reduced CapEx and OpEx compared to traditional gas-to-liquids processes. Advanced syngas upgrading technologies are critical for the successful commercialization of fuel production at a scale relevant for biomass gasification. Research tasks within this project leverage complementary catalyst and process design for (1) the direct conversion of CO_2-rich syngas (15%–20% CO_2 in syngas) to achieve high carbon yields of C4+ hydrocarbons in a single reactor, termed STH, and (2) the subsequent conversion of these hydrocarbons to SAF. Research progress is compared to the Mobil olefins to gasoline and distillate process and the three-step STH process through dimethyl ether previously explored in this project. This research effort supports BETO and ChemCatBio goals, using catalyst and process R&D as a foundation to address risks for process integration and commercialization. The STH pathway generates high-quality SAF precursors with a >70% reduction in GHG emissions compared to petroleum jet fuel. This project assesses catalyst/process durability using real bio-/waste-derived feedstocks in practical reactor configurations with engineered catalyst forms.



COMMENTS

- The goal of this project is to use the conversion of renewable and waste sources of C1 intermediates to produce SAF with improved carbon efficiency and reduced CapEx and OpEx compared to traditional processes.
- The goals of this project are sound, and the scattershot approach (simultaneously investigating multiple processes) makes sense at lower TRLs for similar process conditions. There are clearly identified research challenges: carbon efficiency improvement, regeneration procedures for multicomponent catalyst mixtures, extended operating times, and improved yields. The task management is integrated

across the entire ChemCatBio Consortium and incorporates technical capabilities, TEA, and DEI (at least in theory, as the DEI milestones are not yet determined for this project).

- Progress seems steady, but at a slower rate than projected by modeling. Carbon efficiency is at ~30% (which was the FY 2021 go/no-go) and hasn't progressed further. A regeneration protocol has been established, but the process has not yet been run. Plots lack error analysis, making it difficult to assess the results.

- The impact is strong. This project was about to accomplish technology transfer with the bioenergy industry (research license with Enerkem), as well as publish ~10 papers in top journals and generate patents.

- Approach: The project is focused on C1 feeds (syngas, methanol inputs) to intermediates to ultimately generate SAF. The approach is differentiated from the state of the art in syngas conversion with a focus on funneling chemical intermediates through a methanol/dimethyl ether pathway. A stacked-bed reactor allowed for direct STH conversion. The isoalkane products can then be dehydrocoupled to access SAF. The catalyst design and engineering components that work in concert and reinforce one another to enhance improvements to the overall technology are a highlight of the work. The overarching topics of the project—involving tandem reactions, process intensification, etc.—are recurring themes in the upgrading activities and are viewed as needed strategies to transition the reactions to viable technologies. The presentation could have focused more on the specific management of this project. I don't have any doubts regarding this aspect, but it was not as strong a component relative to other topics. This could be a function of the lead PI having discussed management in the overarching ChemCatBio presentation. I would note that PI Bhan is a great partner for kinetic studies of zeolite catalysts. A forward-looking comment: Given the ability to perform tandem thermal catalysis, in the longer term, this (and other projects) may well consider alternative energy inputs (electro/photo processes) in cases where the economics can work. Given the modularity of these systems, one could imagine funneling intermediates from a thermal reaction to an electro-driven process (as one example). While this is certainly not always feasible, the expanding area of electro-organic synthesis suggests that longer-term opportunities may exist in this space. Perhaps this is more suited for coproduct generation, but it is something worth long-term consideration. The move to more realistic feedstocks is notable and necessary. One question not clear from the presentation is: How does biomass syngas differ from the current feedstock mixtures? Will this be expected to create significant issues? For this reviewer, it was not clear from the slides or presentation. The collaboration with one of the other BETO consortia to obtain the biomass-derived syngas is notable and another sign of cross-talk among consortia. Progress: The outcomes extend beyond prior studies in related HOG systems to include the impact of CO_2 feed stream ratios, optimum regen protocols, catalyst synthesis treatment studies to achieve optimum conversion, and prolonged TOS. These logical investigations generate data to inform further catalyst evolution for a system that can be regenerated to full activity and is robust over long time periods. Progress on all fronts seems promising, as the isoalkane coupling is at the proof-of-concept stage with a similar mixed-bed system. Other goals, such as further studying deactivation and movement toward engineered catalysts, are in line with other efforts in ChemCatBio and can leverage the existing capabilities within the consortium. The goal of moving to biomass-derived syngas to SAF in an integrated process seems at least possible from the results gained from the project to date. Impact: Ten publications is good to strong productivity, with many in high-impact-factor journals (impact factor >10). One patent and numerous presentations by project PIs also suggest successful IP development and dissemination of results to the broader catalysis community. If progress toward goals and milestones continues, the target of direct syngas to SAF, or at least precursors to fuels, will be achievable. Economic modeling suggests that these pathways are certainly worth exploring in an intermediate-TRL effort such as this. Given the group's success with the HOG technology, I'm convinced that the evolved technology developed in this project will have significant impact and will be seen as a commercialization opportunity for the sustainable fuel industry.

- Overall, this project team has made significant progress since the last Peer Review, giving new prospective routes for C1 conversion with high selectivity to either HOG or SAF. They have created materials that have tunable properties and have begun a good approach toward scale-up by establishing good internal and external partnerships.

- This team did an excellent job of centering the audience on the bottlenecks associated with the state of the art in syngas to SAF technology, namely product selectivity, number of unit operations (complexity), aromatics, and monomers as desired products. The team is focused on reducing complexity by converting syngas-type feedstocks directly (in one step) into SAF. This lab-scale work has been published in peer-reviewed journal articles and has resulted in a patent highlighting stacked-bed reactor configurations. The relative size of the stacked packed beds should be disclosed due to CapEx implications. The dual R&D cycle strategy for designing novel catalysts continues to be a progressive approach in process technology development. The technical approach here is to investigate the impact of CO_2 composition in the feed on the STH process to make paraffins; then, once those paraffins are created, they are dehydrogenated and coupled in a single step to SAF-range hydrocarbons. This is a new process-intense route for the team and seems quite interesting. Some key risks were identified: loss of carbon to CO_2, catalyst regeneration challenges, and TOS product yields. Mitigation actions should be provided for each of these. DEIP or EJ strategy was not necessarily provided in detail. It appears that the ChemCatBio DEI resources are being leveraged here.

- The review of the 2021 baseline was good for the audience. The R&D focus from that review dealt with increasing carbon efficiency and reducing CapEx via process intensity. The decrease in CO_2 selectivity and the C efficiency of 32%, as predicted by conceptual modeling, should be validated experimentally. In 2021, the team was able to publish the types of aromatic coke species on the surface of Cu/BEA and develop a regen schedule that enabled complete recovery for over 2 days. This was a major accomplishment. The team also figured out that forming extrudates from the powder catalyst versus depositing copper after the material-forming event results in higher C4 selectivity. The team should report the size of the extrudates and the tube diameters used in the analysis. Some of the work involved collaborations with the thermochemical platform analysis and ACSC projects, leveraging modeling and characterization tools. The direct STH route should still include MFSP estimates (using literature) for the dehydro-oligomerization step, even though the work is at the proof-of-concept stage.

- The C1 team has had major successes and impact in both the journal and patent literature, with a Technology Commercialization Fund being awarded for commercialization of the HOG technology with Enerkem. This technology can also be tweaked to make some kerosene-range molecules. Further, SAF-range material has been demonstrated in the laboratory, passing several key jet fuel specs.

- The project aims to develop engineered Cu/BEA catalysts for direct CO_2-rich STH. They also initiated the effort for isoalkane dehydrocoupling. This project creates a unique approach that integrates foundational catalyst research and applied catalyst engineering. Currently, more information flows from the foundational catalyst research to the applied engineering. It would be more beneficial if applied engineering could generate critical questions that drive the foundational research.

- The project has met its goals and is ready for the next stage of R&D. It would be more beneficial if the team had articulated their R&D plan in the event that the engineered catalysts cannot meet the setup goals, or which avenue they plan to pursue to optimize the engineered catalysts.

- The team already showed that their product could satisfy the criteria for being SAF. The success of this project will help fulfill DOE's SAF Grand Challenge if their R&D activities lead to the scaling up of the process.

- The overall outcome of this project is highly encouraging, as the team has successfully converted CO_2-rich syngas into precursors for SAF using the STH method developed through insights gained from

HOG. The dual-cycle approach, which integrates fundamental studies with the development of engineering catalysts, has proven to be very effective, allowing the team to keep pace with the fuel market shift. The past 2 years of work have yielded impressive results, producing a cost-effective catalytic process with great promise. Moving forward, the team may consider studying reaction kinetics, mass and heat transfer, and the impact of catalyst forming on performance for scaling up.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the many positive reviewer comments about this project's goal, approach, progress, and future plan. We appreciate the note about including error bars and error analysis in our data. Detailed error analysis was omitted here for clarity of the plots, but it is included in our published reports and papers. To the question about how biomass syngas differs from other feedstocks, this project partnered with the FCIC in 2018 and 2019 to assess variability in syngas composition and yield from five top biomass feedstocks. That report was published in the journal *Applied Energy* in 2019. The H_2:CO ratio from biomass is approximately 2.6, which is higher than coal-based syngas (approximately 1.0) and comparable to that produced from steam methane reforming (theoretical value of 3.0). Impurities in the biomass-derived syngas are important considerations, and there are both existing and emerging technologies to remove those impurities for downstream processing. To date, no significant issues with biomass syngas compositions have been identified that cannot be handled with cleanup technologies. This project works closely with the FCIC to stay at the forefront of syngas cleanup technologies to reduce that risk to commercialization for the catalysts and processes being developed in this project. The comment to include MFSP estimates for the early-stage dehydrocoupling step is appreciated, and this is a priority in working with the Thermochemical Analysis project through FY 2025. Relatedly, we appreciate the comment to highlight how information from the applied engineering cycle flows back through catalyst testing. Perhaps not emphasized in the presentation was the direction from the Thermochemical Analysis team to test the STH catalyst system at higher temperatures and pressures (up to 300°C and 5 MPa) than originally targeted (220°C and 0.75–1 MPa) to improve product separation efficiency. This will be emphasized in future reports. The comment to study kinetics, mass transfer, and the effect of catalyst forming was not highlighted in this presentation due to time constraints, but this is an ongoing effort with the CCPC team, with a deliverable at the end of FY 2023 and continuing work through FY 2025. Lastly, with respect to DEIA and EJ, this project supports the overarching ChemCatBio goals, and one project-specific activity was participation in the development of the Justice Underpinning Science and Technology Research (JUST-R) framework, which is an approach to assessing EJ in early-stage research that was recently published in the high-impact journal *Joule*.

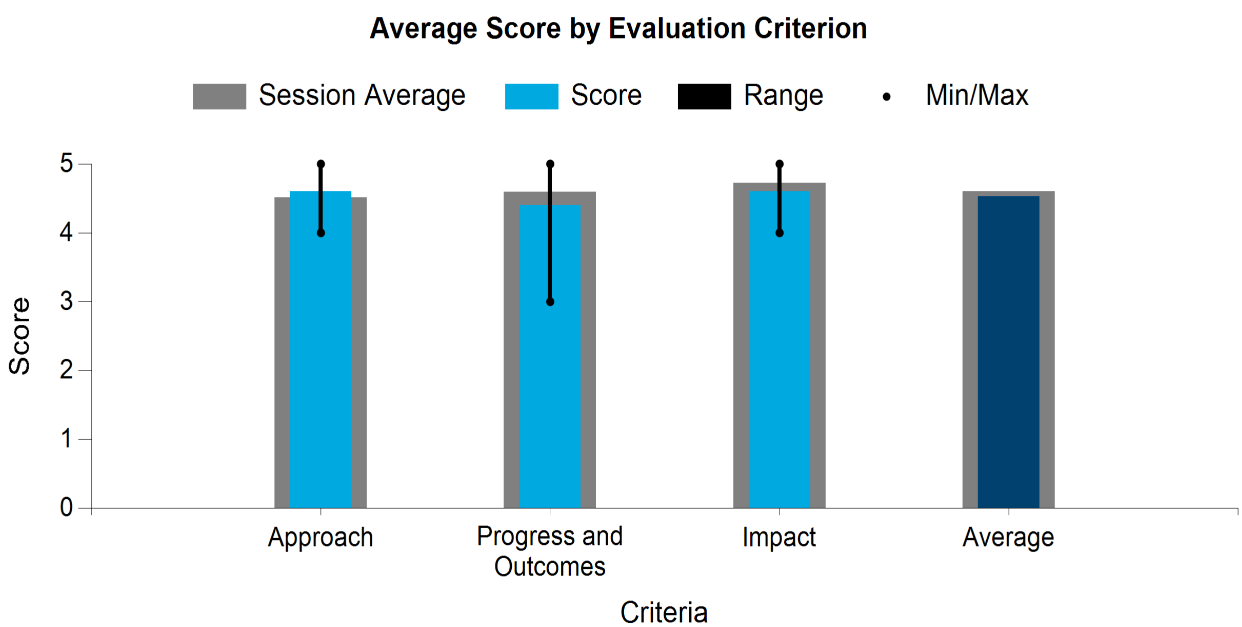
CATALYTIC UPGRADING OF PYROLYSIS PRODUCTS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.1.314
Presenter(s):	Mike Griffin
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,950,000.00

The objective of this project is to advance the state-of-the-art technology for a CFP + hydrotreating process to produce SAF and other biogenic products. Our approach focuses on performing integrated experiments using realistic biomass feedstocks and non-noble metal technical catalyst formulations. CFP is performed in an *ex situ* configuration using a fluidized-bed reactor without co-fed hydrogen. Research advancements over the past 2 years include establishing benchmark yield structures and compositional data for each step of the biomass-to-SAF process, demonstrating the ability to produce a cycloalkane-rich SAF product that meets key ASTM 4054 guidelines, generating benchmark characterization data for technical catalyst formulations with an emphasis on determining the unique composition and combustion properties of biogenic coke, and establishing bio-oil critical material attributes (CMAs) to mitigate the risk of plugging during downstream hydroprocessing. Other impacts from this project include generation of broadly enabling scientific knowledge (12 publications and 12 presentations since 2021), engagement with industry partners (Johnson Matthey, ExxonMobil, and Phillips 66), and identification of a promising pathway to market that addresses emerging demands for biogenic refinery feedstocks.



COMMENTS

- This project aims to develop a pathway to convert woody biomass into SAF and other products by CFP and hydrotreating.
    - Made a pivot in 2021 from fixed-bed to fluidized-bed fast pyrolysis in response to challenges. The jury is still out on hydrotreating, and fraction testing looks good so far but is still an unknown.

- Integrated experimental campaigns with supporting analysis of continuous CFP experiments without co-fed H_2 or noble metal catalysts.
- High O_2 content is difficult to deal with—perhaps coprocessing or a refinery pilot scale?
- Use of realistic biomass feedstocks.
- Technical catalyst formulations.
- Strong management plan for tasks and communication leads to strong collaboration, as shown by publications.
- Included DEI, though weak room for improvement here.
- Progress:
  - Good industrial engagement.
  - Good carbon balances (though no error analysis in tables on Slides 8 and 9).
  - No error analysis on plots.
  - Benchmark yield structures and compositional data for three levels of CFP upgrading.
  - Evaluation of SAF properties.
  - Identification of opportunities to produce a cycloalkane-rich product stream.
  - Characterization data for technical zeolite catalysts.
  - Bio-oil CMAs to mitigate the risk of plugging during downstream hydroprocessing.
  - Defined pathway to market via existing refineries and integration points, which leverages existing infrastructure and workforce.
  - Twelve publications, 12 presentations, two issued patents, and six patent applications.
  - Generated a spinoff project.

- This project was focused on CFP conversion of biomass to bio-oil and subsequent hydroprocessing for SAF applications. The project is commended for the pivot from fixed-bed to fluidized-bed reactors in the past cycle, in part due to the inherent challenges with that set of reactor conditions. The benefits are already evident in the switch, with the ability to perform CFP without co-fed hydrogen and to do the transformation without precious metals. Movement toward use of more realistic biomass feedstocks is another strength of the effort. The project is also involved with multiple collaborations with ChemCatBio partners (Catalyst Deactivation Mitigation for Biomass Conversion [CDM], ACSC, and CCPC). The catalyst characterization work is a particular highlight in the view of this reviewer. The strong connection with various industrial partners is also a positive. Regarding DEI efforts, most aspects seemed pretty standard, and it seems as though the project is waiting on ChemCatBio direction for significant engagement. The energy-justice-related publication is one exception and a clear indication of their efforts in this space. The planned science and experiments are well put together and seek to explore rational structure-property relationship development. Studies of inorganic dopants will certainly impact further catalyst development. The dopant probe students are a specific highlight of the work, which has identified aldehydes as a functionality to monitor in the reactions. Another key aspect of the work is the development of benchmark data for CFP in these new reactor systems, as well as catalytic data for zeolite catalysts. Given the heavy focus in other projects on related zeolitic materials, these specific studies can have an impact on studies across the whole upgrading consortium. In general, promising results from the 2021 pivot were obtained from the CFP, hydrotreating, and fraction testing. The general milestone targets seem achievable, particularly with current results demonstrating good carbon efficiencies, significant GHG reductions, and a promising ability to remove the oxygen content to below detectable limits. Other targets—involving improving catalyst durability and more modest increases in efficiency—seem attainable. The access to predominantly cycloalkane fractions was promising and somewhat unique relative other technologies in the upgrading area, which generally gave isoalkane products. The CMA experiments, designed to determine the effect of contaminants on the fuel fraction properties, were important control experiments. With this information on hand, mitigation methods to circumvent issues with reactive carbonyls in fuel fractions can be pursued. The project, with 12 publications (many in high-impact catalysis journals) and two patents (and six additional patent applications), was very productive. The energy-justice-related publication is another highlight and added dimension of impact. The existing connections with industry are another avenue through which to establish impact with proposed studies. In terms of the technology, there are several advantages to CFP, including the ability to plug and play, unlike other systems. For example, CFP allows distributed pyrolysis to stable bio-oil conversion, which can then be transported to centralized hydrotreating. This modularity is a strength of the effort and is unique relative to some other upgrading projects, which must rely primarily on economies of scale. The direct refinery repurposing connection is another strength, reducing capital costs and also potentially repurposing existing workforces. As such, it is an important technology to investigate at these intermediate TRLs, given the many potential advantages of a viable process in this area.

- The team has done a good job of using a variety of tools to develop a regenerative fluidized-bed system capable of CFP followed by upgrading to SAF. The approach is reasonable, focusing on integrating the CFP and the hydrotreating units while characterizing the CFP oil as a key intermediate. The partnerships are strong, involving major oil and gas companies, catalyst manufacturers, and industry advisors. This work will have a major impact on the industry, allowing existing operating assets of oil and gas companies to be considered for future scale-up and integration for SAF production.

- The team gave a good overview of the 2021 baseline and the research pivot to SAF via catalyst and reactor configuration major changes. The current state of the art suffers from catalyst deactivation, excess hydrogen consumption, and difficult thermal management. The comprehensive approach is to establish a process technology performance baseline, initiate a CFP oil spec sheet, characterize catalytic materials, and investigate refinery economics with strong industry advisory support/CRADAs from the oil and gas and catalyst manufacturing communities, as well as ChemCatBio engagement, which promotes new R&D opportunities. The use of sulfided hydroprocessing catalysts aligns well with existing oil and gas downstream assets. This approach limits the opportunity to develop new materials for this application to some extent. The risks associated with establishing the new baseline using fluidized-bed arrangements were not outlined with any contingency. A DEI lead was mentioned along with several activities.

- The team has made significant progress by designing, constructing, commissioning, and starting up a fluidized-bed-based CFP system. The regeneration cycle was optimized using thermogravimetric analysis/infrared spectroscopy and nuclear magnetic resonance (NMR) to characterize coke type and combustion characteristics for complete restoration of the surface area and total acidity. The team should have provided some insight into the residence times associated with the active riser section and the regeneration side. On the trickle-bed hydrotreating unit, the team should specify any sulfur co-reactants, how the temperature in the reactor is measured, and the amount of carbon going into the gas phase for hydrogen recovery. The final SAF product looks promising with the high amount of cycloalkanes. The identification of the 20 wt % oxygen as the sweet spot in the CFP feed is a good specification based on quality experimental data. The high-throughput CMA spiking experiments appear to be a reasonable approach and tool. More data science (e.g., quantity and processing) discussions were expected here.

- This project opens new opportunities for pyrolysis product upgrading pathways by focusing on the SAF commodity as the end goal. The notion of de-risking downstream hydroprocessing should be clarified relative to early-generation pyrolysis oils. The estimated MFSP and overall process carbon efficiency looks competitive relative to other routes.

- This project focuses on developing a fluidized-bed CFP process. This process utilizes a zeolite catalyst and helps remove co-fed hydrogen, which will have a significant impact on process TEA/LCA and safety.

- The project has an illustration of the production of SAF that meets the ASTM D4054 guidelines for density, viscosity, boiling point, heating value, flash point, freeze point, and volatility. They also establish three CMAs for CFP bio-oil. It would be more beneficial if the team could address how the feedstock varies based on their source and how the variation in feedstock may affect the quality of their final products or the process operating parameters. An omics analysis may be beneficial to enlist the compounds in bio-oil qualitatively or semi-quantitatively. This omics information may help develop a framework to determine the operating parameters of the process based on the feedstock.

- The project has made impressive progress toward the goal.

- The project has developed knowledge and technologies that can benefit the development of fast pyrolysis processes. If successful, this project will help achieve the SAF Grand Challenge. The R&D activities of the team have also led to the development of two other research projects focusing broadly on sustainability. The team has shown commitment to the DEI effort by initiating various activities.

- The progress of this project in producing SAF through pyrolysis of biomass is promising. The use of realistic biomass and fluidized-bed reactors is a significant step closer to achieving success. Collaborating closely with industry and adopting a multitask strategy to address challenges at various stages has helped maintain balanced progress. Over the past 2 years, substantial outcomes have been achieved, including commissioning a reaction system and conducting a relatively long deactivation study, among other scientific achievements.

- The production of SAF from pyrolysis of biomass still appears challenging due to poor miscibility, poor thermostability, and high oxygen content of pyrolysis oils. Coprocessing is a reasonable technical choice to address these challenges after pyrolysis oils have been treated. Collaborating with industry partners to leverage their existing laboratory- or pilot-plant-scale cracking units for coprocessing is recommended. Additionally, modifying the fluid catalytic cracking catalysts or developing new additives could be another approach to improving the utilization of pyrolysis oils.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their excellent feedback and appreciate the positive comments related to our project's approach, progress, and impact. As highlighted by the reviewers, research from this project has led to the development of yield structures and compositional data for an integrated biomass-to-SAF process, demonstrated the ability to produce a high-quality cycloalkane-rich SAF product, and identified CMAs for bio-oil to mitigate the risk of plugging during downstream hydroprocessing. These achievements are a result of a coordinated research effort with ChemCatBio enabling projects and industrial partners, and we would like to acknowledge our collaborators for their contributions. We also appreciate the reviewers' helpful suggestions for improvement and offer the following responses to clarify certain details and outline our plans for future work. Fluidized-bed reactor system: We are pleased to hear the support for our pivot toward utilizing a fluidized-bed reactor system. As highlighted, fluidized-bed CFP can be performed without co-fed hydrogen, utilizes non-noble metal catalysts, and provides greater flexibility in managing catalyst deactivation. It is also true that there are unique risks to this approach. Of primary concern is the comparatively low carbon efficiency of bio-oil versus fixed-bed hydrodeoxygenation. In this project, we plan to address this risk through the development of modified zeolite catalysts that increase carbon efficiency by reducing coking rates and coupling light end molecules into fuel-range products. We are also working closely with collaborating projects to identify opportunities for effective utilization of all byproduct streams (e.g., char). Another important risk is associated with catalyst deactivation, attrition, and regeneration. We are addressing this risk both within the CFP project and through collaborative research with the ChemCatBio enabling projects. This ongoing work focuses on identifying deactivation mechanisms by characterizing pre- and post-reaction catalysts (ACSC), evaluating the unique combustion kinetics of biogenic coke (CDM), and developing regeneration models for riser-type reactor systems (CCPC). Thermal stability experiments: The project team appreciates the positive feedback related to the bio-oil thermal stability experiments and agrees that this approach will provide an excellent opportunity to utilize data science and statistical analysis techniques. Currently, the application of these techniques is precluded by the limited number of experiments. However, ongoing work is focused on expanding the dataset, and we plan to utilize sensitivity analysis and multiple linear regression to identify and predict correlations between bio-oil chemical composition, physical properties, and thermal stability. The reviewers are also correct in pointing out the importance of understanding how feedstock variability impacts bio-oil properties. This represents a central goal within the FCIC, and we coordinate closely with our collaborators to support these efforts. Collectively, the development of feedstock CMAs for biomass pyrolysis (FCIC) and bio-oil CMAs for hydrotreating (this project) will provide a framework to inform quality specifications for the end-to-end process. DEI: Our project's DEIP has three main components: (1) foster an inclusive environment within the project team, (2) promote DEI through research implementation, and (3) benefit underrepresented and underserved communities. Toward these goals, we have encouraged feedback, including conducting anonymous surveys, and have adjusted our meeting structure to make it more inclusive in response to feedback received. We have also developed workshops and "DEI minutes" to raise awareness about citation bias, stereotype threat, and the model minority myth, among other topics. Additionally, members of our project team (including the PI and DEI lead) were collaborators on a recently published manuscript focused on identifying metrics and methods to incorporate energy justice concepts into early-stage research and development (doi.org/10.1016/j.joule.2023.01.007). Later, the input/output method was applied to our project specifically. We have also been fortunate to host two student interns from MSIs as part of the Student Training in Applied Research and Growth Sector STEM Core programs. While we believe these efforts represent strong steps in the right direction, we also recognize that there is room for further improvement and look forward to working across ChemCatBio to ensure that our collective research promotes an energy transition in which benefits are equitably distributed and ideas are widely sourced. Hydrotreating methods: We are happy to provide additional details about the hydrotreating experimental methods. The catalyst is presulfided *in situ* with di-tert-butyl disulfide using industrially established protocols. To maintain the catalyst in a sulfided form during hydroprocessing, hydrogen sulfide is included in the hydrogen gas at a concentration of 60 ppm. The temperature inside the bed is measured by a six-point thermocouple placed along the centerline of the reactor. Carbon losses in the exit gas represent 3%–6% of carbon in the CFP oil and comprise primarily C1–C5 hydrocarbons. Error analysis: Data quality and experimental reproducibility are priorities in our research, and we appreciate the opportunity to provide additional detail on this important point. After commissioning a new vapor-phase catalytic upgrading reactor for CFP, we successfully completed a milestone to demonstrate mass and carbon balance closures of 100% ± 5% and data reproducibility with relative standard deviation of <10% on key metrics. Typical mass and carbon balance closures for the hydrotreating system are 96% ± 2%, and the relative standard deviation on product composition is <2%.

UPGRADING OF C2 INTERMEDIATES

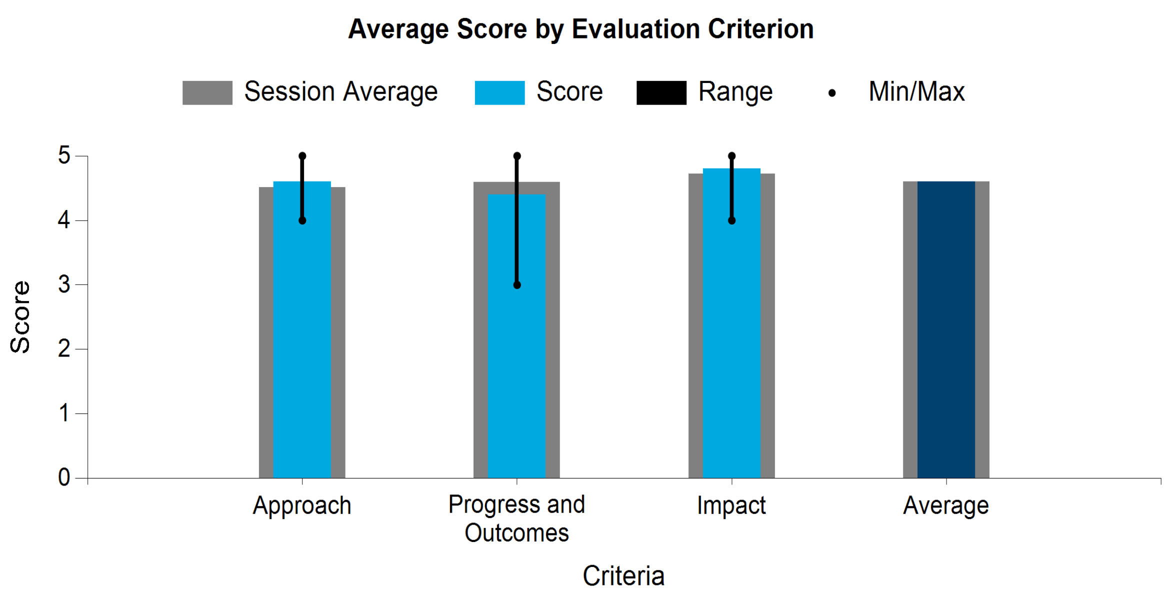
Oak Ridge National Laboratory

PROJECT DESCRIPTION

WBS:	2.3.1.100
Presenter(s):	Andrew Sutton
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2025
Total Funding:	$1,680,834.00

This project is focused on the conversion of intermediate ethanol to jet-range hydrocarbons with integrated routes to coproducts. Ethanol is an attractive feedstock for the production of fuels and chemicals, as it is already produced at commercial scale and can be produced from a variety of renewable biomass and waste sources. In addition, the ethanol "blend wall," coupled with advances in production efficiency and feedstock diversification, is expected to lead to excess ethanol at competitive prices. Initiated in FY 2017, ORNL has performed proof-of-concept and applied R&D, utilized advanced characterization tools to understand key catalytic mechanistic steps and catalyst active site structure-function relationships, and obtained experimental data using scalable fixed-bed reactors to inform models for TEA and LCA.

Efforts at ORNL have culminated in the development of a new biomass upgrading pathway for the direct conversion of ethanol to C4-rich olefins. This pathway provides a more economic route to jet-range hydrocarbons than current technology. The current state of the art for the ethanol-to-distillates process requires four catalytic steps: (1) ethanol to ethylene, (2) oligomerization of ethylene to C4-rich olefins, (3) oligomerization of C4-rich olefins to distillate-range hydrocarbons, and finally, (4) hydrotreating to saturate olefins. Producing C4-rich olefins directly from ethanol with high yield is new and impactful because the produced C4-rich olefins can be selectively oligomerized to distillate-range hydrocarbons, thus eliminating one step. This reduces capital cost requirements, while simultaneously providing energy savings realized by coupling endothermic and exothermic reactions. Further, this project is also evaluating new, promising coproduct options that hold promise in further reducing fuel production costs through the sale of value-added coproducts.



COMMENTS

- Generally, progress has been good. The project has been able to reduce the number of unit operations and demonstrate tuning of the products through catalyst use, and the technology has been licensed by the team's collaborator, Prometheus. It is very interesting to note that the use of miscanthus gets the process to be CO_2 negative. I'm interested to see more details with respect to this. Additionally, the project has demonstrated an excellent C balance of 80%, and more importantly, believes that 100% is possible with recycle. There are remaining issues that have been identified:
  - Deactivation conditions may be too mild to draw conclusions right now—more work is necessary.
  - Nitric acid use and wastewater generation are issues of concern, and should be minimized.
  - Tax credits have a disproportionately large impact on cost (2x in some cases).
- The project has already demonstrated strong commercialization potential, and there is room for further improvement.
- This project is focused on ethanol to higher olefin conversion, using a Cu/La zeolite catalyst, with the lanthanide allowing tuning of the product distribution. The flexibility to dial in distributions suitable for aviation or diesel fuels is impressive. The effort also clearly benefits from a variety of collaborations throughout ChemCatBio; these were also articulated well in the presentation. The work also presented the state of the art and challenges in the space effectively. Also, the push toward engineered catalysts is commendable and in line with evolution of most projects in the upgrading area toward more commercially relevant systems. The mechanistic and contaminant studies are first rate and hopefully provide key insights into the design of next-generation catalysts. While the current catalyst formulation seems very tolerant, I would be curious to know the effects of additional impurities—e.g., trace sulfur. The project management seems well in order and particularly synergistic with the related PNNL efforts with ethanol to olefins. There is clear delineation of projects regarding systems and approaches, meaning knowledge transfer between groups should be relatively seamless. One point for consideration: I think further comment on lanthanide availability might be in order moving forward. Although I realize that this is built into economic modeling, critical element availability and supply chain variability are something gaining scrutiny. Ability to recycle the catalyst or lanthanide might be something to comment on further in future review cycles. Milestones in the project seem to have been achieved or are on a trajectory for success. The current Cu/La catalyst has been demonstrated as scalable, able to be oxidatively regenerated, and tolerant of various feed streams of ethanol. The movement toward engineered catalysts during the next funding period is logical and aligned with most projects in the upgrading section. The versatility and tunability of the catalyst system is impressive and is something I highlight as a true differentiator of the project. The economic modeling as part of ChemCatBio informs knowledge of the system to be cost-effective (e.g., high concentrations of ethanol are required to be economically competitive) while at the same time suggesting significant GHG emission reductions with the system. Fuel testing of the mainly isoalkane products derived from the olefin coupling also appear promising. Here again, the ability to leverage collaborations with ChemCatBio members is key to the timely completion of the fuel analysis and understanding of the system economics. The impact to the broader community is clear, based on the four publications (many in high-impact catalysis-centric journals) and three patents during the prior funding cycle. The licensed tech is also an indication of successful technology development and commercialization potential. If the goals of the project are fully realized, this would certainly have significant impact in the ethanol to fuels/feedstocks space, at least on par with other licensed technologies in the alcohol to jet (ATJ) space.
- As a strategic approach, the project team has been able to forge effective collaborations across ChemCatBio to help elucidate the critical elementary steps in converting ethanol to higher olefins. These

collaborations have led to creating catalyst surfaces that can be tuned to influence overall product distributions.

- The focus is the ethanol to olefins step. The current SOT in the literature is dehydration followed by dimerization. Their sound process-intensity-based approach is to bypass the dehydration step and go straight to butadiene or mixed olefins. It is based on a dealuminated BEA. There are quite a few olefins and oxygenates in the product stream, so the team's approach is to collaborate with the crosscutting enabling technology groups to elucidate the reaction network. The team should spend more time identifying the risks associated with product selectivity control and other potential bottlenecks. The team should be clearer about the DEIP activities and future EJ directions.

- The team showed interesting results on tuning the olefin distribution with lanthanum composition. The connection between structure and activity as characterized by microscopy and X-ray analysis would be useful to show based on the conclusions, as well as surface titration with basic probes to show shifts in total acidity. TOS data showing the impact of regeneration cycles would also be useful. Hydrothermal aging had little effect on product distribution after only 24 hours. With the tools available at ORNL for monitoring material quality, the team should target catalyst synthesis scale-up on the order of kilogram batches. The team is publishing a paper that shows how copper is redispersed when the oxidative regeneration is conducted.

- The original license was with Vertimass, and a licensing negotiation with Prometheus is ongoing. These are clear commercial pathways that the team should be excited about supporting. Further, the impact of this route on the entire bioenergy industry and Gen I ethanol facilities will be quite significant.

- This project is developing catalytic upgrading technologies that enable cost-competitive conversion of cellulosic ethanol to SAF. The project focuses on upgrading zeolite-supported catalysts that enable the direct conversion of ethanol to C3 olefin, which could be used to eventually convert to SAF. The same procedure could be tuned to product chemicals as alternative products.

- The project deploys a collaborative workflow to accelerate the R&D activities. They collaborate with the three enabling teams in the program, as well as the TEA/LCA team, using the results to determine the direction of the R&D activities. They also collaborate with the other C2 project in the program. This collaborative workflow helps advance the research, with significant innovation in both foundational work and technologies. It would be more beneficial if the team could be more proactive in DEI.

- The project developed and tested engineered catalysts, improved catalyst selectivity and stability for C4-rich olefin streams, and conducted calculations for reactor-scale modeling and kinetics for future scale-up. This progress was achieved with a close collaboration with the enabling teams. These efforts successfully demonstrate integrated processing of ethanol to SAF with at least 80% carbon efficiency. There is a clear connection between the deployed approach and the outcomes. The deployment of engineered catalysts and the modeling of reactors illustrate the potential of the processes to be commercialized. The success of this project will help achieve DOE's SAF goal as well as the GHG emission reduction.

- This project has generated several patents that are either in the negotiation process of being licensed to a company or on that track. This record illustrates the impact of the project on industrializing the biomass-based conversion for SAF.

- The project presents a promising new strategy for meeting the shifting market demand for different product distributions from bioethanol by bypassing the ethylene step using tunable catalysts. This approach significantly reduces unit operations and energy consumption. Collaborative efforts with ACSC, CCPC, and industrial partners have led to impressive progress in understanding deactivation mechanisms, scaling up catalyst synthesis, achieving high conversion and selectivity, and meeting GHG reduction goals.

- However, the high water content in the feedstock still poses a significant challenge to this process. Further research is needed to investigate the impact of water on catalyst stability. It is also important to examine the impact of other impurities, such as dimethyl sulfide and dimethyl sulfoxide, on catalyst performance before scaling up. Overall, the outcomes of this project are encouraging, with high conversion, high selectivity, and competitive GGE. With continued research and development, this innovative approach has the potential to make a significant contribution to sustainable energy production.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for the time and thoughtfulness in the feedback they have provided as part of the Peer Review process. We are encouraged by the positive feedback and the appreciation of our work thus far, and we appreciate the opportunity to address some of the points that have been raised. A general point was that DEI progress and EJ involvement was lacking. We agree that this was not mentioned explicitly in the review material, but we are fully engaged with the ChemCatBio DEI team, and a member of our team is a member of that team. We view DEI as very important, and we are continuing to learn ways we can progress. We highly value the information shared from the ChemCatBio DEI team in our consortium meetings. At ORNL, we have been committed to STEM outreach to underserved schools and communities for several years, and we are developing further strategies to remove internal biases, including in hiring, collaborations, and publication citations. In response to the negative CO_2 balance using miscanthus, this takes advantage of the production of dedicated energy crops. This has been published recently, and more details can be found at doi.org/10.1039/D1GC02854E. We also reported MFSPs in this publication and reported updated numbers, taking into account the current blenders tax credit, which offers incentives for producing fuel with a certain GHG reduction relative to petroleum fuels. Even though the TEA in this publication was very competitive, it was provided to show the potential that these tax credits and incentives could have on the SAF industry. In response to the nitric acid and wastewater generation, we agree; it is an important consideration when thinking about scale-up of the catalyst production and an aspect that is rarely considered in explorative research. To use extrudates for our work, we had to scale up the catalyst synthesis, and during this process, we reduced water usage by a factor of 10 and reduced the nitric acid by a factor of 5. This is a significant improvement, and we aim to work with catalyst manufacturers to gain insight into further process improvements as we aim to de-risk this technology for industry adoption. In terms of catalyst lifetime, regeneration, and deactivation, we have an upcoming manuscript discussing the mechanism of deactivation and regeneration, which includes data that we had reported at the previous Peer Review and so did not include it in this review cycle. We do have data for more than 100 hours TOS with multiple regenerations that completely recover the initial catalyst activity. We are excited to scale up this process with engineered catalyst pellets and perform longer TOS experiments that will provide much more relevant data for this system. In combination with this, we have screened multiple typical contaminants that are present in current ethanol production, including methanol, acetic acid, isopropanol, and acetaldehyde, at levels higher than those found in commercial ethanol, with no deleterious effects on yield, conversion, or selectivity. We also have ethanol from a commercial producer that we will screen. The reviewers also mentioned dimethyl sulfide and dimethyl sulfoxide. We have been planning to test for sulfur impurities and will be performing these trials in FY 2024.

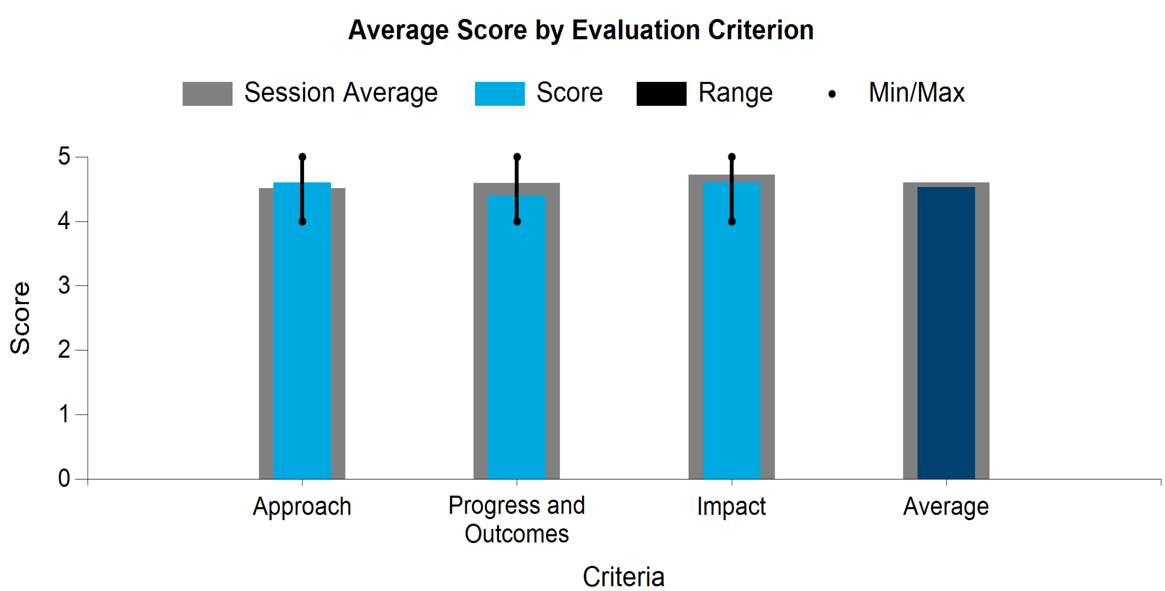
UPGRADING OF C2 INTERMEDIATES

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.3.1.304
Presenter(s):	Rob Dagle
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$751,940.00

This project is focused on the development of a new, cost-effective route to jet- and diesel-range hydrocarbons from ethanol, with integrated routes to coproducts. Ethanol is an attractive feedstock to produce fuels and chemicals, as it is already produced at commercial scale and can be produced from a variety of renewable biomass and waste sources. In addition, the ethanol "blend wall," coupled with advances in production efficiency and feedstock diversification, is expected to lead to excess ethanol at competitive prices. This technology provides an advantage over the current state-of-the-art ATJ technology, with elimination of a unit operation and energy savings realized by coupling exothermic and endothermic reactions. Efforts here have culminated in the development of a new, multifunctional catalyst system for the direct conversion of ethanol to n-butene-rich olefins. Additionally, a second multifunctional catalyst has been developed for the single-step oligomerization of produced olefins to jet-range hydrocarbons. An integrated process demonstration was performed, resulting in the production of a liquid product meeting ASTM specifications for jet blendstock. Ongoing efforts are aimed at further improvements to overall carbon efficiency, as well as engineered catalyst development, using conventional extrudates and kinetic and reactor modeling to accelerate reactor scale-up efforts. The project team is currently engaged in scaling up the catalyst technology developed on this project, employing modular, microchannel reactors. This separate effort leverages recent reactor fabrication advances made using additive manufacturing, teaming with LanzaTech and Oregon State University to take this new process technology one step closer to commercialization.



COMMENTS

- This project is developing a catalytic pathway for direct conversion of ethanol to butene-rich olefin intermediates. The team is moving toward an integrated process demonstration with engineered catalyst development to accelerate the process scale-up effort.

- The project explores two different catalyst systems to convert ethanol to C3 olefins and produce distillate fuels from olefin intermediates and produced fuels with the desired properties meeting target economics. It is a good collaborative effort—both within and outside of ChemCatBio. DEI approach and efforts are conducted via collaboration with the University of New Mexico (UNM). The project risk is addressed in collaboration with partners, with defined mitigation strategies.

- Carbon efficiency and ethanol cost are key cost drivers for improvements in carbon efficiency. The team developed a one-step oligomerization process that incorporates all olefinic intermediates. The team demonstrated integrated processing of ethanol to SAF with a high carbon efficiency of >80%. There is a question about the steady-state performance of catalysts with respect to water. The water content is of concern. More work is needed here—perhaps there could be more interaction with the deactivation project. The process was demonstrated with partial success, but further improvements are required for oligomerization processing: >95% ethanol conversion, 92% C2 olefin selectivity, and 75% C3 olefin selectivity.

- This could enable existing ethanol producers to pivot their product streams toward middle-distillate fuels and renewable chemicals. LanzaTech is commercializing the ATJ process for scaled SAF production developed previously (but this seems to not be from this project). Microchannel reactors enable process intensification and modularity, which is useful for distributed feedstocks.

- The project—focused primarily on ethanol conversion to higher alkenes for conversion to fuels or as valuable coproducts—clearly aligns with broader BETO goals to focus on SAF. It also builds logically from prior efforts by the group in the design of catalysts for ethanol upgrading. This reviewer was particularly impressed with both project collaborations (CCPC, Washington State University [WSU] for fuel testing, and UNM experts in related emission control catalysis) as well as the industrial links, which are established for both the fuel and coproduct components of the work. Extension of the work to greater process integration of the complete process and use of engineered catalysts in the upcoming cycle are warranted and aligned with prior review comments and the natural evolution of the work. Some DEI component exists with the MSI/Established Program to Stimulate Competitive Research (EPSCoR) institution PI, but the project is encouraged in subsequent cycles to provide some additional specifics regarding the interactions to demonstrate tangible connections in this space. The modeling and NMR characterization studies are another highlight. They complement one another, give a better-defined picture of the system, and will hopefully lead to improvements in catalysis design. The additive manufacturing component was brief but is something that should be considered moving forward as an opportunity area, particularly when a DFA/CRADA could arise. There are many directions this area can move—printing catalysts, reactor design (in some cases), etc. Also, given Rapid Advancement in Process Intensification Deployment (RAPID) Institute capabilities and PNNL's role there, the project should look to leverage available capabilities when it is appropriate. The metrics presented were clear. The expanded goals to determine kinetics for reactor modeling and the move to engineered catalysts are consistent with the general shift to these topics in the upgrading portfolio. I view the milestones as a bit aggressive for one project cycle, but they are potentially achievable. The state of the art was summarized well. The presentation also laid out well the progression within the catalyst systems to base metals, understanding of contaminant effects (specifically the role of water in deactivation), and promoter effects on performance. The careful understanding of the effects on the current processes provides pathways for improvement. I also appreciate the transparency about some areas that still need improvement. With this stage of TRL development, it is critical to identify these issues so they can be probed as soon as possible if they end up being a red flag point for the technology. Milestones generally seem on track, as modeling has established the pathway as a viable route to the desired cost metrics. Current targets for FY 2024 and FY 2025 extend to the areas necessary to achieve overall project goals. In particular, it can be highlighted that the results with the single-step catalyst look promising—I look forward to seeing the progression of research and development of this system in a subsequent review cycle. The six publications (the majority of which are in catalysis-focused journals) and the three patents are solid output. The commercial engagement is also a highlight, with partners in both the fuels (LanzaTech) and coproducts (Bridgestone) spaces. It is very rational to pursue alternatives to the ATJ process for the reasons highlighted in the presentation (more versatility, diversity of products/coproducts, etc.). Having scalable alternatives would have clear potential for a commercialization path, much as ATJ is progressing.

- The C2 upgrading team continues to make strides in the area of direct ethanol conversion to C4 olefins for continued oligomerization to SAF. The surface chemistry from a yield perspective remains challenging.
- The team aims to have a bench-scale demonstration of two pathways for converting biogenic ethanol directly to C4 olefins that can eventually oligomerize further to SAF. The approach is to continue developing the catalysts, then provide a process integration proof of concept at the bench scale. The state-of-the-art single-step technology involves catalysts that produce mostly aromatics from alcohols. Here, the team's approach is to design a material that can be highly selective to butenes, as published in a peer-reviewed article in 2020. Several key risks were identified, only for the catalysts, selectivity, durability, and engineered structure performance. The mitigation strategy is to partner with crosscutting functions across ChemCatBio for characterization and insight, which is a great approach. The collaborations include university, national lab, and industry partners. More risks on the integrated process development side should be identified moving forward. The DEIP or EJ plan was not strongly highlighted, except for UNM being an MSI. UNM recently won an award where PNNL helped on the proposal.
- The identification of the butyraldehyde surface intermediates within the reaction pathway as more favorable (in terms of promoting better catalyst performance) was a major accomplishment. The team was able to show how certain promoters mitigate sintering events out to 200 hours on stream. The negative impact of feed water on Cu sintering was experimentally determined. The team was able to demonstrate the entire integrated two-step conversion to SAF, showing 300 hours on stream for single-step ethanol conversion to olefins and several 100-hour regeneration cycles for the oligomerization step. The team disclosed some of the key risks/gaps with the oligomerization step, namely, C2 olefin conversion, regeneration effectiveness, and integration of separation strategies between reaction unit ops. By working to solve the C2 olefin conversion gap, the team developed a multifunctional material capable of handling mixed olefinic feeds for converting to SAF-range material. A patent was filed for this work.
- Based on the most recent progress, the MFSP projection is only slightly above the $3/GGE target, which makes this pathway quite attractive and industrially relevant. Ethanol will continue to be a strong building block in the biochemical/bioenergy industry, with opportunities to valorize into both the fuels and chemical commodity markets. This technology pathway will become more important within the next decade as the ethanol supply becomes challenged, opening up new opportunities for the Gen I ethanol facilities.
- This is one of the two projects focused on developing processes that convert C2 to SAF. This project focuses on the M/SiO_2 (M = Ag/Zr, X) process. The objective is to develop new upgrading technologies that enable the cost-competitive conversion of C2 oxygenated intermediates to distillate fuels and valuable coproducts.
- The team is focusing on ethanol-to-butene-rich olefin catalyst development, olefin oligomerization catalyst development, and the integrated process demonstration. They also plan to conduct TEA/LCA and develop engineered catalysts as their next step in their R&D activities. They have developed a clear plan for risk analysis and mitigation and have shown a commitment to DEI by reaching out to MSIs. They have also developed a framework to collaborate with the enabling teams and the other C2 project.
- The team has illustrated that they are progressing toward new R&D activities. By collaborating with CCPC, they have discovered that proximity of small Cu nanoparticles and ZrO_2 interfaces facilitates the

desired route via a butyraldehyde intermediate. In collaboration with the CDM team, multiple catalyst design strategies were investigated, leading to catalysts providing >95% ethanol conversion, 92% C2 olefin selectivity, and 75% C3 olefin selectivity. They also analyzed the impact of real feedstock on catalytic performance. This progress is appropriate and will help achieve the goal of this project, as well as DOE's goal for SAF and GHG emission reduction.

- Ethanol is a large amount of biomass raw chemicals. This project aims to develop processes that can convert ethanol to SAF. The progress of the project has illustrated its potential to be commercialized. More efforts will be needed to analyze the impact of real feedstock on the catalyst performance and duration.

- This project has made significant progress in exploring a new route to directly produce C3 olefins from ethanol. A good risk and mitigation approach was employed, with close collaboration within ChemCatBio and academia. This has resulted in a promising catalyst system developed through rational catalyst design based on mechanistic studies using state-of-the-art techniques.

- Although the addition of dopants has improved the stability of the olefin catalyst, further enhancements are necessary, particularly in the presence of water in real feedstock. Using accelerated deactivation as a pretreatment step for catalysts before activity screening is recommended to identify catalysts with higher potential for commercialization.

PI RESPONSE TO REVIEWER COMMENTS

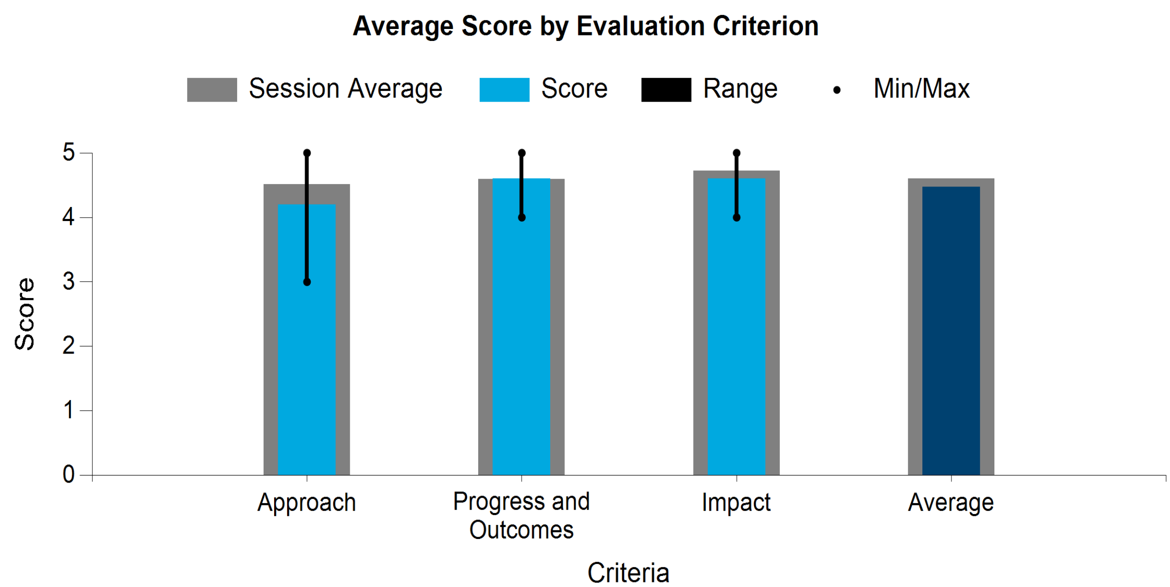
- We appreciate the positive comments from the reviewers highlighting the following: our innovation approach over current ATJ processing; the use of ethanol as a strong building block for renewable fuels and chemicals; strong collaborations both within and outside ChemCatBio, which includes industrial links; our DEI approach via collaboration with UNM; the use of partnering to mitigate technical risks; the use of modeling and NMR characterization to identify the favorable surface intermediate (butyraldehyde) within the reaction mechanism; the discovery of how the catalytic properties can be tuned to facilitate the favored pathway, with CCPC collaboration; the use of multiple catalyst design strategies to improve performance; our progress toward reducing Cu metal sintering; the evaluation of real feedstock on performance; our determination of water having a negative impact on catalyst performance; our transparency about some areas that still need improvement, including better separation between reaction units; the extension to include process integration, including a 300-hour two-step conversion demonstration; the future development of engineered catalysts and kinetic and reactor modeling; the development of a new, patent-pending, multifunctional oligomerization catalyst; the potential for commercialization; our solid publication and patent outputs; clear metrics; and our well-laid-out presentation. Regarding reporting more details about our collaboration with UNM: Here, we are focused on new catalyst concepts for improving catalyst durability, leveraging UNM's unique synthesis and characterization capabilities. UNM's expertise in designing thermally stable single-atom catalysts can be extended to metal clusters relevant to our catalyst system. By providing suitable support structures, it is possible to make these catalysts more thermally stable and regenerable. UNM will prepare new formulations that PNNL will test for reactivity. UNM's unique microscopy capabilities will also be leveraged to characterize spent samples. With this collaboration having just kicked off in April 2023, we will share progress in the next review. Regarding the comment that more work is needed to mitigate catalyst deactivation, particularly in the presence of water that is present in real feedstocks, we agree. Improving catalyst durability is certainly a key part of this research. Water in the feed has been identified as having a negative influence on catalyst durability. We note that water in the feed can be removed prior to conversion, if necessary, as commercially practiced. Thus, water removal is a risk mitigation to the overall processing. However, a significant amount of water is also produced during the reaction. Thus, we will continue to develop a more water-tolerant catalyst. Further, we will work with the CDM and use accelerated deactivation as a pretreatment for catalysts before activity screening (as one reviewer suggested). Regarding the comment that more risks should be added for the integrated process development side: Indeed, these risks were not highlighted in the risk table. However, when discussing results for the two-step processing, we highlighted key challenges that remain. These include (1) better interstage separation, and (2) improved oligomerization processing to incorporate the smaller amount of ethylene produced, along with butylene, into jet-range hydrocarbons in one step. These are what we consider to be the key risks to the integrated processing. That is why we worked to develop a patent-pending oligomerization catalyst. In subsequent work, we will work to improve interstage separation, and then demonstrate improved integrated processing. Regarding the expanded goals for kinetics for reactor modeling and the move to engineered catalysts being “a bit aggressive” for one project cycle, we agree that the broadened scope is challenging. This will be alleviated in part through partnering with the CCPC for kinetics and reactor modeling, where this scope will largely lie. The engineered catalyst development will be a key portion of the scope for this project. The reviewer was correct to point out that these expanded goals are consistent with the general shift to these topics in the ChemCatBio portfolio.

CATALYTIC UPGRADING OF BIOCHEMICAL INTERMEDIATES

National Renewable Energy Laboratory, Pacific Northwest National Laboratory, Oak Ridge National Laboratory, Los Alamos National Laboratory

PROJECT DESCRIPTION

The biochemical conversion of biomass via sugars and related intermediates to fuels is a primary conversion pathway within the BETO program. This CUBI project addresses critical barriers to the catalytic conversion of sugars and sugar-derived intermediates into SAFs and coproducts. Specifically, efforts are focused on key fuel intermediates that are identified in the 2018 BETO biochemical conversion design report, namely biomass-derived sugars/furans that do not require a biological conversion step, along with carboxylic acids and fermentation-derived 2,3-BDO. First, we are developing a pathway that upgrades biomass-derived sugars directly through dehydration to furans, followed by condensation and HDO. Complementary pathways upgrade platform molecules (carboxylic acids, BDO) derived from biomass-derived sugar fermentation. For the carboxylic acids project, we focus primarily on ketonization, HDO, and cyclization for the production of SAF. Regarding BDO upgrading, CUBI has two complementary research tracks: BDO upgrading (1) via methyl ethyl ketones and (2) through reactive extraction via dioxolanes. In this presentation, we will highlight these routes toward SAF from a technical perspective as well as through a summary of TEA and LCA. By pursuing coordinated and independent research directions and collaborating with complementary projects, the CUBI project strives to develop viable routes toward SAF production.



COMMENTS

- Common comments for all projects:
  - One thing that was rather challenging about reviewing this project, which was split across multiple labs, who each gave their one presentation as a part of a large block, was keeping everything straight, as we went all the way through and did questions at the end. Additionally, the lack of a consistent format across the component presentations made it difficult to follow a cohesive story.
  - TEA and LCA: Overall, it was difficult to separate out approach, progress, and impact for each pathway.

- As the name implies, this project is focused on upgrading intermediates derived from biochemical pathways. The potential diversity of products used as intermediates to access SAF is greater than in other projects, which also adds a layer of complexity to the catalytic methods employed. Issues with contaminants for real broth-derived products or waste streams is another issue that ultimately must be addressed. The attempt to use such realistic streams and the handling of mixed feedstocks in some cases is noteworthy. It would likely only be pursued in the context of a national lab project like this one for de-risking to the point that it could be of interest as a viable technology to industry. Given the many layers of scientific diversity in the project, economic modeling provides another key pillar to the effort. Furfural, carboxylic acids, and BDO are major platform molecules of focus, with each lab concentrating on a particular substrate or reaction pathway. General comments here precede specific lab-by-lab notes. With the spectrum of reactions involved in CUBI, the need for collaborations across ChemCatBio is clear. In general, these connections are evident and well utilized across other BETO consortia (SepCon) and within ChemCatBio. The breadth of these interactions is what one would expect for an effort spanning biochemical inputs and chemical upgrading. I would also note that the many industrial interactions are vital to the project and provide some indicator of potential for transfer of successful technologies. The initial DEI statement is broad and not really descriptive as to specific actions taken within the project. While individual labs sometimes included information with specific actions (ORNL), the unevenness of this in the presentation is something to remedy in a future cycle.

- Discrete overall milestones of CUBI involved developing a viable butyric acid in FY 2023 and the BDO pathway in FY 2024, along with an end-to-end pathway that met discrete fuel and efficiency/GHG metrics. The goals are in line with moving from concept to demonstration and, ultimately, further down the technology development slope. Overall, viability seems present in all pathways. In general, all aspects of CUBI demonstrate a reasonable degree of productivity in the publication and IP spaces, with a distribution of 1–2 publications per topic and one patent during the evaluation cycle. The ORNL aspects are one area I would specifically highlight, as the VFA ketonization is being scaled/licensed by Alder, and output in the dioxolane area is significant, particularly on the IP generation side. I also commend the NREL component that examines the paper sludge as a feedstock—this has some loose connection to the topic of a prior university project in ChemCatBio. It is gratifying to see that prior knowledge is being leveraged (when appropriate) within the consortium to advance technology development. I believe it is a great sign when companies want to continue working with their partners past the funding phase of a given project. This, combined with CUBI's many industry interactions, bodes well for the ultimate integration of technologies developed within the project. In general, I think that many of the pathways are reaching a critical juncture to begin the process of exploring scaling, shifting to realistic feeds, etc. I look forward to seeing the results of the next funding cycle and how these processes translate through the next phase of development.

- The CUBI team has improved in communicating the approach and benefits of this project at a high level to the public and peer review community since its inception. The presenters were able to keep the audience centered on which part of the SAF pathway involves the CUBI research focus. The opportunity to cyclize ketones to aromatics without the use of hydrogen for use in SAF blends should be impactful and industrially important, as realized by the industrial fuels startup partner licensing the patent. The project has always been challenged by its tendency to take on too many pathways at once, with those pathways having significant CapEx. The team did an excellent job of organizing quite a bit of research work and science. They should continue to prioritize the resources allocated to various pathways as ranked based on factors such as technical/business risks, TEA (CapEx, OpEx), LCA (% GHG reduction), etc.

- The approach of upgrading sugars either biologically or thermochemically to SAF-range products is very clear and succinct. This project continues to have a strong technical approach of increasing the molecular weight of biochemical intermediates using a combination of aqueous transformations and traditional thermochemical deoxygenation where necessary. The state of the art was difficult to determine across all the projects. The partnerships and collaborators are strong and promising, covering a comprehensive approach to developing the technology that includes TEA, LCA, multiscale modeling, separations, feedstock optimization, etc., as well as leveraging ChemCatBio's crosscutting services. The team should not lose focus on generating the spec sheets for key biochemical intermediates and their corresponding pathways, as this has always been the underpinning of the project. The project has always been challenged by its tendency to be too expensive and take on too many pathways at once. The increased emphasis on project planning and organization is apparent. An external collaboration should be prioritized to enable a pathway's potential of success to be ranked based on factors such as technical/business risks, TEA (CapEx, OpEx), LCA (% GHG reduction), etc. The current state of the art of producing biochemical intermediates and/or their corresponding SAF pathways was not presented. For the quantity of research conducted, the number of risks/gaps was not clearly identified, and mitigation actions were not stated. A small table was presented in the appendix dealing with research interests for catalyst performance and reactor parametric studies. A good effort to hire interns and co-ops was mentioned.

- Generally, it looks like steady improvements in the economics continue across the various pathways explored. Additional cost reductions were identified in most pathways, with most hovering in the \$2.5–\$3 range. Some pathways incur minor to moderate cost increases (dioxolane pathways), but reap the benefit of significant (10%) GHG reductions. Because the individual pathways are intimately tied to the economic modeling throughout the development process, I have little doubt that the feedback loop between the modeling and the science will result in progress in the technology and economic viability.

PI RESPONSE TO REVIEWER COMMENTS

- General responses: Given that the CUBI projects (2.3.1.101, 2.3.1.102, 2.3.1.103, and 2.3.1.104) presented together, and that many of the reviewer responses addressed the project at large, we will provide a single, collective response to the reviewers' general comments, followed by task-specific responses in the appropriate sections. First, we would like to thank the reviewer panel for taking the time to provide their valuable feedback, thoughtful comments, and suggestions on our project. We appreciate the review panel's generally positive assessment of this project and the research activities occurring at each laboratory. Although presentation time constraints can make balancing all aspects, such as a comprehensive background for each section, challenging, future presentations will aim to outline the current state of the art. Along with this, we will place a greater emphasis on the potential risks and gaps in future presentations. We will work on improving the consistency of our presentation format and will aim to provide more detail to help reviewers understand the overall approach, progress, and impact for each pathway. The responses below generally follow the format of a reviewer comment in quotations followed by a brief response.

- "The attempt to use such realistic streams and the handling of mixed feedstocks in some cases is noteworthy. It would likely only be pursued in the context of a national lab project like this one for de-risking to the point that it could be of interest as a viable technology to industry." We thank the reviewer for pointing this out and agree that integration with upstream projects and the use of real streams is of critical importance to the industry at large.

- "The CUBI team has improved in communicating the approach and benefits of this project at a high level to the public and peer review community since its inception. The presenters were able to keep the audience centered on which part of the SAF pathway involves the CUBI research focus." As this is a large and complex project, we will continue to work to harmonize our communications moving forward. Although in some ways, it may seem that CUBI is five independent projects that simply share a project title, in reality, we find great synergies within this group of researchers and collection of projects. We strive to ensure that this synergy comes through in our presentations.

- "The initial DEI statement is broad and not really descriptive as to specific actions taken within the project. While individual labs sometimes included information with specific actions (ORNL), the unevenness of this in the presentation is something to remedy in a future cycle." We agree. While DEI initiatives are formally managed at the consortium level, we would like to emphasize that each lab participating in this project incorporates DEI principles into its strategies, policies, practices, and decision-making processes. This commitment helps create a more inclusive and equitable research environment, leading to better science, increased collaboration, and positive societal impact. We agree that in the Peer Review presentation, some individual labs included information on specific actions regarding DEI strategy, but there was unevenness in the overall presentation. To address this concern, we will emphasize and improve communication on the DEI aspect in future CUBI presentations and include specific actions, initiatives, and strategies implemented to promote diversity, ensure equity, and foster inclusion within the project.
- "The current state of the art of producing biochemical intermediates and/or their corresponding SAF pathways was not presented." We agree with the reviewer that this will be an important component to expand upon in future presentations. We opted to leave out a detailed discussion of upstream pathways because they were covered in other projects during Peer Review. Although these upstream research activities fall outside of the research purview of CUBI, with highly integrated projects like this, we understand the value of discussing the pathway as a whole as opposed to compartmentally.

CATALYTIC UPGRADING OF BIOCHEMICAL INTERMEDIATES

National Renewable Energy Laboratory

WBS:	2.3.1.101
Presenter(s):	Jeffrey Linger; Jacob Miller; Ashutosh Mittal
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,350,000.00

COMMENTS

- This part of CUBI is focused on the conversion of VFAs to SAF through ketonization followed by HDO to create fuel molecules or SAF precursors. The background makes a clear case for the opportunity to pursue wet waste fractions beyond the oil phase that is currently utilized. The current cycle goals revolve around scale-up of prior demonstrated reactions and transition to flow conditions. Both are necessary for a viable process to be developed and are the right targets to pursue at this stage. The role of water in deactivation of the catalyst was an important (while perhaps negative) result. Follow-up studies do indicate one can accept deactivation if a sufficiently economical catalyst is used. The concept demonstration of HDO to an arene fraction is significant and establishes the complete pathway. The next cycle will be critical for determining whether the process can be transitioned to a scalable and economical system.

- The VFAs project is one area I would specifically highlight, as the VFA ketonization is being scaled/licensed by Alder, and output by the dioxolane area is significant, particularly on the IP generation side. I also commend the NREL component that examines the paper sludge as a feedstock—this has some loose connection to the topic of a prior university project in ChemCatBio. It is gratifying to see that prior knowledge is leveraged (when appropriate) within the consortium to advance technology development. I believe it is a great sign when companies want to continue working with their partners past the funding phase of a given project. This, combined with the many industry interactions for CUBI, bodes well for the ultimate integration of technologies developed within the project.

- Mixed sugars to SAF: This portion of CUBI is focused on sugar dehydration, condensation, and HDO to access SAF. Current efforts involve exploring the parameter space of these steps (solvent/reagent use in particular) to reduce cost metrics. The parameters selected to explore—a new solvent, use of a base catalyst that favors mono-adduct formation, understanding deactivation in conditions that mimic broth-derived intermediates, and optimized catalysts for HDO—seem logical and like good target spaces to explore. In general, I think that the division of pathways is very logical, and the projects are pursuing rational parameter optimization for the stage each technology is at. Although some of these are at an earlier stage of scaling relative to other ChemCatBio projects, it is important to have the diversity seen here in a portfolio of projects with the breadth of the consortium, particularly when you hope to use the true spectrum of platform molecules that can be provided by biomass-derived sources.

- Mixed sugars to SAF: This activity exceeded cost-driven metrics, with paper-derived waste sources looking promising. The move toward cyclic hydrocarbons is more exploratory, but is warranted from the perspective of an improved property of the fuel product.

- The TEA improvements were clearly identified, with significant improvements in $/GGE for (1) the furan path, due to condensation reactor optimizations; (2) the VFA path, due to ketone recovery upstream HDO; (3) the BDO/MEK path, due to improved MEK separation; and (4) the BDO/butene path, due to dioxolane phase separation efficiency. The replacement of the precious metal catalysts for VFA HDO seems like it should have resulted in a lower $/GGE reduction than 1 cent/GGE. There was a slight increase in the MFSP, even with the dioxolane recovery improvement. The stability of the solid base catalyst and adduct yields was quite impressive for furfural conversion. The platinum-supported HDO catalyst with >20 wt % loading of precious metal showed high yields. More R&D on reduced or zero precious metal loaded supported catalysts is necessary and should be a collaboration with the ChemCatBio ACSC team. The peer-reviewed published article highlighting the modeling efforts on ketonization was insightful regarding water inhibition and the interstage design implications of a commercial reactor. There is still much more to complete in order to de-risk such design configurations with no pilot-scale experimental validation for the reaction rate effectiveness factor. Operating the ketonization plugged-flow powder bed reactor for up to 70 hours on stream was a reasonable start to understanding the long-term stability risks. The MFSP estimate before the stabilized rate for ZrO_x catalyst deactivation should be higher than 4 cents/gallon, especially because the ketonization catalyst lost 80% of its initial activity. The proton Zeolite Socony Mobil–5 (ZSM-5) ketone upgrading experiments were promising. The progress is at an early stage, with low conversion, short TOS, and small reactor beds. The proof of concept has been completed at the bench and prototype lab scale.

- There was a significant shift (>$5 GGE) in the MFSP estimate when using BDO feedstocks in 2021 versus the dioxolane pathway in 2023, which should be explained by the catalyst performance being comparable.

- The presentation was very comprehensive and organized. This was greatly appreciated given the number of R&D activities within this project. This project could almost be its own consortium focused on various upgrading, solvent recovery, and catalyst regeneration strategies.

- This project was reported under the umbrella of CUBI. It focuses on R&D activities to enable industrialization of VFA-SAF processes. The team conducted an in-depth, scale-up-oriented study of the ketonization step, mainly in two directions: (1) reactor design and (2) catalyst deactivation. They discovered water as the main factor that inhibits the desired reactions in a process using engineered catalysts and developed an industrial-scale reactor model with the integration of a multistage reactor and interstage water removal via separation. Their R&D activities led to the development of a flow reactor process for light ketone upgrading to replace the condensation step. Aligning with their research activity, they have shown their commitment to DEI by recruiting researchers from underrepresented groups. It will be beneficial if further R&D activities can reduce the complexity of the reactor model. For instance, would a reactive membrane concept work for this process? It may also be beneficial if future R&D activities can understand the heat/mass transport in this reactor model, which may help develop principles for scale-up. Overall, the project has illustrated the appropriate progress that can help achieve its goal. The project has also demonstrated its impact by (1) developing a new reactor that can help achieve DOE’s SAF Grand Challenge, if it can scale up and industrialize, and (2) illustrating its commitment to DEI.

- The CUBI projects demonstrate excellent teamwork and numerous promising processes. All of the processes have successfully met their targets and have become increasingly eco-friendly and efficient compared to 2 years ago. TEA/LCA plays an important supporting role in evaluating both the technical and economic aspects of the projects to make go/no-go decisions. The furfural upgrading project has made significant advancements by utilizing non-azeotropic solvents and heterogeneous basic catalysts and achieving a 31% reduction in GGE. The VFA to SAF project has progressed even further with industrial-scale reactor modeling, utilizing the equilibrium activity of the catalyst, and working with an industry partner to build a 1-gallon/day demo unit. These are all very encouraging outcomes. Further research is recommended to gain a better understanding of the processes, such as studying the deactivation mechanism to assist with rational catalyst design. For example, in the case of furfural upgrading, a common issue associated with solid base catalysts is leaching. Thus, multiple cycle runs are necessary to assess the stability of the catalysts.

PI RESPONSE TO REVIEWER COMMENTS

- "The platinum-supported HDO catalyst with >20 wt % loading of precious metal showed high yields. More R&D on reduced or zero precious metal loaded supported catalysts is necessary and should be a collaboration with the ChemCatBio ACSC team." We agree with the reviewer panel's assessment that the current platinum-supported HDO catalyst with a high loading of precious metal has shown promising results, but further research and development are needed to explore the potential of reduced or zero precious metal loaded supported catalysts. Based on reviewer recommendations, collaborating with the ChemCatBio ACSC team will be pursued. By leveraging their expertise, we will be able to identify ways to improve the performance of the catalyst while reducing the use of precious metals, thus making the process more cost-effective and sustainable in the long run. Moreover, we have been working to develop effective and robust non-precious-metal catalysis for HDO, and we believe that the impact of this advance would be more easily recognized in comparison with the current state of the art, which is the use of expensive precious metal catalysts.

- Regarding de-risking VFA ketonization: We appreciate the reviewer's comment regarding the status of de-risking the VFA ketonization step, particularly with regard to pilot-scale experimental validation of the catalyst effectiveness factor. Luckily, our upcoming FOA with Alder Fuels will allow us to perform this work.

- "The team should not lose focus on generating the spec sheets for key biochemical intermediates and their corresponding pathways, as this has always been the underpinning of the project." We agree with the reviewer that specification sheets of CMAs for our biochemical intermediates are crucial to generate. Currently, the still-evolving nature of the biochemical processes supplying our intermediates complicates the process of making spec sheets. However, as these processes become optimized, we can perform targeted studies to determine allowable concentrations of contaminants, etc. in each intermediate upgrading progress.

- "It will be beneficial if further R&D activities can reduce the complexity of the reactor model. For instance, would a reactive membrane concept work for this process? It may also be beneficial if future R&D activities can understand the heat/mass transport in this reactor model, which may help develop principles for scale-up." We appreciate the reviewer's comment about reactor heat and mass transport and model complexity. There was not time in our presentation to specify, but our model does capture heat and mass transport phenomena on the particle and reactor scales. Luckily, ketonization reactions are roughly thermoneutral (ca. 0 to +15 kJ mol^{-1}, depending on acid reactant identity); this prevents major thermal gradients on the particle scale and results in a net temperature decrease of ca. 10°C across the length of an adiabatic reactor running at 100% conversion. Our model also captures the effects of internal and external mass transfer on the pellet scale. The internal mass transfer limitations were discussed in the presentation (effectiveness factors can be as low as ~0.5), but there are negligible external mass transfer limitations, provided that flows are close to the turbulent regime. We will consider alternative reactor designs such as membrane reactors in the future.

CATALYTIC UPGRADING OF BIOCHEMICAL INTERMEDIATES

Pacific Northwest National Laboratory

WBS:	2.3.1.102
Presenter(s):	Vanessa Dagle
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$449,614.00

COMMENTS

- The R&D is focused on three pathways: dehydration, aldol condensation, and HDO. This aspect of CUBI involves BDO dehydration to MEK, MEK to olefins, and subsequent oligomerization/hydrogenation to produce SAF. Major areas explored in this cycle include understanding contaminant impact on conversion, adjusting the economics to changes in process, and demonstrating the pathway to obtain adequate samples for fuel testing properties. The need to study contaminants is clear with the switch to realistic feedstocks. Subdividing the role of organics versus inorganics is important, as mitigation may proceed differently for each category of impurities. Here, collaboration with other ChemCatBio-wide effects (catalyst deactivation) is critical.

- Progress: Discrete overall milestones of CUBI involved developing a viable butyric acid in FY 2023 and the BDO pathway in FY 2024, along with an end-to-end pathway that met discrete fuel and efficiency/GHG metrics. The goals are in line with moving from concept to demonstration and, ultimately, further down the technology development slope. Overall, viability seems present in all pathways. The activity demonstrated full pathway progression to access fuel fractions with reasonable to promising properties. The next cycle will be key to translating the knowledge gained on contaminants to determine the ability to circumvent any issues related to the real feedstock.

- The team did an excellent job of experimentally demonstrating the negative effect on catalyst stability of processing real BDO feedstock versus surrogate. There was a significant decrease (>30%) in the MFSP 2030 progression due to improvements in per-pass conversion for MEK upgrading and alkene oligomerization. Key oxygenated and metal feed impurities were well characterized in collaboration with the ACSC team. The proof of concept for the liquid-phase conversion of 2,3-BDO is an important result. The team should discuss how trace oligomers in Step 2 for the BDO/MEK route go into the water phase and what the future concept is for water treatment. For liquid-phase BDO chemistry, the time of the regeneration cycles and whether vaporization is required should be explained.

- The 2,3-BDO/MEK pathway has good promise, even with the risks associated with feed impurities. This route could use more industrial engagement and support to enhance commercial interests. The presentation was very comprehensive and organized. This was greatly appreciated given the number of R&D activities within this project. This project could almost be its own consortium focused on various upgrading, solvent recovery, and catalyst regeneration strategies.

- This project was reported under the umbrella of CUBI. It focuses on a BDO-MEK-SAF process. This project focuses on the impact of the impurity of the feedstock on catalyst stability, particularly the impact of potassium. The conversion from a model feedstock to a real feedstock is a key step to determining the potential of a process to be industrialized. The project has shown the change in the catalyst performance due to this change and has identified the impact of the feedstock impurity. It would be beneficial to collaborate with enabling projects like CCPC or catalyst synthesis to reversely develop catalysts that can endure this impurity, or to collaborate with upstream or separation teams to either tune the feedstock or develop a cost-effective process for pretreatment. The project shows that some progress has already been made in this direction. The project also shows an updated TEA and has initiated the LCA. The TEA/LCA will play an important role in determining the potential of industrialization for this process. The coproducts play a role in reducing the overall cost. It would be beneficial to evaluate whether the coproducts and SAF have a similar market size. The team also shows a liquid-phase upgrading of BDO to MEK. They have tested three catalysts under various conditions. This exploration has illustrated that the liquid-phase conversion may be a viable path. Overall, this project has illustrated appropriate progress to achieve its goal. The detailed R&D on the effect of feedstock impurity on process performance and catalyst stability will play a critical role in the industrialization of this process. The knowledge and technology may be transferrable to the other projects within the Catalytic Upgrading program. The new liquid-phase process opens another possible way to industrialize the BDO-MEK-SAF process. This project has illustrated its impact by (1) developing a BDO-MEK-SAF process that can help accomplish the SAF Grand Challenge if successful, and (2) conducting R&D activities on feedstock impurity, which will be a big roadblock for commercializing biomass-based chemical conversion processes.

- The progress made in upgrading 2,3-BDO to SAF via MEK has been significant, using feedstock that contains impurities. The systemic study in collaboration with ACSC on the impact of organic and inorganic impurities with TOS was impressive. This study is crucial, as it provides guidance for feedstock specification and catalyst design. It is also encouraging to see that the feasibility of this route has been demonstrated by this project.

PI RESPONSE TO REVIEWER COMMENTS

- PNNL (2.3.1.102): We thank the reviewers for their time and feedback. We appreciate that the reviewers understand the value of the BDO/MEK pathway to SAF, that they highlight the relevance of the work from this pathway, and that they acknowledge the progress made.

- "The team should discuss how trace oligomers in Step 2 for the BDO/MEK route go into the water phase and what the future concept is for water treatment." Water is removed from the process prior to Step 2 as opposed to after Step 2. Indeed, MEK can be easily separated from water using conventional distillation. The MEK solution contains trace amounts of some compounds, but traces of olefin oligomers were neither detected nor expected. The main trace compounds detected include iso-butyraldehyde, iso-butanol, and butadiene. The catalyst for Step 2 is a $ZnZrO_x$-based catalyst with unique redox and acid properties that allow for hydrogenation/dehydration and aldol condensation, which lead to the desired olefins. Traces of alcohols, aldehydes, ketones, and acids are converted into olefins over the $ZnZrO_x$ catalyst. Traces of butadiene are expected to be converted into butenes due to the presence of hydrogen and the mild hydrogenation properties offered by the catalyst.

- "For liquid-phase BDO chemistry, the time of the regeneration cycles and whether vaporization is required should be explained." The team recently started liquid-phase upgrading and presented the results obtained for 40 consecutive cycles in a batch reactor. The catalyst was not regenerated between cycles. Catalyst durability and potential regeneration needs will be investigated in future work conducted in a fixed-bed reactor.

- "To further reduce the energy cost of the process, in addition to the use of renewable natural gas, it is recommended to consider the use of waste heat from other processes." We agree with the reviewer that other sources of renewable energy could be used to reduce the energy cost in addition to the use of renewable natural gas. For this preliminary life cycle assessment, renewable natural gas and renewable H_2 were considered because we already had access to the associated costs.

- "It would be beneficial to collaborate with enabling projects like CCPC or catalyst synthesis to reversely develop catalysts that can endure this impurity, or to collaborate with upstream or separation teams to either tune the feedstock or develop a cost-effective process for pretreatment." The team is already collaborating with ACSC and CDM, and it interacts with the upstream biological team. In fact, the results for the organic and inorganic impurity studies have already been shared with the biological team producing the fermentation broth, which has been investigating and has already identified solutions for some of the impurities.

- "The coproducts play a role in reducing the overall cost. It would be beneficial to evaluate whether the coproducts and SAF have a similar market size." All the pathways under CUBI involve adipic acid coproduct from lignin upgrading, and it is reducing the cost. The BDO pathway has also been investigated for the possibility of diverting some of the MEK from SAF production to the coproduct market to investigate the potential for decreasing the need for lignin upgrading. The SAF market is much bigger than the MEK coproduct market, and only a small fraction of MEK should be diverted to the coproduct market if this is the chosen pathway in order to avoid saturating that coproduct market.

CATALYTIC UPGRADING OF BIOCHEMICAL INTERMEDIATES

Los Alamos National Laboratory

WBS:	2.3.1.103
Presenter(s):	Claire Yang
Project Start Date:	10/01/2015
Planned Project End Date:	09/30/2025
Total Funding:	$250,000.00

COMMENTS

- This project aims to convert fermentation-derived 2,3-BDO into SAF with a distillate MFSP of $2.50/GGE at maximum and a GHG emissions reduction of 70%. Conversion of BDO to a protected dioxolane has advantages in processing through a straightforward separation, if the dioxolane can be upgraded economically and the aldehyde used can be recovered. This half of the dioxolane project is centered on exploring the dioxolane structure space by varying the aldehyde to understand the impact on separations and upgrading. A range of dioxolanes were prepared, with linear/branched structures, on scales that were amenable to subsequent upgrading studies. The ability to deal with materials derived from realistic fermentation broths is another goal—even if the majority of impurities stay in the broth, there may be impacts to the chemistry you are unaware of until working under those conditions.

- Improvements in the acid catalyst allow for a significant reduction of the excess aldehyde used to form the dioxolane and improve process economics. At the same time, the family of desired structures was prepared and scaled for further upgrading. The modeling is promising, suggesting that the pathway could approach or exceed desired GHG reduction goals.

- The industrial version of the dioxolane production process could resemble traditional alkylation units if the mineral acid technique is favored. An entire section was dedicated to discussing the formation of alkenes from dioxolanes. This was a good way to organize this part of the content. Dioxolane is really a BDO carrier, which is fascinating. The team should disclose the extent to which metal ions penetrate the dioxolane phase.

- The CUBI team has provided a promising pathway for sugars to SAF with immediate commercialization potential, as evidenced by a published paper and design report. The team should mention any efforts engaging ASTM at this early stage. The dioxolane intermediates research still has progress to make in terms of raising more technical awareness of the opportunity.

- This project was reported under the umbrella of CUBI with several other experimental projects that focus on developing processes to produce SAF using intermediates from biomass conversion. This project focuses on 2,3-BDO upgrading via dioxolane intermediates. The team reports a very promising reactive extraction process. This reactive extraction process was developed using normal acid catalysts and liquid-liquid phase separation with the dioxolane products with high purity. The team then used this dioxolane as the platform chemical to develop SAF products. The reactive extraction process has potential because it does not require expensive noble metal catalysts. The reduction of the cost and GHG emissions for the production of dioxolane will help make the SAF production more competitive in terms of price and will reduce the overall GHG emissions for the final SAF products. This process is based on a liquid-phase process. The recycling, storage, or remediation of the liquid phase may influence the commercialization potential. It would be beneficial for commercialization for the team to conduct NMR or another analysis to identify side products in this process and discuss with other consortia, like SepCon, to develop related processes. It is also interesting to note that the dioxolane derivatives produced in this process may have some potential electrochemical applications. 1,3-dioxolane is one of the most commonly used electrolytes for lithium-ion batteries. Although the market for electrochemical applications is smaller than the SAF market, the ability to produce such compounds from biomass could be interesting. The ability to tune the structure of dioxolane derivatives by adding different chemicals may pave the way for producing electrolytes with specific conductivity. It may also have some potential applications in the electrochemical conversion of CO_2 and the production of H_2. Overall, this project has illustrated suitable progress in producing various dioxolane derivatives via the developed reactive extraction processes. The team also presented significant progress. The team showed process integration under the guidance of TEA, examined the catalyst stability, and developed a pretreatment that can enhance catalyst stability. It has been observed that catalyst stability is an overarching challenge over the whole Catalytic Upgrading program. It would be beneficial if the program could develop general principles or guidance that would help mitigate catalyst deactivation. This project has demonstrated its impacts by (1) developing a process that can help address DOE's SAF Grand Challenge, and (2) inventing a likely biomass-based process to produce electrolyte products for electrochemical applications.

- BDO upgrading via dioxolane intermediates could be a game-changing process toward the formation of SAF via BDO. The formation of dioxolane is an important step, as a significant drop of GGE has been achieved downstream using dioxolane as feed. The progress that has been made in the development of dioxolane since 2021, including the identification of feasible precursors and catalyst development, is promising.

- Further research is needed to study the deactivation mechanism of resin-based catalysts. Leaching of the acidic group is a common cause for deactivation of those catalysts in liquid-phase reactions. In searching for alternate acid catalysts, liquid acids may raise concerns regarding corrosion and environmental impact. Alternative non-resin solid acids, such as sulfonic silica/zeolite or carbon-based acids, may provide better stability. Has any research been conducted to evaluate their effectiveness in this process?

PI RESPONSE TO REVIEWER COMMENTS

- LANL (2.3.1.103) responses: "Improvements in the acid catalyst allow for a significant reduction of the excess aldehyde used to form the dioxolane and improve process economics. At the same time, the family of desired structures was prepared and scaled for further upgrading. The modeling is promising, suggesting that the pathway could approach or exceed desired GHG reduction goals." We greatly appreciate the acknowledgment of the process' potential and successes to date. Issues related to contaminants and other such factors when using real fermentation broth, as the reviewer raises, are absolutely a key factor moving forward and the major point of focus. Isolation of dioxolane directly from the broth has already been and will continue to be carried out for downstream processing in the LANL BDO upgrading approach. Both organic and inorganic contaminants/impurities have been analyzed by high-performance liquid chromatography and inductively coupled plasma mass spectrometry. Further testing is also underway with real fermentation broth to establish what effect this has on reaction parameters, such as the acid strengths and required loading amounts, as well as the resulting conversion and dioxolane yield. This testing also ties into broader investigations into different types of acids, which will be essential for further process analysis and modeling to help de-risk potential future process scale-up in industry. Additional work is underway to look at the effect of different acids on the minor organic components that remain in the fermentation broth as well.

- With regards to metal ions penetrating the dioxolane phase, this is a good point the reviewer raises, but it will potentially be affected by the reaction systems used (such as the acid and its quantity). As such, this has not currently been determined, but it is certainly something to be established in our next step once the acid type is determined. We appreciate the reviewer's comments on leveraging traditional alkylation units in the industrial version of the dioxolane production process if the mineral acid technique is favored based on TEA and LCA.

- We appreciate the reviewer's comment regarding raising more technical awareness of this promising dioxolane pathway opportunity for industry engagement. We are currently planning on working with the

BDO fermentation team at NREL and the dioxolane upgrading team at ORNL to package this technology with IPs and bring it to potential industry partners.

- "The recycling, storage, or remediation of the liquid phase may influence the commercialization potential. It would be beneficial for commercialization for the team to conduct NMR or another analysis to identify side products in this process and discuss with other consortia, like SepCon, to develop related processes. It is also interesting to note that the dioxolane derivatives produced in this process may have some potential electrochemical applications. 1,3-dioxolane is one of the most commonly used electrolytes for lithium-ion batteries. Although the market for electrochemical applications is smaller than the SAF market, the ability to produce such compounds from biomass could be interesting." The reviewer raises a good and key point with regard to future commercialization—namely, that the contents of the residual aqueous phase (post dioxolane isolation) are important to understand and consider. Current work using actual fermentation broth is indeed aimed at looking into the residual organics within the aqueous phase both before and after reaction with different acids, to determine how the choice of acid may affect this aspect. We appreciate the reviewer's suggestion of connecting with the Separations Consortium. This dioxolane technology has indeed been brought to Separations Consortium, and the process was examined by the SepCon team. One manuscript (doi.org/10.1021/acs.iecr.2c04307) has been published based on this reactive extraction process for separating 2,3-BDO from fermentation broth. We will continue working closely with the Separations Consortium to further address some aspects of acid type selection and potential pretreatment options.
- We thank the reviewer for acknowledging the progress made but also for raising the potential of the formed dioxolanes as solvents in electrochemical applications. This is something we haven't explored yet. This could indeed add further value and could be another avenue of contribution to the process. While perhaps outside the scope of the current work, it is definitely an avenue the authors are keen to explore further and hopefully pursue in the future.

CATALYTIC UPGRADING OF BIOCHEMICAL INTERMEDIATES

Oak Ridge National Laboratory

WBS:	2.3.1.104
Presenter(s):	Andrew Sutton
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2025
Total Funding:	$1,227,920.00

COMMENTS

- This project aims to adapt a BDO conversion approach to utilize dioxolanes as a BDO synthon.
- The second half of the project, which is focused on dioxolane, involves its conversion to olefins and ultimately to SAF. Given the PI's other ChemCatBio project, this coupling to the related technology makes complete sense. The project is exploring optimization of reaction conditions, including temperature, the viability of various dioxolane intermediates, and demonstration of aldehyde recovery. These are all logical to explore at this stage before attempting to move forward with further scaling of a potential process. Progress: Discrete overall milestones of CUBI involved developing a viable butyric acid in FY 2023 and the BDO pathway in FY 2024, along with an end-to-end pathway that met discrete fuel and efficiency/GHG metrics. The goals are in line with moving from concept to demonstration and, ultimately, further down the technology development slope. Overall, viability seems present in all pathways.
- It is reassuring that the various cyclic intermediates are effectively interchangeable with BDO in upgrading, and the renewably sourced aldehydes might be used at some stage. Optimization of reaction conditions—temperature, demonstration of aldehyde recovery, etc.—are logical and move in the right direction. The next key steps of moving to fermentation-derived intermediates, shifting to longer TOS, and understanding ways to improve the economics of aldehyde recovery are logical and necessary. The fuel properties of the upgraded products also appear promising.
- The team should provide a little insight into or hypothesis on the increased MEK formation over Cu-ZSM-5 with branched versus unbranched dioxolane feeds. The nature of the protons left on the zeolite and their ability to acidify dioxolanes back to BDO should be explained. An explanation of MEK as an intermediate for enhanced paraffin formation in the reaction network could be helpful as well. The olefin product yields (X, S) were impressive for the data presented, regardless of dioxolane precursor. The team should report the TOS information as well.
- The CUBI team has provided a promising pathway for sugars to SAF with immediate commercialization potential, as evidenced by a published paper and design report. The team should mention any efforts engaging ASTM at this early stage. The dioxolane intermediates research still has progress to make in terms of raising more technical awareness of the opportunity. The SAF analytical data seems very believable with the challenge on flash point, which can be overcome easily. There is a clear advantage of being able to process hydrous BDO as a feedstock. The presentation was very comprehensive and organized. This was greatly appreciated given the number of R&D activities within this project. This project could almost be its own consortium focused on various upgrading, solvent recovery, and catalyst regeneration strategies.
- This project was reported under the umbrella of CUBI. It focuses on de-risking the process of converting 2,3-BDO to SAF via the dioxolane derivatives developed in another project under the same umbrella. This project focuses on examining how the quality of the final SAF products relates to the various conditions of the dioxolane feedstock produced in the other project (like BDO versus dioxolane) and the process operation parameters, such as temperature. Such correlation will be important for determining which technology to focus on when conducting the R&D activity for scale-up. It would be beneficial if

the team could show how the selection of catalysts could affect the SAF products from various dioxolane feedstocks. It may also be beneficial to collaborate more closely with the teams focused on separation and recycling to develop a viable process under the guidance of TEA/LCA. The team already illustrates this direction by investigating the recycling of aldehyde. Overall, this project has illustrated appropriate progress to develop a BDO-dioxolane-SAF process that has the potential to be industrialized. The success of this project will help meet the SAF Grand Challenge for DOE.

- The project to upgrade BDO via dioxolane intermediates has made significant progress in its second phase, building on lessons learned from earlier work. The project benefits from well-structured project management and planning. Most importantly, the results have been very promising, with high conversion and selectivity toward olefins using a Cu/ZSM-5 catalyst without any evidence of coke formation.

- How to integrate this process with the synthesis of dioxolane is not clear at this point. I look forward to more progress in the overall process design.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for their time and all the positive feedback on our project. The questions they raised have been very useful as we plan the next stage of this work and have already stimulated thoughts on improvements to our approach and aspects where we need to focus more attention. In this regard, there are specific points raised that we would like to expand upon.

- "The team should provide a little insight into or hypothesis on the increased MEK formation over Cu-ZSM-5 with branched versus unbranched dioxolane feeds." The reviewers raise a very interesting point from a fundamental standpoint. MEK generally increases with increasing size of the aldehyde used in dioxolane formation, although a direct correlation between branching and MEK formation is not evident. A potential hypothesis for this is that, due to the size of the aldehyde, this exhibits a longer time in the zeolite framework due to confinement effects, leading to increased coke formation and partial catalyst deactivation for MEK reduction to the alcohol. This is just a hypothesis, and we aim to elucidate this in more detail.

- "An explanation of MEK as an intermediate for enhanced paraffin formation in the reaction network could be helpful as well." Alkanes are present in negligible amounts unless the temperature is increased, which drives the alkane reduction to alkenes. This over reduction results from the formation of alkenes from either the aldehyde or the BDO/MEK intermediate, which are indistinguishable from each other in this process.

- "The dioxolane intermediates research still has progress to make in terms of raising more technical awareness of the opportunity." We have a set of publications on this process ready to submit that will allow us to present a complete portfolio of this technology from fermentation to SAF, including newly updated TEA and LCA. We also continue to work with the separations and fermentation teams to present a comprehensive vision for this application.

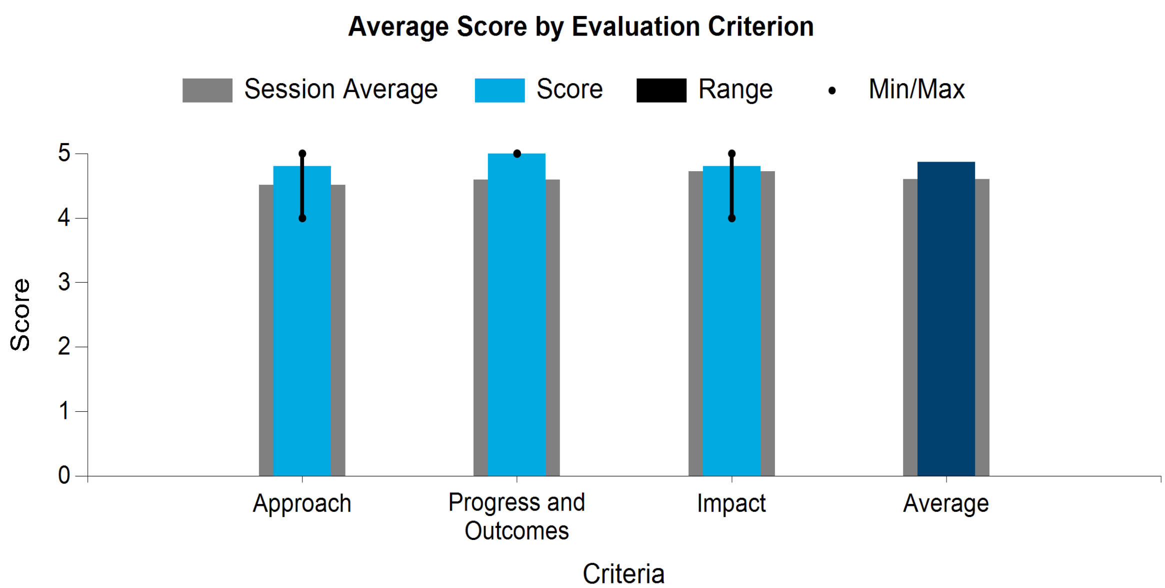
CONSORTIUM FOR COMPUTATIONAL PHYSICS AND CHEMISTRY – CHEMCATBIO

Oak Ridge National Laboratory

WBS:	2.5.1.301
Presenter(s):	Jim Parks
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$2,021,157.00

PROJECT DESCRIPTION

The CCPC is an enabling consortium of BETO that utilizes computational modeling to support the achievement of goals in ChemCatBio and other consortia such as the FCIC and SepCon. It comprises six national laboratories (ORNL, Argonne National Laboratory, Idaho National Laboratory, National Energy Technology Laboratory, NREL, and PNNL).



COMMENTS

- The CCPC is a BETO consortium made up of six national labs that applies multiscale computational science to enable bioenergy successes in other BETO consortia. The consortium's primary goal is to develop and apply a fundamental-science-based computational tool set that enables and accelerates the discovery and optimization of cost-effective catalyst materials for bioenergy applications, the translation of catalyst discoveries to higher TRLs, and the cost-effective scale-up of bioenergy technologies relevant to industry. The CCPC Tool Set Applied includes atomistic scale modeling (periodic DFT) for elucidating reaction mechanisms, theory and experimental characterization for identifying key reaction intermediates, DFT calculations, grand canonical free energy minimization, chemical bonding analysis to investigate structural and chemical changes during reaction over both catalysts, and *ab initio* molecular dynamics simulations plus enhanced free energy sampling to ascertain the mechanism and thermodynamics of deactivation. The impact and relevance of the CCPC Tool Set Applied include the determination of optimal reaction conditions for enhanced catalytic activity and selectivity, elucidation of reaction mechanisms of reductive etherification of n-butanol and 4-heptanone on Pd/$NbOPO_4$ catalyst, catalyst optimization for SAF production via CUBI, and a first-of-its-kind set of contaminants/poisons database for bioenergy applications. In addition, a full mechanism for deactivation and regeneration of ORNL's catalyst reveals strategies for preventing deactivation and/or accelerating regeneration, and new open-source code enables high-fidelity mesoscale simulations to optimize catalyst architecture for reactor configuration commercial performance targets. The CCPC also developed modeling tools to screen potential catalyst architectures before synthesis, and 3D X-ray reconstructions of commercial catalysts can also be directly imported for detailed performance simulations. Additionally, COMSOL bed models were developed for deconvolution of combustion kinetics and mass/heat transport effects from temperature programmed oxidation data complemented by spent and partially regenerated particle/coke characterization. Impact: CCPC models enable industry partners to advance bioenergy via CCPC's DFO program.

- CCPC is another enabling project, spanning five labs, that brings the power of multiscale modeling to ChemCatBio and other BETO consortia. The ambitious scales of the effort are impressive, as is the incorporation of the power of high-performance computing (HPC) into the effort. For such a broad but core enabling capability, it is critical that the effort evolves to meet the needs of ChemCatBio. It is clear in many ways that this is the case, based on adjustments from cycle to cycle on funding allocations to various computing scales. While this is a work in progress, this reviewer does strongly advise continued assessment of these levels to ensure that the signature aspect of CCPC (the significant investment in cross-scale modeling) is not lost. One piece missing from the presentation was a high-level description of the management of CCPC. Particularly given the scope and size of the effort, some details regarding how day-to-day management of the group occurs was a missed opportunity. In addition, I think that prior review questions regarding the ability to provide some type of metric for the degree of catalyst acceleration should not be lost to the wind. While I would agree that it is not easy, efforts to do so (even if difficult or unsuccessful) should at least be documented and disseminated. Regarding progress, let me be clear that CCPC checks all the boxes to me—the collaborations are tangible and varied across ChemCatBio projects, the funding allocation shifts to account for evolution in consortium project needs, advanced computing methods are being implemented (AI/ML/data science), and interactions with the data hub are vibrant and robust. The diversity of examples highlighted across ChemCatBio efforts was impressive, particularly the crossing of atomic, meso, and reactor scales. While the distribution of highlights will likely evolve in future cycles with the greater focus on reactor modeling, it is clear that a strength and signature of the effort its diversity and ability to walk between scales. I encourage CCPC not to lose this focus despite the heavier emphasis on the larger length scales. One question that could have been better articulated in the presentation involves allocation of time between consortia within CCPC. Some comments on this topic could provide broader context for reviewers. I think it is a legitimate question to discuss more broadly, as CCPC is a support engine for so many other BETO efforts. The HPC discussions were enlightening, and the focus on lessons learned was excellent, as it provides a starting point for productive use of new resources. The anticipated strategies for effective HPC use seem like the right ones. In particular, the Advanced Scientific Computing Research/Basic Energy Sciences collaborations on code development and leveraging the basic science programs' expertise with HPC (in theory) seem like clear wins for CCPC in advancing the HPC components of the project. One opportunity area mentioned in other review comments relates to modeling associated with additive manufacturing. As there are opportunities on the experimental side in this space, some of which were demonstrated by DFA projects reviewed this cycle, I believe there are opportunities connecting theory to these systems, whether they involve catalyst synthesis or reactor design. In particular, developing real-time AI/ML responsive systems is something that should at least be considered. Perhaps this is still at more of a fundamental phase, but I do believe this type of real-time feedback between theory and experiment is not far off and can have an impact in many arenas, one being the manufacturing space. The 35 total publications are quite impressive. In the future, a high-level breakdown of the percent of these reports that are collaborative with PIs in CCPC projects versus stand-alone reports would be valuable. I don't doubt the collaborative nature of the effort, but it provides a simple quantifier for evaluation. It is good to see review comments from past cycles being implemented, especially regarding working more with industrial partners. From the vignettes presented, the impact these collaborations have on the companies was clear (the Pyran 1,000x scale-up comes to mind as one signature example). The somewhat flexible degree of tech transfer and the experience of working with both large and small industrial entities was a nuance that came out clearly in the presentation and Q&A; I had underappreciated this. One point to consider: Given the now extensive pivot to reactor modeling, is there some way to develop tools in this space that could be combined with other data hub efforts accessible to the broader catalysis/engineering community? Currently, this seems like a potential gap in the suite of tools offered by that project and one that could be incredibly impactful. As a whole, it is clear that CCPC is having a significant impact on ChemCatBio, the greater BETO consortium portfolio, and its industrial partners.

- The team has done a great job of developing DFO projects and moving the HPC initiatives forward. More atomistic studies have been conducted, providing key insight into C=0 and C-C bond activation and most probable surface structures.
- The fact that the CCPC is able to stitch the modeling across multiple scales, coupled with experimental validation, makes this team very unique. They have a strong collaborative approach where they are doing work with several consortia. They are the oldest consortium in the BETO portfolio and can be considered state of the art. Their strength is how they adapt and collaborate with others. This flexibility enables them to stay on the leading edge of technology and solve important problems creatively. The team continues to stay flexible, working with more industry partners while solving problems at the atomistic level. More emphasis on the goals and objectives within the project plan over the next few years can be bolstered with additional commentary on DEIP and EJ activities.
- CCPC continues to bring major value across all of ChemCatBio, working a variety of projects across multiple scales using different *ab initio* and modeling tools. The agreement between the DFT predictions and the characterization experiments for the VFA work could be interesting. CCPC has been involved in several successful DFO funded collaborations. The structure-activity relationship between palladium and etherification rates was simulated along with surface mechanistic detail. Similarly, the overlay of experiments and modeling calculations would be useful for that discussion. Spillover surface calculations for unsaturated bond activation provided good insight and should be connected back to the key synthesis parameters responsible for controlling it. The formation of CuH active sites as migrating from silanol nests is an important observation and result. The oxidation mechanism for regenerating the proper Cu-Si distance should be explored further. The Guerbet reaction kinetic modeling will be useful for the community when published eventually. The reaction network selected should be verified and justified. Catalyst deactivation simulations using HPC matched experimental images very well. The modeling work with Pyran seems to be helpful for scale-up and should include a few experimental data points. The scale-up modeling with Catalyxx appears to be proceeding well. The larger 5-ton reactor radial temperature profile should be provided along with the axial analysis.
- The Johnson Matthey partnership for creating and modeling extrudates appears to be promising. CCPC continues to demonstrate successful DFO projects, as indicated by collaborations with Forest Concepts, Pyran, and Catalyxx. All of these projects have a clear path to contributing deeply to commercial technology development. The team should consider how to collaborate with the data hub project as well as an industrial partner to provide multiscale modeling software tools at the commercial level. By leveraging HPC capabilities to engage the external bioenergy community, the team will establish a lasting impact and legacy.
- CCPC develops and applies a computational tool set to support catalyst design and deployment, as well as process scale-up.
- CCPC is a consortium composed of six national labs. They provide computational support ranging from DFT for catalyst design to mesoscale modeling for reactor design. They provide unique enabling technologies to accelerate the development and deployment of catalysts for bioenergy-related conversion. Their role in this program is unique, especially in an era in which computation is playing a more and more important role in the R&D activities. CCPC has shown a successful way to manage the

diverse efforts in the team. It would be beneficial to be more creative in developing activities that contribute to DEI and workforce development.

- CCPC has illustrated impressive progress from all scopes. One note is that the effort of CCPC is shifting from catalyst design to reactor process modeling. This shift is reflected by the funding allocation and the ongoing projects. At the DFT for the catalyst design aspect, CCPC has illustrated the success of several projects, including revealing the deactivation mechanism of catalysts and the mechanism for reductive etherification on Pd/$NbOPO_4$ catalysts. On the mesoscale modeling, CCPC has also illustrated their outstanding abilities, including analyzing the effect of particle size, shape, and porosity on the performance of engineered catalysts. These accomplishments, which have been achieved by closely collaborating with the other forces in the program, are accelerating the development and deployment of catalysts and help fulfill DOE's goals for SAF and GHG emission reduction. It would be more beneficial if CCPC could be more proactive or take a more leading role in the catalyst design and development efforts. It would also be beneficial if CCPC could adapt more advanced computational technologies, such as deep learning, to enhance their R&D outcomes.

- The computation-based design of catalysts and the reaction process demonstrates a clear connection between CCPC's effort and DOE's goals for SAF and GHG emission reduction. The approaches used by CCPC establish a clear connection with their outcome. CCPC may not generate any products that can be commercialized immediately or directly. However, such efforts play a role that cannot be replaced in this era, when we are witnessing the growth of computation.

- CCPC has been a leading force in computational catalysis, providing critical support to accelerate biomass conversion projects through long-term investment and support from BETO. The collaboration between national labs and computational experts with strong bioenergy backgrounds, who have shifted resources toward scaling up, has proven to be highly effective in supporting biomass conversion projects. Cosponsoring computational projects with industry has also been an excellent approach to optimize resource utilization. CCPC's numerous contributions and impressive achievements are commendable. The scaling up assistance provided by CCPC to Pyran is an excellent showcase.

- Moving forward, in addition to continuing its current efforts, such as mechanistic studies, upgrading data hub, and realistic catalyst structure, CCPC should pursue research in both fundamental and applied directions. It is essential to maintain a balance between these two research directions, as a lack of fundamental understanding could hinder progress in applied research. Thus, it is vital to continue funding fundamental studies, especially those that incorporate AI and ML techniques.

PI RESPONSE TO REVIEWER COMMENTS

- The CCPC team thanks the reviewers for their comments. Notable positive comments from the reviewers include compliments on the number and variety of collaborations and related successful outcomes, including collaborations that extend beyond BETO (e.g., the Basic Energy Sciences program), the unique and important role that the CCPC serves in the BETO program, and the multiscale modeling approach of the CCPC. The CCPC is encouraged to maintain our approaches in these areas based on the positive feedback. The reviewers offered a number of guiding comments that the CCPC values as constructive feedback. While complimentary of the multiscale approach of the CCPC, reviewers advised actively balancing the research across the multiple scales to maintain both fundamental discovery science and scale-up efforts. The CCPC shares the concerns of potential misbalance across the scales of research, and in particular, the current risk to underserving the atomic-scale catalysis research that is critical to the ChemCatBio catalyst discovery cycle. Reviewers also encouraged more emphasis on AI/ML approaches. Again, the CCPC agrees with this feedback and seeks to advance further on the successes utilizing AI/ML to date, and to do so by further leveraging the unique HPC resources in the national lab system. The reviewers also suggested further collaboration with the data hub project or industrial partners to make multiscale modeling tools available to the community. The CCPC has made available to the public open-source code of models developed previously in the spirit of this feedback, and the CCPC will consider what more can be done in this area with the data hub project and industry partners. Additional suggestions from the reviewers related to outreach and impact included recommendations to outline more specific goals and objectives for DEI and workforce development. Again, the CCPC appreciates this feedback and will look to define, incorporate, and achieve such objectives. Overall, the CCPC appreciates the constructive remarks and guidance from the review panel, as the recommendations are in line with the CCPC's own vision and priorities moving forward. Any additional resources provided to the CCPC will be utilized to strengthen the balance of multiscale research, advance CCPC tool sets with AI/ML and HPC, extend the impact to the broader bioenergy community, and advance DEI and workforce development activities.

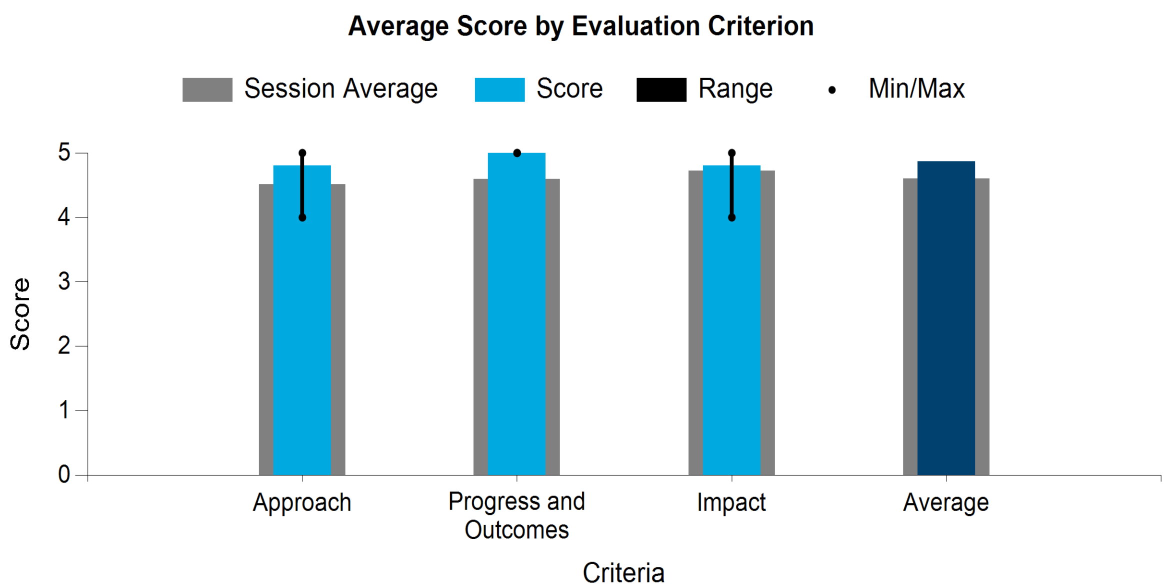
ADVANCED CATALYST SYNTHESIS AND CHARACTERIZATION

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.5.4.304
Presenter(s):	Susan Habas
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$581,473.00

The ACSC project, in close collaboration with the ChemCatBio enabling capabilities, (1) provides actionable insight into catalysts under realistic process conditions for each of the Catalytic Technology projects, (2) addresses overarching catalyst durability challenges central to ChemCatBio, and (3) adapts and applies new synthesis methodologies and *in situ*/*operando* characterization capabilities to meet the needs of the Catalytic Technology projects. The outcome is a reduction in the time required for the Catalytic Technology projects to meet transportation decarbonization targets. The ACSC project contributed to the demonstration of a fourfold acceleration in the catalyst and process development cycle for the ethanol to olefins process within the Upgrading of C2 Intermediates project. It did so by leveraging the knowledge, capabilities, and expertise developed within ChemCatBio for the Upgrading of C1 Building Blocks project. The outcome was a threefold acceleration in the time leading up to licensing of the technology, highlighting the impact of the collaborative and integrated resources of ChemCatBio on technology maturation. The enabling capabilities will leverage the capabilities and expertise developed in these efforts to provide similar insight into engineered catalysts, accelerating the catalyst and process development cycle and reducing commercialization risks for catalytic technologies.



COMMENTS

- The synthesis and characterization work was excellent. This is a key enabling technology/project for the success of ChemCatBio.
- This project had strong support of ChemCatBio, direct engagement with all projects, and joint milestones with all catalysis projects.

- This project enables evaluation of catalytic performance for engineered catalysts and develops structure-property relationships. Clear benefits to the catalyst development cycle can be seen.
- The synthesis and characterization are world-class. There is evidence of direct industry interactions. Outputs included 18 publications, eight external presentations, five direct-funded industrial engagements, webinars for community outreach, and novel characterization techniques.
- This enabling project is focused on accelerating catalyst and process development through contributions in synthesis, advanced characterization, and microscopy. The effort spans three lab partners with expertise ranging from a variety of synthetic methods to X-ray methods to multimodal microscopy. Discrete examples from multiple projects demonstrate the critical role of ACSC in its enabling capacity. The project overview in the presentation highlights the feedback loop between all capabilities. Even though this effort involves lab groups, this reviewer is impressed at the clear signs of integration across ACSC and the interactions with other upgrading projects. Part of this may involve the management and project structure, where joint milestones with individual projects create a level of dual ownership. Regardless, the synergy is a clear strength of ACSC. In prior review cycles, ACSC was challenged to quantify their ability to accelerate technology development. They answered this call, showing a fourfold reduction in development time. This demonstrates their responsiveness to reviewers and paints a clear picture of the project's value to the consortium. Furthermore, the group is attempting to be responsive to ChemCatBio's evolution and other review comments, with a movement toward more industrially relevant catalyst formulations. The current partnerships cultivated with catalyst providers should help make this transition a smooth one. The types of advanced tools that may be needed could evolve, particularly the analysis of spatial resolution as one moves to extrudates. There are many impressive things to note about ACSC, but I would particularly highlight the following. The first is their expertise in the synthesis and characterization of a broad range of materials—from Cu zeolite to carbide/nitride supported materials. This suggests that, as ChemCatBio interests continue to shift, there is complete flexibility in the catalysts accessible to the group. The second strength is the range of scales characterized—from individual active sites to bulk materials. This is a significant challenge but is critical to accomplishing consortium goals. ACSC, with access to a broad swath of advanced tools within the national lab complex, clearly meets this need. Finally, the annual reevaluation cycle to reinvigorate the methods used is another key strength. This is a great general operating procedure and has recently led the synthetic push to advanced engineered forms of catalysts as well as the micro-X-ray absorption spectroscopy technique. A few areas of consideration include the following. First, there is potential for greater interaction with the RAPID Institute/incorporation of advanced additive manufacturing techniques. Although the consortium has implemented such methods in specific projects, this group is poised to leverage this area in unique ways. I understand that specific systems are more amenable than others, but I encourage the group to look to exploit this area given the opportunities provided to synthesis and reactor design. Second, while electrocatalysis was mentioned somewhat in passing, long-term evolution could involve hybrid thermal/electro or fully electro technologies. I would encourage ACSC to remain agile in the types of materials studies (revisiting carbide/nitride materials at some stage, perhaps) and characterization methods employed so that opportunities in the space of nonthermal energy inputs can be fully realized by the group when they present themselves. No significant DEI component was articulated, but it was communicated that the ChemCatBio-wide strategy will be implemented. I don't have doubts that the next cycle will show increased focus on this area. The specific examples provided in the presentation highlight the defined contributions of ACSC to other ChemCatBio efforts. I would highlight one, the University of Southern California/ACSC collaboration, which altered cost/energy inputs in the synthesis of MoC catalysts, resulting in a 50x increase in throughput, which is quite impressive. I would also note that external partners, like this one, are well chosen based on area of expertise, which likely results in the interactions being so fruitful. The significant enabling highlights provided for each of the major task areas were impressive. They provide a comprehensive picture of the acceleration of a suite of technologies across ChemCatBio and establish ACSC as a signature crosscutting effort for ChemCatBio. Evolution from prior cycles is also evident. Time to development

with collaborative projects can now be quantified. Also, the pivot from certain techniques—neutron vibrational spectroscopy as one example—is well justified based on the evolving needs of the consortium and is responsive to the science and technology required in individual projects. In addition, the data and catalyst tools being developed in ChemCatBio are integrated into ChemCatBio efforts, as the CatCost tool was highlighted as a value add for Ni nanoparticle synthesis. I have mentioned the acceleration charts elsewhere, but the level of detail is impressive and provides unequivocal evidence of the value ACSC provides to the consortium. Although these charts are timely to prepare, I think continuing to evolve the current example or also expanding on another system in future cycles would continue to demonstrate the unique value the project provides to the broader portfolio. The 18 collaborative publications—the majority if not all of which are with other consortium project PIs—is a testament to the project's role in the broader effort. Prior reviews indicated that interaction with the industrial partners in DFAs was a missed opportunity, and in this cycle, five such projects involved ACSC collaborations. The responsiveness to review and BETO directions is clear. Two patents also resulted from the work directly in ACSC. The ability to develop separate IP from the other projects is impressive given the prescribed role of ACSC as such a collaborative endeavor, which indicates a level of independent technology development within the project. The impact in all facets—when measured by output, level of collaboration with other projects, or connection with industrial partners—is excellent.

- The ACSC project continues to be one of the most successful endeavors within the BETO portfolio, focusing on the problems that enable catalysis R&D to accelerate and using tools that help elucidate the critical mechanisms and root causes behind the bottlenecks in material synthesis. The core of the success of this project partly stems from choosing the right collaborators and problems to pursue, thus allowing for actionable deliverables to emerge in a timely manner.

- ACSC continues to be a strong project with a solid approach, supporting all aspects of ChemCatBio with advanced synthesis, *in operando*, imaging, and spectroscopic tools. The team's work is the heart of the catalytic upgrading effort. They work directly with ChemCatBio projects and try to respond to urgent requests as well. The use of micro-X-ray absorption spectroscopy for studying engineered forms is a next-level approach and tool for ACSC. The project team clearly understands how to plan and accelerate catalytic material research. More discussion around the instrument reliability program for these indispensable resources should be offered, as well as the DEIP and EJ commitments.

- The team continues to use advanced characterization tools to provide critical insight into the development of heterogeneous catalytic materials across the entire ChemCatBio Consortium. An excellent, detailed, and thorough chronology was provided, highlighting the impact the ACSC project had on normal catalyst development cycles from formulation inception to material technology licensing. A normal cycle could range from 7–10 years, as in the case of the Cu/BEA system, versus 3–5 years for the Cu-Zn-Hf/BEA system. This is a major accomplishment, and fundamental research questions were also answered along the way. Another key accomplishment was using *in situ* Fourier-transform infrared spectroscopy to identify a low-temperature oxidative regeneration cycle for the STH materials. It was interesting to observe how a small degree of sintering creep tends to help the C4= selectivity with each regeneration cycle. The team should explore this phenomenon more and collaborate across ChemCatBio to enhance understanding. There was excellent characterization work provided for the Pt/TiO_2 deactivation during pointing to metal poisoning and surface instability during CFP upgrading. The team should be clear regarding the re-dispersion aspects of the regeneration protocol allowing for full recovery and should show the changes in exposed surface area. The role of fully reduced metallic copper on diol deoxygenation chemistry should be clarified a little further and is quite interesting. The team should further explore how to use the non-carbidic coke to their advantage during the metal carbide regeneration cycle.

- Significant and important peer-reviewed journal articles and project reports have been generated from this project. There have been 18 peer-reviewed publications since the last Peer Review. Fifty percent of the industry projects in ChemCatBio utilize the ACSC. The IAB gave excellent feedback. They are currently helping BETO reach its goals by characterizing catalysts for key routes. They are also helping with the SAF Grand Challenge, as well as the CO_2 electrochemical reduction techniques.

- ACSC is an enabling project in the Catalytic Upgrading program. The goal of this project is to provide actionable insights into catalyst development challenges under realistic process conditions by leveraging world-class synthesis and characterization capabilities across multiple DOE national laboratories. This is an unreplaceable asset in the whole program.

- The project's R&D activities focus on two directions: direct engagement with specific projects to assist the synthesis and characterization of catalysts and overarching challenges in catalyst synthesis and characterization. Both directions are important to the success of this project as well as the whole program. The team has illustrated their ability to balance the two directions well. They also developed three modes for the experiment projects to collaborate with ACSC, casting their different needs. However, keeping the balance between the two directions is an important factor and needs careful management in the future. With more research activity extending to engineered catalysts, it is critical to still build a close connection between the efforts addressing the direct engagement and those addressing overarching challenges. The team has illustrated their commitment to DEI. It would be beneficial if they could be more proactive in workforce development.

- They have successfully improved the synthesis of several catalysts for several C1 and C2 projects. They also collaborate with the other enabling team to analyze the catalyst deactivation mechanism and develop actionable technologies to mitigate the deactivation. This progress is appropriate and helps achieve the SAF and GHG emission reduction goals set by DOE. They have shown a clear risk analysis and mitigation plan to help seize the success of their project. It would be beneficial if the team would address more overarching challenges in catalyst synthesis via these direct engagements. It would also be beneficial if the team could consider deploying additive manufacturing, high-throughput technologies, or even AI to help accelerate the design of synthesis pathways for catalysts.

- The ACSC project enables the other projects to possess catalysts with the desired properties. This is the enabling technology that makes the other experimental R&D activities possible. It also provides a crucial technology to lower the cost of catalyst preparation and extend catalyst lifetime, making commercialization possible.

- The ACSC platform leverages expertise to expedite the development of catalytic processes through synthesis and characterization. It combines cutting-edge *in situ* techniques for both bulk and surface analysis with computational modeling to identify active sites and deactivation mechanisms, along with throughput and statistical tools, resulting in a powerful approach for catalyst development. The platform's project management is exceptional in supporting multiple projects with rapid response times, and the outcomes have been remarkable, reducing catalyst development time by a factor of four.

- This platform should continue to serve as a driving force for new projects. Bottlenecks in resources should be identified, and additional funding should be allocated if necessary to ensure that critical resources have backups, especially during unprecedented challenges like supply chain disruptions during the pandemic.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful insight and constructive feedback. Notable positive comments included (1) the critically important role of the ACSC project as an enabling capability within ChemCatBio for accelerating the catalyst and process development cycle as well as tackling overarching catalysis research challenges, (2) the successful management of the ACSC project and its integration with the Catalytic Technology projects and industrial partners, and (3) the responsiveness of the team to the evolution of consortium and previous reviews, with a transition toward more industrially relevant engineered catalyst formulations. We also appreciate the enthusiastic responses regarding quantification of the catalyst and process development cycle. This effort, in collaboration with other enabling capabilities and Catalytic Technology projects, enabled us to set a baseline for the time required to develop next-generation catalysts that meet target metrics, and then to exceed this time by a factor of four for a related catalyst system by leveraging the knowledge, capabilities, and expertise within the consortium. Going forward, this same approach will be applied to engineered catalyst formulations. Success in this next development cycle will require, as the reviewers have noted, continued adaptation and demonstration of characterization techniques with spatial resolution across multiple length scales and cost-effective, scalable synthesis methods informed by industry partners that provide targeted catalytic performance while reducing risks associated with commercialization. In addition to continuing to develop *operando* characterization capabilities and expertise that keep pace with the evolving needs of ChemCatBio, the reviewers highlighted synthesis expertise for a broad range of materials as a strength. The reviewers advised addressing overarching catalyst synthesis challenges in conjunction with relevant characterization to flexibly respond to new catalytic technologies. As suggested, we will continue to explore new catalyst materials such as transition metal carbides and their utilization and incorporate additive manufacturing or high-throughput technologies in conjunction with AI/ML techniques to help accelerate the design of synthesis pathways for catalysts. This is an ongoing goal of the collaboration with the University of Southern California, which was noted by reviewers as a strength, and we will continue to foster this partnership. Further, our partnerships will be leveraged to develop project-specific goals and objectives for DEIA and workforce development, as suggested by the reviewers, in addition to targets that will be implemented consortium-wide. For example, providing training in catalyst characterization for students has been highlighted as a need by current and prospective partner institutions and can provide a framework for broader outreach. Overall, we appreciate the positive feedback and constructive guidance from the reviewers and will seek to continue balancing our commitment to direct engagement with the Catalytic Technology projects to answer pathway-specific questions with our efforts to tackle overarching catalysis challenges that can provide broad value to the bioenergy community.

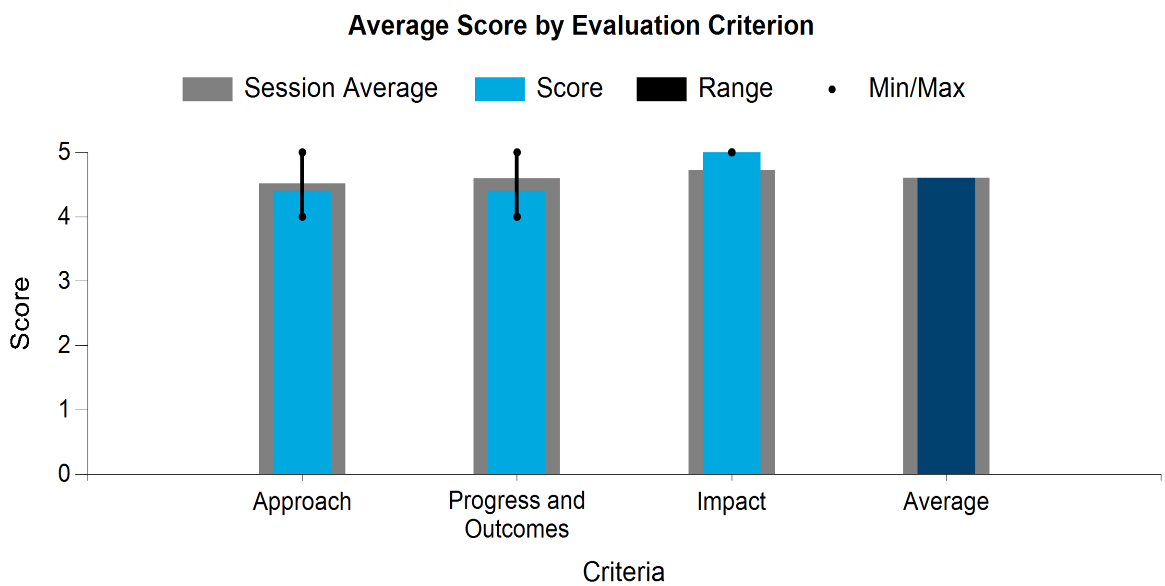
CATALYST DEACTIVATION MITIGATION FOR BIOMASS CONVERSION

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.5.4.501
Presenter(s):	Huamin Wang; Karthikeyan Ramasamy; Katarina Younkin; Michele R. Jensen
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$332,910.00

Catalyst Deactivation Mitigation for Biomass Conversion will enable the accelerated development of commercially viable catalytic processes for biomass conversion to SAF technologies by tackling catalyst deactivation issues that have the potential to impact multiple BETO-funded programs. Significant challenges exist for developing catalysts with long lifetimes for bioenergy applications due to some unique problematic properties of biomass-derived feedstocks. This project, an enabling capability of ChemCatBio, serves as an R&D team specialized in identifying catalyst deactivation mechanisms and developing solutions for improving catalyst lifetime. We coordinated and worked collaboratively with various projects to address some overarching catalyst deactivation challenges and to support specific technologies in expanding catalyst lifetime. Examples include (1) a comprehensive study on the impact of water on different types of catalyst active sites and mitigation strategies, and (2) enhanced understanding of the deactivation mechanisms leading to new catalysts with improved stability for ethanol and butanediol conversion. We provide fundamental insights into catalyst longevity to guide the rational design of robust and industry-relevant catalysts. We directly address catalysis barriers to improve catalyst lifetime and achieve ChemCatBio's goal of accelerating catalyst development and technology readiness for industrial application.



COMMENTS

- The ChemCatBio project aims to provide foundational insights and actionable recommendations for extending catalyst lifetime in biomass catalytic conversion, enabling cost and risk reductions of catalytic processes for BETO conversion technologies. The project's relevance lies in addressing the critical need for catalyst stability in catalysis and biomass conversion R&D and avoiding pitfalls during technology maturation. The goal is to increase awareness of catalyst deactivation issues and focus on catalyst stability within ChemCatBio through a collective and collaborative effort. The approach involves a systematic study of catalyst deactivation, including multiple approaches to understanding the deactivation mechanism, providing actionable recommendations, and developing regeneration methods to address deactivation. Progress has been made in addressing overarching catalyst deactivation challenges, such as the impact of water on multiple catalysts, regeneration methods for coke removal, and the impact of catalyst scale-up on stability. The project has improved catalyst lifetime for specific ChemCatBio catalysis technologies, such as C1 upgrading, C2 upgrading, CUBI, and CFP. The impact of the project is significant in terms of improving catalyst lifetimes, achieving cost and risk reductions for conversion technologies, filling gaps, and providing a knowledge base for rational design of more stable catalysts. Ultimately, this project will lead to accelerated catalyst and process development, a better understanding of catalyst deactivation issues, and the development of tools and methods to evaluate stability more quickly.

- Studying targeted catalyst deactivation across consortium projects is a critical need, particularly given the inherent challenges of biomass use as a feedstock (mixed and variable feed, water content, etc.). The specific emphasis of the effort on characterization/advanced tools to understand structure and induced changes in catalyst composition is a sound approach and aligns well with the existing strengths of the national-laboratory-led consortium. While deactivation studies have ties to basic understanding of catalyst function, they also have direct cost benefits. I would specifically highlight the strong focus on stability, which is key for scalable/deployable technologies. The approach is well aligned with an effort that seeks not to duplicate industry/field practices (with more focus on activity and selectivity), but to lay the foundation for reducing the catalyst development and deployment cycle by focusing on a gap between the research and development/deployment spaces that is sorely in need of being addressed. The major areas of focus—coking, contaminants, and water—are logical. At the same time, the overview did a good job connecting the broader areas to science questions that must be studied to gain the type of knowledge that can impact catalyst design and optimization. The deactivation pathways of a process influence all aspects of the system—whether it be feedstock inputs or the catalyst itself, along with reactor engineering. As the consortium continues to evolve and the types of problems examined increase in complexity, this project is encouraged to continue to think beyond just improvements in the catalyst piece, and to also consider feedstock and reactor improvements to performance. The pivot toward the study of primarily copper zeolite catalysts and engineered systems is appropriate given prior review feedback and the heavy reliance on these systems by ChemCatBio. The upcoming cycle seems focused on the study of more realistic catalysts, greater collaboration with theory, and perhaps exploring reactor advances. These all seem like reasonable directions to pursue. In particular, the nature of specific catalyst formulation will add a layer of complexity beyond prior studies of powder-based systems. One aspect that can perhaps be further explored as complexity builds is the nature of feedstock streams and the impact on catalyst performance. This is perhaps addressed to a degree with the contaminants theme, but I believe there could be valuable studies that explore the impacts of feed mixtures on catalyst behavior beyond what is currently done. Additionally, more time could have been spent with a forward-looking lens, specifically on the changes and challenges anticipated in moving to a heavier emphasis on the study of engineered catalysts. The management plan is suitable and connects, as it should, with broader consortium themes while also being integrated with key aspects of individual projects. Sufficient details were provided on more community-facing activities (perspective on deactivation, etc.) and contributions to individual consortium projects during the last project cycle. Looking forward, the project should also be thinking about moving beyond deactivation in zeolites, especially with some focus on the use of non-PGM systems necessitating exploring other catalyst/support systems. Being ready to enable study of deactivation involving alternative energy inputs (nonthermal) and new catalyst systems will be important to advancing the broader goals of ChemCatBio. DEI efforts were mentioned in passing. There is an opportunity to have some impact in this space, given the collaboration with an MSI/EPSCoR institution. The project would benefit from further fleshing out the details of the interactions and outcomes in a subsequent review cycle. The track record in prior cycles of identifying discrete topics (inorganics impact as one example) and making measurable progress improvements on specific consortium projects is notable. As an enabling capability of ChemCatBio, the synergy of the deactivation effort appears to be increasing, and future plans would continue to strengthen these ties. The specific examples presented reinforce interaction with other projects in the consortium, as one would expect. The well-organized vignettes demonstrate clear value across various projects in the consortium. What could be better delineated in the slides is a discrete degree metric of improvement in some of the catalyst systems. It is not clear in most cases how new, improved catalyst formulations impacted the stability, conversion, etc. Scaling factors (double lifetime, etc.) would be a rough way to disclose the impacts, and project members are encouraged to state these in future cycles. The science focus of the work is strong, but some type of metric of improvement, even if crude, is desirable. The publication of five papers, all in high-impact-factor journals, is commendable. The review article in particular, along with the blog, provides ways to extend project impact beyond just specific ChemCatBio projects. Furthermore, the inclusion of contaminants in the property database is notable and provides a broader resource to the catalysis community. Development of standard deactivation protocols could also be incredibly impactful. As a suggestion, the project could look to expand awareness of the effort through regular webinars as a visual complement to the blog. For the level of support of the activity, the work has an outsized impact on both the ChemCatBio projects and the broader catalysis community that should be commended.

- The team has provided a very focused approach for dealing with the key catalyst deactivation technical gaps facing the ChemCatBio community, with an emphasis on coke, water, and feed contamination in both powder and engineered forms. Much progress has been made with developing regeneration techniques and understanding reactor loading profiles.

- The project has a very clear and methodological approach to studying and understanding deactivation. This is a well-designed project. The team is working across ChemCatBio in a close manner, making sure the work is relevant to the deactivation concerns. The technical approach is to first identify the deactivation problem, determine the mechanism, develop a mitigation approach, and then verify the solution. The interwoven challenge of contaminants, water, and coke is a good way to simplify the mission. The team will also get more involved in the engineered structure stability efforts moving forward. Unfortunately, the state-of-the-art deactivation programs are often proprietary to commercial catalyst manufacturers. The team can either engage the IAB further or collaborate openly with catalyst suppliers on targeted initiatives. The project plan appears to be clear and focused with reasonable objectives. The team should continue to highlight the DEIP and EJ efforts, as PNNL is known to be highly active in this area.

- The project has informed ChemCatBio about key modes of deactivation and solutions to rectify and regenerate the catalyst. The use of model catalysts to understand real catalysts under real reaction conditions is often very tricky. The team was able to pull it off for the Pt/TiO_2 system, developing a regeneration method that involves removing potassium impurities. It is good to see the collaboration with CUBI start to define the 2,3-BDO feed spec sheet with respect to sugar, potassium, and water levels, using deactivation severity as the standard. The concept of an axial deactivation reactor profile is an effective analysis with important unit configuration implications. The team should disclose the coprocessing feed content level with an acceptable impact on the diesel hydrotreater performance. The dependence of Cu dispersion on the water content in ethanol was a good observation, and the results of improved stability should be shared if available. The situation with water and surface modification should be a high priority for this project, with an emphasis on stabilization solutions. For the Pt/TiO_2 system, they identified five modes of deactivation contributors: poisoning, sintering, coke, bulk crystalline phase change of the support, and attrition. The team learned that water must be managed in the ethanol feed to mitigate the Cu sintering.

- The deactivation project expands beyond ChemCatBio and will provide key information for the entire global catalyst community, as indicated in the high-impact publications released. The review article recently published on deactivation due to the conversion of biomass was an excellent contribution to the research community. By gaining more fundamental, root-cause, mechanistic information, the team should continue to pursue opportunities to bolster the predictive power of models in short time scales.

- This enabling project targets an overarching challenge for realizing bioenergy: catalyst deactivation. The goal of the project is to provide foundational insights and actionable recommendations for extending catalyst lifetime in biomass conversion.

- This project deploys an integrated and collaborative effort to address the catalyst deactivation issue. They work closely with ChemCatBio projects for specific catalysts. They also collaborate with other enabling projects, including CCPC, ACSC and Data Hub. They have also built close communication with stakeholders, developed joint milestones, and set up go/no-go decisions to help manage the projects. Their research targets specific catalysts such as $Cu/ZrO_2/SiO_2$ and Y/Beta for ethanol to butenes or zeolite catalysts for CFP. Meanwhile, they address overarching stability challenges when studying those specific catalysts. They focused on three interwoven challenges: contamination, water, and fast coke formation. They started to shift from model catalysts to engineered catalysis due to the need of the program. Overall, this project has deployed appropriate approaches to conduct their R&D activities. They showed clear management and an efficient way of communicating with the other groups. It would be beneficial if they could be more proactive in their DEI efforts.

- The project has illustrated impressive progress in supporting ChemCatBio efforts and addressing the overarching challenges related to catalyst deactivation. The team has helped identify potassium as an important feature to reduce catalyst lifetime, as well as revealing the mechanism and developing actionable methods to mitigate the deactivation. It would be beneficial if the enabling projects could be tied together more closely and build a cross-process platform or knowledge base that can address some overarching challenges that are common in multiple processes.

- Catalyst deactivation is one roadblock to commercializing the biomass conversion process. This project utilized an integrated and collaborative approach to address the deactivation challenges with the aim of extending catalyst lifetime. These R&D activities have shown a clear impact on enabling commercialization of the biomass conversion process and helping DOE achieve its goals in SAF and GHG emissions. Although most of the R&D activities focus on specific catalysts, the overall goal focuses on several overarching challenges. Resolving these challenges will help improve the design and deployment of the catalysts. It would be more beneficial if the project would prepare the harvested knowledge and data in a digital format that could be used for the AI design of catalysts.

- Developing a project that specifically addresses the deactivation challenges in catalytic upgrading during biomass conversions is a strategic approach to promoting both fundamental understanding and commercialization. Although complicated, with many variables, the deactivation mechanisms share common features for heterogeneous catalysts. The outcomes of this project are impressive, not only in terms of the progress in identifying the deactivation mechanisms, but also in terms of the fruitful regeneration efforts. The learnings from this project will not only accelerate the biomass conversion projects, but also benefit the entire catalysis society. However, one challenge with the deactivation study at the benchtop scale is developing lab deactivation protocols that can predict the performance and lifetime of a catalyst in commercial units. Typical deactivation protocols for automobile emission control catalysts and fluid catalytic cracking catalysts could be used as references. Cyclic reactions at low and high temperatures can be conducted without modifying the reaction systems to quickly assess the sintering or coking issues of catalysts. For future investigations, it should be useful to invest in a fixed-bed steamer with a horizontal tube furnace. Such equipment requires minimal capital investment and enables efficient deactivation under high temperatures, high steam, and other poison gases for multiple samples. Furthermore, collaborating with industry partners can assist in developing deactivation protocols.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their support for the project, their thoughtful insight, and their constructive feedback. We agree on the importance of addressing catalyst deactivation, a key roadblock in commercializing the biomass conversion process. The central goal of this project is to overcome these challenges, aiming to enhance the design and deployment of the biomass conversion process. By doing so, we can contribute to DOE's goals in SAF production and GHG reduction. We are grateful for the positive comments regarding the impact of our work on the ChemCatBio projects and the broader catalysis community, the outcomes of this project related to identifying in-depth deactivation mechanisms and fruitful regeneration methods, and our collective and collaborative effort to address the overarching deactivation challenges. We will continue to work closely with other enabling projects to utilize diverse tools, tackle the most impactful catalyst stability challenges, and balance overarching challenges with the specific needs of catalysis projects. We agree with the reviewers that this project should continue to provide specific metrics of improvement in certain catalyst systems, and we are looking forward to working closely with catalysis project teams to quantify these aspects. We agree with the reviewers about the importance of engaging with industry to access existing state-of-the-art deactivation programs. We are actively interacting with our IAB and industrial partners, including a catalyst company through our accelerator partnership, to facilitate industry engagement. Developing standard deactivation protocols is another valuable suggestion from the reviewers, and we are actively exploring this possibility. We are committed to sharing our generated knowledge with industry and catalysis R&D communities through various channels, including publications, workshops, webinars, ChemCatBio technology briefs, and Data Hub. To support DEIP initiatives, we will maintain our collaboration with the MSI institution and actively engage in our consortium-level efforts.

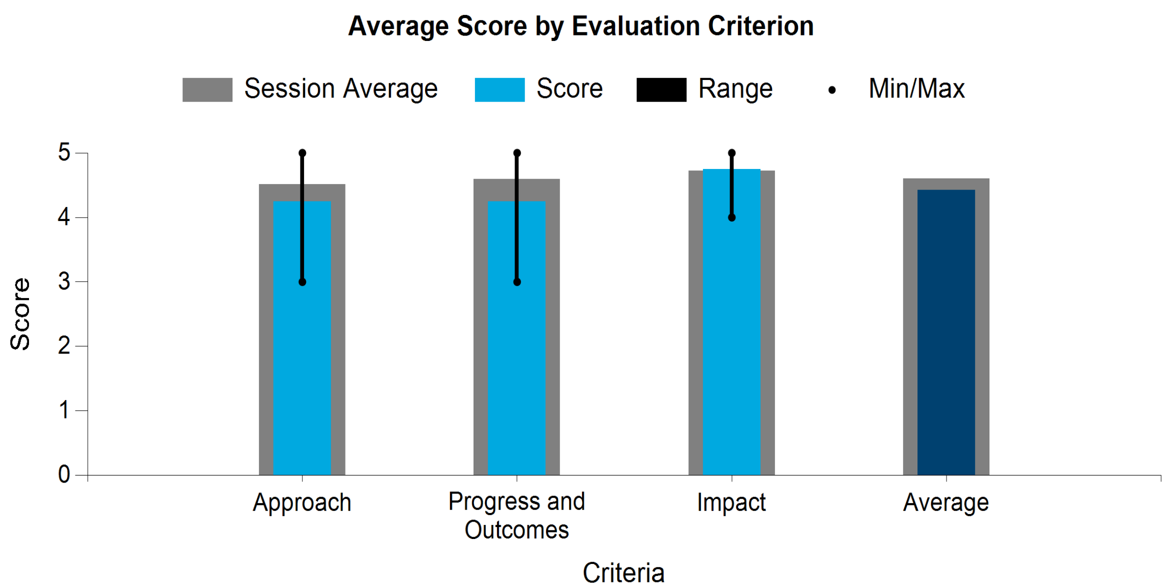
CHEMCATBIO DATA HUB

National Renewable Energy Laboratory

WBS:	2.6.2.500
Presenter(s):	Frederick Baddour; Carrie Farberow
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2025
Total Funding:	$150,000.00

PROJECT DESCRIPTION

The ChemCatBio Data Hub project accelerates the catalyst and process development cycle by providing (1) a secure repository and plug-ins for centralized data storage and sharing and (2) advanced analytics tools to provide predictive capabilities for research and development. In FY 2020–2022, the project was focused on the development of a Catalyst Design Engine, a pathway-independent tool that evaluates the trade-off between the predicted performance and material cost of catalysts for producing a diversity of end products from biomass and waste resources. Realizing this vision requires that the building blocks of the Catalyst Design Engine, namely CatCost and the CPD, are powerful, intuitive, expert-vetted tools with substantial buy-in from the research community. Toward this goal, the CPD has added a user guide, opened to community uploads, upgraded the user interface, and progressed the development of a unique “reference species interconversion” feature that enables comparison and pooling of broad adsorption energy data. A new dataset containing binding of contaminants relevant to catalyst deactivation has been generated through collaboration with CCPC and will be made publicly accessible in the CPD. During the next 3-year project cycle, efforts will focus on the development of transformational tools, expansion of the database, and integration with AI/ML methods for predictive applications.



COMMENTS

- The goal of this project is to accelerate the catalyst and process development cycle through development of analytics tools and to harness and curate catalyst data.
- This project takes the approach of integrating technology data (performance and properties), catalyst cost estimation, and ML to create a database that can be used to accelerate future catalyst design and process development. The data hub is intended as a data sharing tool and a framework for collaboration, in addition to serving as a repository for data that can be used for research beyond the scope of this project.

The project has a strong, logical approach, starting with intra-consortium data sharing, then opening up the database and analysis tools to the public, and finally, allowing public user interaction—all while handling the administration and software development for the code base and tools for the data hub. There is a diverse project team that brings significant and curated experience. The management plan for accomplishing the work and the communication between team members seem strong and include agile methods. Additionally, having routine interactions with the user community means the tool is being developed in response to how it will be used.

- Exceptional progress has been made on this project. The CPD exists as a free and public R&D resource. The initial release contains DFT-computed data plans that include allowing for user uploads (subject to quality control) in a future iteration. To date, 10 experts have been interviewed for feedback on the database. This is a good start, but additional interviews at additional experience levels are still necessary. The researchers have created a public Wiki-style documentation website that details how to use and search the CPD and a public webinar to engage the research community. Additionally, they are working to develop a data curation plan. This is very exciting, as I see great potential for this database.

- This project has already demonstrated impact and has great potential for further impact. The ability to compare data in the published literature or enable a comparison of experimental data to DFT calculations is huge. There is so much potential to save duplication of efforts (and the associated money) as well as to aid the catalyst community in faster and cheaper catalyst discovery. Additionally, this data hub should make it easy to identify outlier datasets and help the catalyst community converge.

- The team has a solid approach that focuses in the near term on optimizing the application programming interface development process to enhance user query experiences as the property database expands. This work will impact the catalyst development community as more reference data is uploaded along with the user training documentation.

- The team spent a good amount of time walking the audience through the risks associated with the project. The team should continue to coordinate and collaborate with larger industrial information technology organizations to leverage the capability and accelerate the work. In terms of data curation and quality, partnering with organizations like the National Association of Manufacturers could be an important relationship if not already explored. This project will always enable more innovation in the field of catalyst development using automated computer science. There was no mention of DEIP or EJ standards related to this project. There is a huge opportunity here due to the coding and information technology gap across the United States for disadvantaged communities.

- Effective user guide documentation takes a significant number of man-hours to properly prepare for public consumption. The data hub team was able to pull together a web-based user guide with searchability. The team should expound more on the data quality and verification aspects of the curation plan and even consider automation for this part of the process. It is probably a good idea to include usage analytics for the tools that are released. The reference species interconversion tool continues to be a very strategic feature for the project. The team did an excellent job of walking the audience through a species interconversion activity. More examples like this would allow progress to be evaluated more easily in the future.

- The data hub, when finally executed with fully functional tools and algorithms, will have a significant impact on the scientific community, as catalysis is at the core of process technology development. The team should continue to raise awareness of BETO's commitment to this technology development and continue to engage the power user community.

- This project provides a unique asset to the Catalytic Upgrading program. It will build a cyber-infrastructure that could be used for future ML research of catalyst design and deployment or for enabling the search of existing catalysts. This cyber-infrastructure is expected to change the paradigm of catalyst R&D. This specific project indeed has a limited budget, which may impact its progress. With this limited budget, it would be more beneficial for the project to engage the AI community and to leverage the existing capacity of the community. Some open competitions on Kaggle or the other platform may help identify suitable ML models. It would also be beneficial to develop a concrete plan for data integrity and safety when reaching out to the community.

- The ChemCatBio Data Hub is a highly valuable platform for the catalysis society, and it is vital that this effort continues to expand. The approach and project management of the data hub are fantastic, with a very clear development plan that includes risk management strategies to reduce data gaps. The breakdown of the budget is helpful for reviewers, making it easier to evaluate the project's progress and resource allocation. I strongly recommend providing more funding to support the growth and expansion of the data hub. With the assistance of AI, the data hub could become an even more comprehensive resource for the catalysis society, including more digested information such as safety data sheets and U.S. Environmental Protection Agency and U.S. Department of Transportation regulations related to raw materials and products. More promotion of the platform will attract more users and partners, leading to increased collaboration and innovation in the field of catalysis. This approach will not only help avoid duplicated work but will also ensure that the platform remains a relevant and effective resource for the community. Overall, the ChemCatBio Data Hub is a critical asset for the catalysis society, and it deserves continued support and investment.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments on our project management and approach. The reviewers were optimistic about the value of the ChemCatBio Data Hub as a resource for the catalysis community. In particular, the reviewers noted the benefit of reducing redundancy in catalysis research, the ability of the data hub to serve as a collaborative framework that supports accelerated catalyst discovery, and its utility in helping the community reach consensus. They noted the continued strategic importance of unique features like the reference species interconversion tool for the CPD. The reviewers further highlighted the importance of engaging with industry experts both in the information technology industry and in catalysis communities to accelerate development and remain responsive to the needs of catalyst researchers. We were glad to hear the broad support for these areas, which have been a major focus of the project, and we will continue to keep these engagements as priorities to provide guidance to the project. The reviewers also provided a number of helpful suggestions to guide the project. They highlighted the importance of leveraging existing tools and capabilities within the AI/ML community, which aligns with the FY 2023 Q4 milestone for this project, "Define scope and conduct gap analysis to advance toward the Catalyst Design Engine Vision," which will establish the road map for utilizing AI/ML features within the CPD. Toward the goal of data growth and quality, the reviewers suggested exploring relationships with catalysis organizations like the National Association of Manufacturers and highlighted the importance of the data curation plan under development within the project. The reviewers suggested including usage analytics for the tools developed within the project. We agree with the reviewers that usage analytics will be increasingly valuable as the database becomes more integrated with the catalysis community and may offer a source of additional development guidance. We are continuing to evaluate these approaches and agree that they are promising avenues for accelerating data growth while maintaining data integrity. In conclusion, the reviewers highlighted that the project has advanced substantially since the 2021 Peer Review and has demonstrated significant impact. They reiterated the value of continued development of the data hub platform and emphasized the importance of sustained community engagement. We appreciate this assessment and the reviewers' numerous helpful comments, which we will integrate into project plans as we continue the development of data tools to accelerate catalysis research.

LOW-PRESSURE HYDROGENOLYSIS CATALYSTS FOR BYPRODUCT UPGRADING WITH VISOLIS

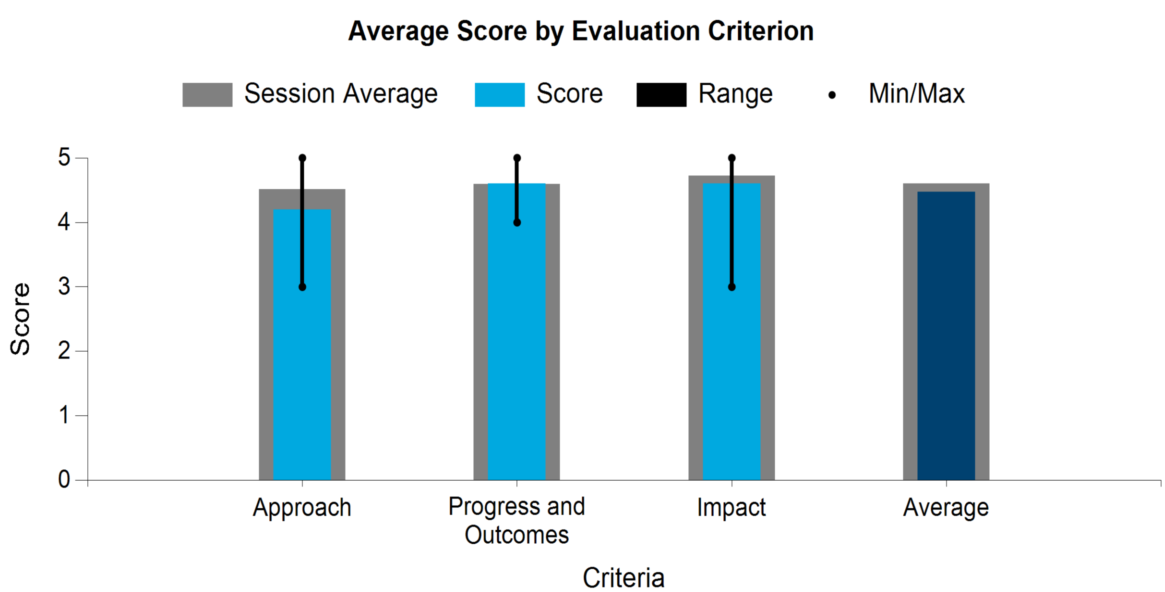
Pacific Northwest National Laboratory, Visolis

PROJECT DESCRIPTION

WBS:	2.3.1.700
Presenter(s):	Karthikeyan Ramasamy
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2022
Total Funding:	$205,000.00

In late 2017, ChemCatBio invited industry to partner with national laboratories and leverage ChemCatBio capabilities. Visolis, a small company coupling bioengineering with chemical processing, answered the charge with a hybrid process to produce high-value monomers at near-theoretic yields. Visolis has previously demonstrated demo-scale (6,000 L) fermentation to produce an intermediate with low projected costs at a commercial scale. The development of hydrogenolysis to convert the bio-derived intermediate to the desired monomer was proposed to ChemCatBio. A major production cost in hydrogenolysis is the requirement for very high pressures—typical pressures for hydrogenolysis exceed 25 MPa. In earlier work, Visolis and PNNL demonstrated complete conversion of the fermentation-derived intermediate with a selectivity of over 90% at 200°C and 12.5 MPa, but facilities capable of operating at such high pressures are expensive. Lower hydrogenolysis pressures improve capital and operating costs.

The Phase I objectives were met by demonstrating a stable and robust hydrogenolysis catalyst in FY 2020 for the conversion of the fermentation-derived intermediate to a high-value monomer at >80% selectivity under 5 MPa pressure. Objectives of the Phase II effort are to understand and develop mitigation strategies for the feedstock impurities on the catalyst stability and engineer the catalyst to the extruded form for scale-up studies. The team will also provide TEA for a pilot-plant design using Aspen Plus process models and discounted cash flow analysis.



COMMENTS

- Supporting a biotech startup by developing a hydrogenolysis catalyst is a very interesting demonstration of catalyst development for a private commercial entity. Not a lot of detail was given on the approach. Progress and impact are excellent based on the corporate partner being pleased with the final product.

- The approach is as follows: This DFA project with Visolis seeks to develop low-pressure hydrogenolysis catalysts to convert a small molecule intermediate derived from fermentation to a value-added monomer. Within the work plan, the roles of PNNL/the company are clearly delineated in the presentation, with PNNL handling synthesis, combinatorial screening, and attempts to convert to a flow process. Phase II seeks to move to engineered catalysts, which aligns well with prior review suggestions to move to more realistic systems. While generally lacking any details, the presentation did highlight nicely the power of throughput screening methods, which were well suited for this project. The slides and presentation lacked a degree of detail that was desirable as a reviewer. In particular, some specifics regarding the rationale behind results would have demonstrated fundamental understanding of the systems and ability to perhaps apply knowledge to other systems. As an example, regarding the role of water in promoting increased selectivity—positing some rationale for the observation would provide a better-developed picture of the work without compromising IP. This was a moderate weakness of the project. In terms of progress, the project has met milestones in both phases—developing a successful low-pressure catalyst with at least reasonable durability in Phase I and seeking lower PGM content, understanding containment tolerance, and developing mitigation routes in Phase II. These goals were achieved with the discovery of a system that had excellent water/acid tolerance, a demonstrated ability to scale catalyst synthesis, and robust catalyst stability. The lack of details makes some aspects of evaluation difficult. For example, the need for the key synergistic promotor and the lack of any idea of the general elements involved might mitigate PGM loading savings. The projected cost reductions mitigate this concern, but some level of detail could be provided. The impact for Visolis is clear, given that their expertise is more in the fermentation area. The benefit to experts in catalyst synthesis and high-throughput discovery was crucial. However, it was less clear what the benefit was to the PNNL researchers. Some further comments on the experience and how it benefits future research projects would enhance the presentation. The connection to engineered catalysts could also be in line with evolution of the broader upgrading portfolio, but this was generally inferred and not expanded on in any significant detail.

- As a catalyst development and testing community needing acceleration in R&D, more projects should embrace combinatorial catalysis. This project team did a great job of using these tools.

- Combinatorial catalysis is an excellent approach for this project and will always open new opportunities for discovery and innovation with heterogenous catalyst design. The team did not mention the need for data science and data management that truly accompanies any combinatorial program. There appears to be a significant breakdown of scale-up development work that is missing in the approach from catalyst discovery to testing catalyst stability. The state-of-the art hydrogenolysis catalyst for C6 upgrading was not mentioned. The industrial partner originally started with $CuCrO_x$, and the national lab discovered the current catalyst platform. The project plan in Phase II was completed and was aggressive in moving from reduced PGM loading in engineered formed catalysts. The team should outline the real technical risks and gaps associated with making this work viable. There was no mention of a DEIP or EJ perspective with this work, especially from the industrial partner perspective.

- The project team demonstrated how an effective industry collaboration with an appropriate and effective tool in combinatorial testing accelerated the catalyst development. This was done in a batch combinatorial system at PNNL. The lowering of the platinum group promoter loading should have gone through a maxima in product selectivity. The TOS for this TRL level seemed appropriate, approaching 500 hours with a stable selectivity. The catalyst seems to be stable in the presence of two organic acid contaminants. It is difficult to determine what a surrogate feed and real feed is for the project to evaluate the impurity study. Lactone appears to be an important intermediate side product. The point at which water is not helpful to the product distribution should be determined. The 50-cm^3 reactor with extrudates was deemed a scaled-up unit at a 25x factor. The dehydration-based undesired side product rate appears to rise and ultimately decrease over time. There seems to be a period under 200 hours where the surface is unstable. An overlay of the carbon balance would be useful here.

- The team mentioned that the project has moved on, and there is an ongoing collaboration with a scale-up partner. There was no data or design information shared on this activity. There should be some type of resource benefit to ChemCatBio in this combinatorial approach that covered formulations in extrudate structures. This project has a very clear commercialization pathway as the TRL matures. This route provides a solid addition to BETO’s chemical process technology portfolio.

- This project serves as an example of successful translational research. The team successfully converts a catalyst discovered in foundational research to a viable catalyst for real industrial applications. The team has deployed various methods, such as combinational methods, to help accelerate the deployment of catalysts for industrial applications. This project has met all its goals and is ready to be completed with success. Due to the lack of detail, it is challenging to address whether this project will help achieve DOE’s SAF Grand Challenge. However, based on the information shared by the presenter, this project is ready to enter the next level by scaling up with an industrial partner. This R&D activity illustrates the potential benefit of this project in enhancing the sustainability of the energy or chemical supplies.

- This project serves as an excellent example of successful collaboration between BETO and industry for the commercialization of bioproduct upgrading. The approach and outcomes are highly impressive, with the development of a cost-effective catalytic process for hydrogenolysis, and the proven stability of the engineered catalyst is very encouraging. The R&D support from BETO highlights the potential of this program to serve as an incubator for many startups in industry. Although the project has been completed, following up on the progress at Visolis to validate the technology would be beneficial to finalize the TEA. In case Visolis is unable to scale up the process for any reason, it is important to ensure that the learnings from this project are available to other interested entities.

PI RESPONSE TO REVIEWER COMMENTS

- The project team would like to express our gratitude for the insightful comments provided by the reviewers. We sincerely apologize for the lack of detailed information related to the product streams, the role of water in promoting increased selectivity, and the breakdown in scale-up development work from catalyst discovery to testing catalyst stability during the Peer Review presentation. This limitation is primarily due to the constraints of confidentiality imposed by our industrial partner. However, once the novelty of the project is protected by a patent, our objective is to make the information accessible to the public and document all relevant details in the data management hub operated by ChemCatBio. We acknowledge the impact of high-throughput screening methods in this project. Combinatorial catalysis has proven to be an excellent approach, accelerating catalyst development and creating opportunities for innovation. We agree that incorporating data science and data management into our combinatorial program is crucial, and we will ensure we address these aspects in our future work. We appreciate the reviewer’s recognition of the direct funding opportunities from BETO to support the industry in the commercialization of bioproduct upgrading. The development of a cost-effective catalytic process for hydrogenolysis and the proven stability of the engineered catalyst are encouraging outcomes from this project. We agree on the importance of following up on the progress at Visolis to validate the technology and share project learnings with other interested entities for the TEA. We will ensure that we provide updates and share relevant information on this ongoing activity. Thank you for suggesting that we outline the benefit to the PNNL researchers and explain how the experience gained from this project benefits future research projects. We will incorporate this information in our future presentations to provide a comprehensive view of the project’s impact on our team and its relevance to future opportunities. We would like to express our gratitude for your comments regarding the importance of DEI and EJ perspectives. It is important to note that this project was funded prior to the implementation of the DEI programs in BETO, and as such, it did not have a direct milestone specifically dedicated to DEI and EJ aspects. However, we fully recognize the significance of these perspectives and are committed to integrating them into our projects to ensure a more inclusive and equitable approach.

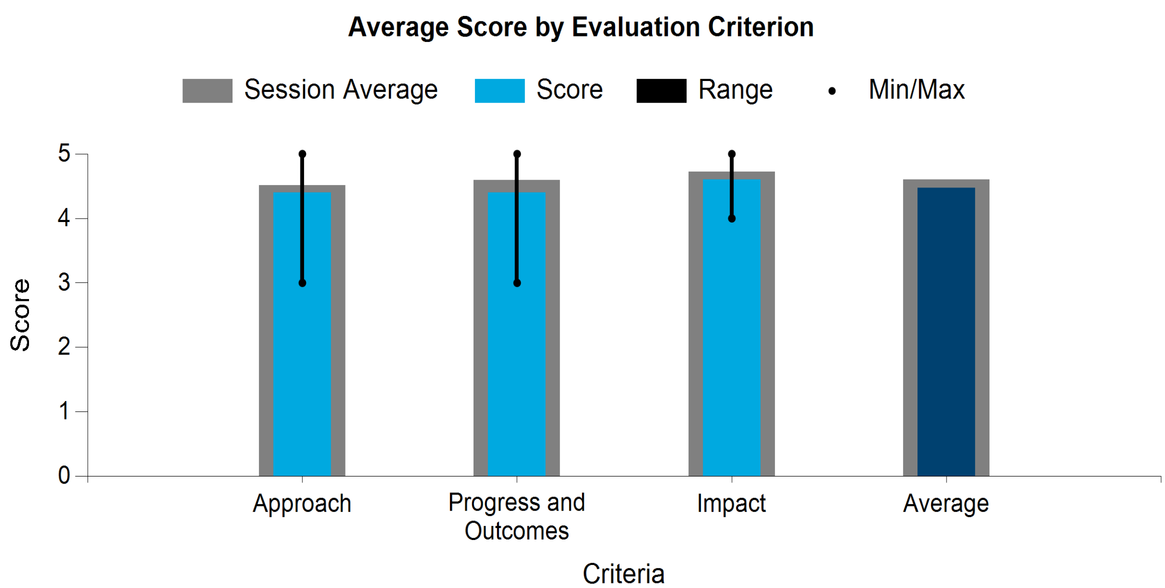
CATALYTIC PROCESS INTENSIFICATION OF BIO-RENEWABLE SURFACTANTS PLATFORM WITH SIRONIX

Los Alamos National Laboratory, Sironix

WBS:	2.3.1.704
Presenter(s):	Claire Yang
Project Start Date:	07/01/2017
Planned Project End Date:	09/30/2023
Total Funding:	$282,000.00

PROJECT DESCRIPTION

The size of the global surfactants market is projected to reach $52.4 billion (U.S. dollars) by 2025. Surfactants are the key active ingredient in cleaning and personal care products and are one of many petrochemical products that could be supplemented with biomass-derived materials. Sironix Renewables LLC has invented a new class of surfactants, called oleo-furan surfactants (OFSs), which utilize the unique properties of biomass by linking the function of bio-based furan building blocks with natural oils to provide 100% bio-based multifunctional and eco-friendly cleaning and personal care products. This project is helping Sironix Renewables de-risk their process scale-up for new product development and maturation. The Phase II joint research project with Sironix Renewables is designed to leverage the catalyst development resources and catalytic reaction engineering of ChemCatBio with the surfactant's platform of Sironix Renewables to accelerate the DOE-invented and DOE Small Business Innovation Research-funded technology toward market commercialization. Technical goals accomplished include the development of new catalysts and reaction pathways of various furan-based structures to lower production costs with environmentally benign materials, process improvements to achieve the efficient scale-up strategy of existing surfactants, and detailed TEAs to guide experimental efforts and measure market potential.



COMMENTS

- This is an interesting project, as it seems to consist of the development of a catalyst to enable a process for private industry company Sironix. In terms of the project goal, "reducing barriers to scaling up Sironix technology by addressing catalytic upgrading and process intensification challenges," it would be interesting to know the value of this work beyond this specific instance. The project scores very well in progress and impact. The development work is complete and the technology has been transferred to the company such that development of detergent formulations is currently underway; in addition, a laundry product partnership has been achieved.

- This DFA project, on a no-cost time extension, leverages LANL and ChemCatBio capabilities to further guide Sironix as they develop oleo-furan-derived surfactants and value-added chemical intermediates. The choice to pursue bio-based surfactants certainly aligns with BETO goals of exploiting bio-derived molecules for use in products. The focus in this phase on scaling the technologies is consistent with consortium efforts focused on more downstream aspects of technology development and deployment. The capabilities at LANL provide an obvious value add for Sironix, given the combination of reactor capabilities, catalyst synthesis, and TEA. It does seem like this project could have benefited from an even tighter collaboration with the consortium, specifically regarding the characterization capabilities of other parts of ChemCatBio. However, at this later stage, the synergy shown between catalyst development and economic modeling is a key element of the work that is vital for success of the project. In particular, it appears that prior review critiques of using economic modeling to guide decision-making were heard and implemented in this subsequent cycle. Aspects of project management appear well in order and were articulated clearly in the timeline/milestone slide. Further evidence that the project is effective stems from the desire to submit a no-cost time extension to continue the fruitful collaboration. No DEI efforts were specifically called out. Provided that this is an existing project that is sunsetting, the lesser emphasis on this area might be the direct result of the current ramp down of the work.

- Improvements across the various phases of the project are clear. These improvements include moving from batch to flow synthesis, developing new reactions informed by TEA, and exploring new processes that access novel chemical building blocks of potential interest. While the catalysis has clearly evolved to be enabling for chemical formation, it is also promising to see that the target products show utility for the desired applications. The economic modeling was clearly instrumental in identifying areas for improvement on the catalyst synthesis and process sides. The issue of feedstock variability is an interesting and critical one for this particular space. The ability to recognize the opportunity to prepare a former costly reagent as a valuable coproduct is clever while also making the entire process more economically viable. Stressing flexibility in processes and products increases the likelihood of a sustainable and successful business model.

- As mentioned above, Sironix benefits from the project in critical and unique ways. The business is continuing to make inroads because of the ability to be flexible in the intermediates produced and the routes used to access OFSs. The proposed pivot toward high-end markets makes sense and is likely necessary to compete (at least perhaps in the short term) economically with well-established companies in the surfactant space. Less clear are some of the benefits to LANL. While the presentation brought out this impact to some degree, more commentary on transferrable insights that LANL gained in the catalyst synthesis, testing, and modeling arenas—even if statements are general due to the nature of the project—would more effectively demonstrate knowledge gains for both partners.

- The iterative design approach for the project has been an effective R&D strategy enabling a new class of furan-tail intermediates to be synthesized. Small batches have been transferred in the industrial collaboration, suggesting a process with viable economics.

- The project appears to have a successful approach that involves close collaboration between the laboratory and industry partners, where frequent design and material synthesis iterations at small scales are critical. The state-of-the-art OFS catalysts need improvements in lifetime, cost, and yields, and the corresponding process design CapEx needs a reduction, which is the core of the goals in this project. The process intensity approach was explained in this work switching from batch to flow reactors. A new process design based on new chemistry was launched in 2023, and it seems like this would introduce a few new risks in the project. There were no critical risks identified for moving the project forward to the next level. No comments were made concerning DEI or EJ.

- The project team made good progress on finding a fatty alcohol feedstock replacement for reacting with furans along with a new catalyst and a patent to cover it all. An additional patent was filed that looked at using furfural, furfural alcohol, and furoic acid as precursors, along with a new catalyst. The team should look at scaling up and delivering intermediates in the 100 gram to 1 kilogram range now. This will require the use of additional quality control R&D tools.
- The project team already has a good industrial partner with a product with decent margins. The project is closely tied to the business objectives and has a great opportunity for success. This pathway offers the BETO community a new route into existing niche chemical production markets. Once the volumes are scaled, the economics will improve dramatically.
- This project reports an effort to develop and commercialize bio-based surfactants. It is currently under non-cost extension.
- The project uses an iterative design cycle to meet the project goals. The cycle includes TEA-based process viability determination, tail options and chemistry definition, catalyst synthesis, characterization and evaluation, and surfactant production and testing. This iterative cycle turns out to be a practical and efficient approach to evolving the products.
- The project has patented catalysts for Phases 1–3 and has developed new OFS platform chemicals. They also delivered 10 grams of new materials to the industrial partner.
- If successful, the project will enable the company to enter a $12-billion U.S. market. The R&D activities have led to three patent applications, several awards for green technology, and partnership with several top players in the field. The surfactant market is a highly divided and competitive market. It will be critical for the company to produce the first profitable production.
- This project is a great example of the successful partnership between ChemCatBio and industry, resulting in remarkable outcomes in the conversion of biomass into value-added products. The project management has been exceptional, with a well-defined timeline and a comprehensive approach to risk mitigation. The progress made over the past 2 years in catalyst upgrading and process optimization is impressive. The successful advancement of this project also serves as an excellent case study for fine-tuning the TEA model to more accurately predict the costs of a process.
- The story of this successful project should be included in promotional materials to raise public awareness and support for this kind of collaboration.

PI RESPONSE TO REVIEWER COMMENTS

- First, we appreciate the review panel's overall positive assessment of this project with the progress and impact we made in supporting bio-advantaged product development with Sironix. Here, we will provide some insights on the higher-level question from the reviewers: Why were DOE funds used to develop a key technology for private industry? This is a great opportunity called a DFO that is designed specifically for industry and academic partners to utilize ChemCatBio's capabilities. This funding opportunity provides resources for partners to collaborate with ChemCatBio's investigators for developing novel catalysis processes and creating new capabilities and approaches to improve the lab's capabilities in the catalysis and conversion portfolio. This DFA project sits in the industry partnership portion of the consortium. This project with Sironix serves as a successful example in this regard by leveraging LANL's capabilities in catalyst development and TEA-guided reaction process improvement and intensification to help address key challenges and reduce barriers to accelerated commercialization for performance-advantaged bioproduct industry partners. We understand the reviewer's concern that the technology being demonstrated appears specific to Sironix. While this research has clear benefits to the commercialization of Sironix's OFSs, the development of alternative feedstocks to provide a domestic source of renewable furan, furfural, and furfural alcohol has applications across a wide variety of bio-advantaged products. The key building block of OFSs is furan or 2-methylfuran. Furan is produced by the decarbonylation of furfural. 2-methylfuran is a byproduct of the hydrogenation process for producing furfuryl alcohol. The major use of furfural is the production of furfuryl alcohol, which is used as a binder for foundry sands. In 1991, the United States produced 49,000 tonnes of furfural and 25,000 tonnes of furfuryl alcohol per year, accounting for 36% and 23% of world production. By 2001, domestic furfural production dropped to 8,000 tonnes/year, or 4% of the world market, and domestic furfuryl alcohol production dropped to 5,000 tonnes/year, or 4% of the world market. Today, the United States produces no significant quantities of furfural or furfuryl alcohol. China processes 80% of the world's installed furfural capacity, and they produce 70% of the world's furfural. Both the United States and the European Union have issued dumping findings against Chinese furfuryl alcohol production. LANL has developed a new process for converting corn bran, which is a byproduct of corn ethanol production, into furfural. This work was part of a BETO-funded project to develop a sustainable source of JP-10. Our TEA for this process indicates that it is competitive with Chinese-produced furfural. Sironix is one of several companies interested in a reliable domestic source of furfural. Helping Sironix develop a new market for furfural-derived chemicals may help revive a domestic furfural industry, which will also benefit domestic ethanol producers. Each year, multiple consortia within BETO provide DFOs for industry and academic partners to utilize their capabilities. Proposals will leverage the consortium's world-class capabilities to address challenges as identified by successful applicants from industry and academia. The DFOs have been demonstrated as a good strategy to accelerate technology maturation and commercialization to benefit the community with new inventions; in this project are surfactants, which are one type of bio-advantaged product. At LANL, we are planning to propose more projects with Sironix and other industry partners in the coming years to meet their needs with the capabilities we have developed and are developing in the lab. In addition, ChemCatBio DFOs are open to all U.S. companies and universities. We appreciate the reviewer's acknowledgment of our efforts in catalyst development and TEA-guided process improvement, and the priority of better serving Sironix's needs and key challenges to commercialization. More proposals have been submitted looking for funding support and collaboration opportunities on process development and scale-up for newly invented surfactant production. Due to time constraints, we didn't get a chance to present our DEI efforts along with our technical progress in this project. The project brings together a diverse team in terms of gender identity, racial and ethnic background, and career stages. The LANL PI has been working closely with the LANL workforce and pipeline program on hiring postdocs and student interns from MSIs to help with surfactant platform molecule synthesis. As part of efforts to reduce hiring and workplace bias, Sironix has developed hiring practices targeting the recruitment of a diverse set of STEM professionals through a series of proactive practices involving equitable job advertising, bias reduction in hiring material review, interviewing practices, and candidate pool selection guidelines. As part of this project work, Sironix will continue to refine policies for hiring, work, promotion, and pay, as well as employee protections that ensure confidential reporting and zero tolerance for all forms of abuse. In addition, Sironix will be implementing new initiatives for the development of equitable and inclusive business practices, including improving their outreach to and representation of underserved communities. This will entail increasing minority representation on the company's board of directors by hiring one additional member and providing at minimum one additional language translation for Sironix's website, newsletter, and other public-facing materials originating internally from Sironix. We agree with the reviewer that additional comments on the knowledge gains yielded for LANL over the course of this project would be helpful. To this end, LANL is benefiting from this project not only by expanding capabilities in catalyst design and increasing the TRL of catalytic conversions and surfactant development, but also by widely opening the door to developing other performance-based bioproducts. For example, the patented chemical reaction and process we developed during this project can also be applied to produce chemical herders to help prevent petroleum oil spills, to produce pesticides that can help address global security challenges, etc., which align well with our mission at LANL. This project is undoubtedly a win-win for both parties. A systematic risk assessment of OFSs has not been performed. This task was beyond the scope of the current CRADA. However, the process engineering done in support of the TEA has provided insights into potential problem areas. The overall process involves a combination of standard unit operations and processes that are well understood and not of particular concern. Sulfur trioxide production for sulfonation is an example of such a process. Other parts of the process are new and pose risks to the project. Our current work helps mitigate the risks associated with producing the backbone molecules. Key reactions in the process are very exothermic. Heat removal from these reactions at a commercial scale is a concern, as is the thermal stability of the reaction products. Other areas of concern include the following: (1) two separation processes key to purifying the product have not been tested at scale, and (2) sulfonation of the furan with sulfur trioxide has not been tested. Producing kilogram quantities of the oleo-furan intermediate would need more funding support. At the end of this project, we will provide Sironix with our recommendations concerning scaling the production and purification of the intermediate to kilogram quantities. The focus of our recommendations will be on the processing steps involving new chemistry. We also submitted new proposals seeking to address the scale-up challenges of the newly developed technologies. The TEA has provided a good understanding of which areas of the process have the greatest impact on capital investment. Our current work in developing alternative chemistry and exploring alternative tails to attach to furan and furfural derivatives is an effort to reduce capital investment. Some of the alternatives that we are currently considering will simplify the process, and the simplifications have the potential to reduce capital investment by 50%. We agree with the reviewer that the 100 gram to 1 kilogram scale is the primary target for intermediates, as well as for surfactants and formulations to facilitate application testing. Sironix's assessments during this project provided proof of concept for the commercial viability of the newly invented surfactants. In our new proposed project, LANL and Sironix are aiming to work cooperatively to increase the scale of intermediate and surfactant production to meet these volume targets. Sironix has access to the quality control and R&D tools required for this product, either in-house or with the use of available facilities at Washington Clean Energy Testbeds. We thank the reviewer for the recognition of our useful and effective iterative design cycle and for providing positive feedback. We are also expecting to see Sironix and its partner manufacturers produce the first profitable production in the near future, and we would be happy to provide more technical support along the way. We appreciate the positive feedback from the reviewer. The laboratory produced materials as part of the R&D 100 submission for this work. These materials included written materials as well as a video. The suggestion to raise public awareness of this work is appreciated, but it needs to be subject to Sironix's business strategy. We should review and update the materials generated for the R&D 100 award if appropriate. A good first step would be an article in the laboratory's magazine, *Los Alamos Science*, and visibility for the work on the laboratory's external website. We will also try to submit this success story to an outlet targeting trade and professional publications, such as *Chemical Engineering Progress* and *Chemical & Engineering News*.

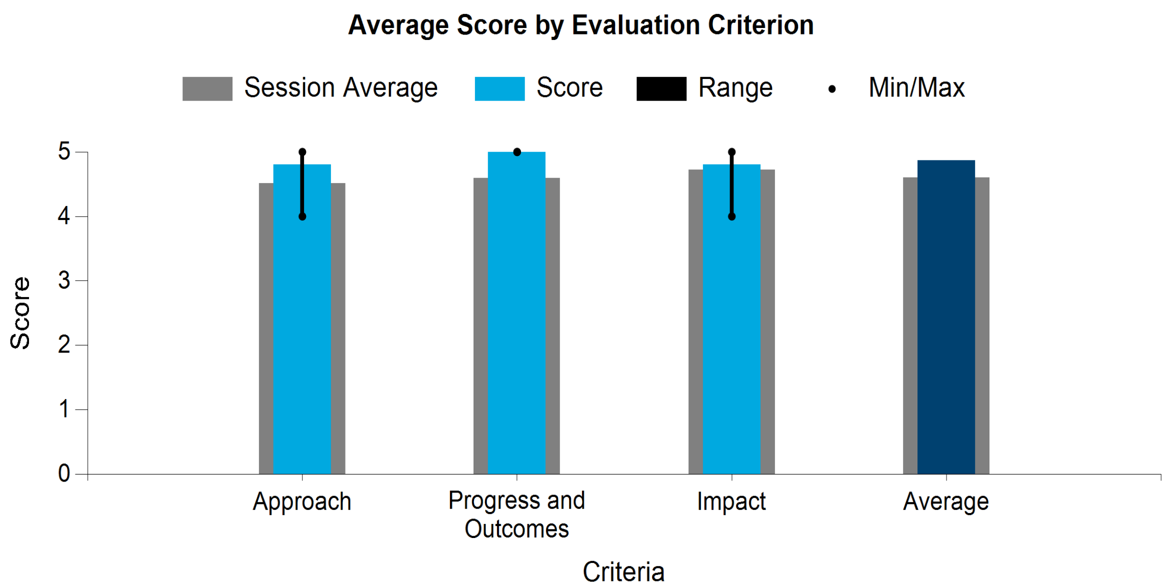
CATALYST DEVELOPMENT FOR SELECTIVE ELECTROCHEMICAL REDUCTION OF CO_2 TO HIGH-VALUE CHEMICAL PRECURSORS WITH OPUS 12

National Renewable Energy Laboratory, Opus 12

WBS:	2.5.4.707
Presenter(s):	Frederick Baddour
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2022

PROJECT DESCRIPTION

Cost-effective electrochemical CO_2 reduction (ECO_2R) is considered one of the holy grails of green chemistry. However, widespread commercial fuel and chemical production via ECO_2R is limited due to the lack of a suitable reactor design and catalysts with high selectivity to the desired products. This technology has the potential to convert CO_2 into a range of molecules that would benefit the biofuels and bioproducts industry. Within the bioenergy industry, more than 45 million metric tons per year of CO_2 are generated from existing domestic biorefineries. With projections of abundant and inexpensive renewable electricity, utilization of this domestically produced CO_2 to make fuels and chemical products has the potential to significantly enhance the economic viability of these operations. Twelve's core innovation is a reactor design that enables ECO_2R in a polymer electrolyte membrane (PEM) electrolyzer. A novel polymer blend and transition metal nanoparticle catalysts on carbon in the cathode layer transform a PEM water electrolyzer into a PEM CO_2 electrolyzer. The goal of this project as a follow-on Phase II DFO is to implement stereolithographic 3D printing to rapidly prototype advanced millifluidic elements to develop a versatile platform for the preparation of nanostructured CO_2 electroreduction catalysts at throughputs >10 g per day. This production capability will enable the systematic evaluation of catalyst properties and ink preparations for membrane electrode assemblies (MEAs) >600 cm^2.



COMMENTS

- This DFA project seeks to advance high-throughput synthetic methods to permit scaling of MEAs for electrolyzer synthesis. With the expertise at NREL in catalyst synthesis and characterization, this project seems a natural partner with ACSC PIs and their capabilities. The electrolyzer target of CO_2 to CO is a strong near-term goal to advance CO_2 conversion to viable fuels and chemical feedstocks. The potential versatility of the process and plug and play in biorefineries and standard refineries is another clear strength. Given that this is in Phase 2 with the same parties, it is no surprise that the communication lines seem appropriate. Use of the data hub for collaboration provides another value add to the database, given that it allows secure communication channels for data exchange between the lab and industrial participants. The use of CatCost further highlights the integration of the tools developed by ChemCatBio into the ethos of all research the consortium performs. Furthermore, the slides clearly delineated the roles of Twelve and NREL. It was also evident that there was mutual benefit from the interaction, as Twelve scaled catalyst synthesis while NREL was able to hone microfluidic synthesis, which may well impact non-DFA funded projects. *In situ* analysis to understand catalyst synthesis is another highlight of the work and something that can be done in a multimodal fashion, as NREL can, in a select number of organizations. The additive manufacturing component of the work was a highlight and hopefully something the consortium can continue to leverage in this and other projects. Given the success here, exploring and integrating 3D reactor printing and reactor design may be worth additional consideration in certain instances with other consortium efforts. The direct connection with theory in reactor design further highlights the utilization of the consortium's full suite of capabilities in DFA projects and is a resounding response to prior review comments. In the long term, opportunities may exist to connect such synthetic methods as described here to high throughput, or to couple data science with responsive reactors to further decrease the time needed to optimize the systems. The consortium is encouraged to push current capabilities in this space when the opportunity arises with potential future DFA projects that align with these areas. DEI was not explicitly called out from broader consortium interests in the space. For an existing project with an external partner focus, this is perhaps not too surprising relative to some of the continuing efforts that rely heavily on national laboratory or university leadership. For new DFAs, some level of effort to disseminate DEIPs would be expected.

- The project results clearly speak for themselves—the flow system has been demonstrated with good to great results. The catalyst and MEA can be scaled and shown to maintain comparable reactivity. While Phase I focused more heavily on identifying potential catalyst improvements and provided the basis for targeting a specific catalyst, Phase 2 moves toward scaling. This is very much consistent with prior review suggestions to move in the direction of advanced catalyst synthesis with an aim toward technology development and deployment. The choice to explore microfluidics was a sound and well-rationalized one for nanocatalyst synthesis. The results demonstrate not only successful synthesis on the desired scales, but also decreased throughput time and time needed for grafting. As performance was not impacted, the project is considered a resounding success.
- The Phase I and Phase II collaborations were critical to the development of a viable catalyst for the assembly, while also providing a path to the needed scaling to continue to pursue the electrolyzer technology. The project also has clear benefits for the consortium, providing experience with additive manufacturing and microfluidics that can be leveraged in other nanocatalyst synthetic schemes. Experience with the full cycle of catalyst development and scale with these systems could prove invaluable if/when new catalyst architectures are explored for AOP projects. Also, the DFA project enables the pursuit of methods and capabilities that are not mature enough for AOP-type projects but could complement work in these major areas in future cycles. The products stemming from the work (one paper accepted in a solid-impact-factor journal, one paper in preparation, and two patents) represent a solid output, given the IP considerations and ultimate desire to develop the technology. The project is also clearly evolving consortium interests, moving from batch-type synthesis to reactions in flow. The increasing comfort level with such systems can only reap benefits in general for DFA and AOP projects alike. Furthermore, this reviewer was unaware of the robustness of the 3D printed resins and reactors—this versatility should be exploited (when feasible) in other synthetic examples that could further benefit consortium efforts in other areas.
- Here, the work was focused on the Phase II objectives, which were to create catalyst synthesis methods that can be scaled. NREL provides the catalyst and reactor design, characterization, and modeling, while

the industrial partner performs the assembly and performance testing activities across multiple scales. To accelerate the research, NREL takes an innovative approach of fast-prototyping continuous flow material synthesis reactors for nanoparticle production. These nanoparticles make up the ink used in MEA fabrication, and the material synthesis microreactors can provide a way to scale up. The team did not provide a clear comparison with the current commercial synthesis method for the same type of nanoparticles to show all the technical benefits. There is no question that this approach opens up a variety of innovation pathways for material design and modeling. The only key risk mentioned was the inability to create a material synthesis scale-up process. The project plan appears to be reasonable with the close collaboration and iterative technical feedback between the teams. No DEIP or EJ discussion was provided by the lab or industrial partner with relevant goals within this project.

- The team did an outstanding job of using the 3D printing and additive manufacturing tools, as well as the computational design tools, to fabricate microfluidic elements. The microchannel design features of these elements were selected through literature research, COMSOL analysis, and interactions with CCPC. All these activities are great examples of using advanced tools and collaboration to complete critical tasks and advance the work. In the last 2 years, by using this method, the MEA geometric surface area was able to be scaled by 30x and the nanoparticle production rate increased by 7x. Further, the technique was a clear way of adopting process intensity batch-to-continuous strategies successfully. The results were compelling, showing no difference in performance between batch and continuous methods.

- This project clearly shows how a close collaboration between labs and industry can be advanced using innovative approaches with direct application to the final process technology. This route has significant promise for both BETO and the decarbonization climate technology community. The work went directly into the business strategy, impacting the scaling objectives, which are at the core of technology development for high-tech startup organizations. The team was able to include material quality features in the synthesis process by using spectroscopic property correlation techniques that are very common to industrial processes. The team should discuss more of what it would take to put together a real material synthesis process design for this micro-fab approach based on 90-degree micromixers.

- This project reports aim to de-risk the commercialization of CO_2 electrolysis by developing high-throughput synthesis methods for high-performance nanocatalyst production. This project is with Opus 12 (Twelve).

- The project has two phases of R&D activities. The Phase 1 activities developed a better catalyst and effective supporting methodologies to retain particle size and morphology at increased loadings. The Phase 2 activities involved designing and fabricating millifluidic reactors using additive manufacturing techniques, evaluating the impact of millifluidic reactors on catalytic properties, demonstrating an end-to-end process for nanoparticle catalyst synthesis, and supporting MEA fabrication and performance evaluation. This innovative approach has illustrated that it could be used to accelerate the industrialization of catalyst deployment. Such an approach may also be used to accelerate catalyst selection and upscaling in the other projects.

- The project has made appropriate progress toward addressing its goal and has accomplished the setup tasks properly.

- Electrochemical conversion would be an exciting direction to develop a sustainable process with GHG emission reduction. This project has illustrated its close ties with DOE's targets of reducing GHG emissions. The development of a millifluidic-based high-throughput approach could have a significant impact on catalyst design and deployment. It could be beneficial for ACSC to see this technology, and it could be leveraged to accelerate catalyst synthesis and characterization in a broader spectrum.

- The design and implementation of a high-throughput millifluidic system in this project demonstrates the exciting potential for future labs. The combination of high-throughput stereolithographic 3D printing, online spectroscopy monitoring, computational modeling in reactor design, and integrated processes is an impressive approach. The results, including a 6.6-fold increase in throughput and 40x scale-up, are convincing.

- Although the cost-effectiveness of further scaling up these techniques is unclear without a cost breakdown, the insights gained from this project can be leveraged in future projects. For example, the project team could collaborate with CCPC to design and fabricate novel catalysts using the techniques developed in this project.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments on our project management, communication, and industrial engagement. The reviewers were positive about this project's demonstration of accelerated technology development through close collaboration between labs and industry. They also noted the clear linkages between this project and DOE's decarbonization and GHG emission reduction targets. Further, the reviewers highlighted the benefits of the crosscutting capabilities that were developed within the project and their interest in seeing these technologies leveraged within AOP projects to the benefit of ChemCatBio. Notably, the developed expertise in the additive manufacturing of reactors and millifluidic synthesis were encouraging outcomes of the project and were indicated as valuable capabilities that could benefit the consortium more broadly. We share the reviewers' optimism and excitement about the potential impact these developed capabilities could have on ongoing work in the consortium and will continue to seek opportunities to leverage them to address targeted catalyst deployment challenges. In conclusion, the reviewers highlighted that the project has advanced substantially since the 2021 Peer Review and demonstrated significant impact. We appreciate this assessment and the reviewers' numerous helpful comments.

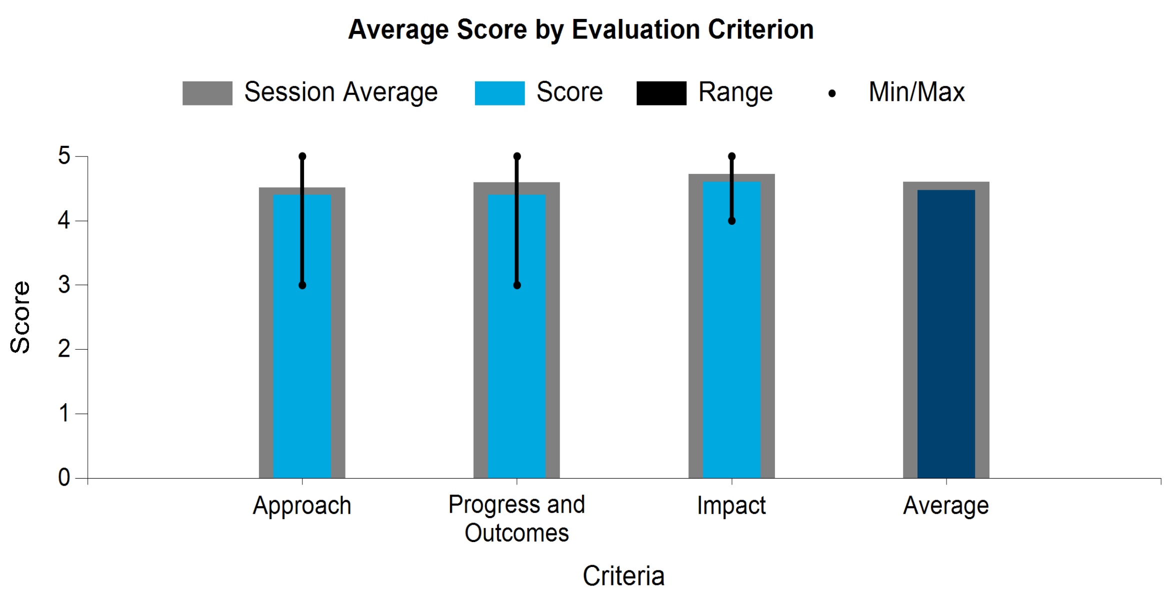
SYNGAS-DERIVED MIXED OLEFIN OLIGOMERIZATION FOR SUSTAINABLE AVIATION FUEL

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.3.1.318
Presenter(s):	Karthikeyan Ramasamy; Katarina Younkin; Michele Jensen
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$472,139.00

To meet the immediate need for decarbonization of the aviation industry, leveraging existing commercial processes and feedstocks will be the most efficient path toward producing SAF in the near term. Syngas is one of the most attractive feed sources because it can be derived from a broad range of renewable and waste feedstocks via gasification while benefiting from existing infrastructure throughout the petrochemical industry. Of the existing industrial processes for transforming syngas to synthetic fuels, none produce aviation fuel efficiently. However, methanol synthesis followed by methanol-to-olefin processing offers an already established and active commercialized pathway to produce mixed light olefins, primarily ethylene and propylene. This mixture can potentially be directly oligomerized to jet-range products in a single reaction step. If demonstrated with high yield and selectivity, elevating this single operation unit to industrial scale would complete an end-to-end commercial pathway for producing SAF from syngas derived from various ecologically disadvantaged feedstocks. To achieve this goal, this project will develop a C2–C5 co-oligomerization catalyst and demonstrate an efficient path to generating SAF from syngas via a mixed olefin intermediate.



COMMENTS

- This project develops a process to produce SAF from syngas-derived mixed olefins, demonstrating a commercially viable path to achieve a 70% reduction in GHG emissions.
- The project aim is to design/develop a catalyst that enables integration of metal and acid catalysis pathways for co-oligomerization of C2 and C3 to produce SAF. The highly collaborative research team

includes PNNL, WSU (fuel property analysis), and Haldor Topsoe (catalyst development). The DEIP is to "hire at least one student from groups underrepresented in STEM," which I find to be a pretty weak plan. First, it really has to be more than one student, as the data clearly shows that hiring just one of any minority group puts an undue amount of pressure on them, and keeps them in a high-pressure "spotlight" situation. Ideally, the group would be on the order of at least three. This also gives them some ability to form a support community and not feel isolated. Second, just hiring them without a clear mentoring plan or programming in place to support them is not a great way to set them up for success.

- The project has had solid progress so far. The first milestone (September 2022) was met, and the September 2023 milestone is on track. The team developed the hybrid catalyst system and optimized reaction conditions to achieve C2–C5 co-oligomerization with more than 75% selectivity to jet-range products. The team still needs to demonstrate the durability of the catalyst, and is planning to test for ~500 hours.
- This project demonstrated a co-oligomerization process with mixed olefin (C2–C5) feedstock to produce hydrocarbons in the jet fuel range. This meets the standard at = 50% blend level.
- The approach is as follows: This project is focused primarily on one step of the syngas-to-fuels conversion chain—co-oligomerization of the olefins generated in the process—while also attempting to demonstrate linkage of all associated reactions to provide significant quantities of hydrocarbon fractions for further testing. The focus on mixed streams of olefins makes complete sense to mimic the potential feeds from methanol to olefins (MTO). The same can be said of a strategy focused on the need for multifunctionality in catalyst design, given the mechanisms that will be accessed in the oligomerization process. Furthermore, the reactor/bed engineering focus of the work is appropriate given the collected data. The roles were clearly defined in the presentation. The WSU connection for fuel testing is a vital component, given their expertise in fuel testing, and the project's milestones heavily focused on obtaining adequate amounts of hydrocarbons for blend testing. In the proposed cycle, the move toward an integrated sequential process and the use of engineered catalysts are logical and align with increasing the complexity of the consortium projects. Understanding deactivation in these systems is critical to sort out, given that the process may be very different in the sequential versus hybrid bed catalysts. This project represents a clear opportunity to interact with the deactivation project to advance understanding of the reaction system and continue to increase the efficacy of the transformation. The DEI component—support of a summer college research student from an underrepresented STEM background—is commendable. Hopefully the student can link to the broader opportunities provided to Science Undergraduate Laboratory Internship and other summer research students at PNNL. In terms of progress, the results are primarily a function of reactor bed manipulation, as the mixed catalyst in a single bed is less effective than a sequential approach. It is gratifying to see that the mixed streams behave much as the lighter olefin feedstocks do. The initial milestone of providing the needed quantity of the mixture for blend testing was achieved. The reviewer also acknowledges that the setup used to provide the mixed olefin feeds is an impressive tool in this work and one that took nontrivial effort to establish. The property testing also yields some promising initial results, and provides the ability to tune properties to the desired ranges with some modifications to the system. The challenge now is to integrate all parts of the syngas-to-fuels pathway to provide the desired product and to do so at longer times. Economic modeling will also be explored further to guide subsequent cycles. Given the progress to date, moving to these more ambitious milestones is appropriate. In terms of impact, the desired move of the technology from TRL level 2 to 4 seems like a manageable yet impactful step in moving from development toward scalability during the project timeline. If all milestones are achieved, the syngas-to-fuels pathway will be demonstrated and a better understanding of the economics of the process will be achieved. For one cycle of a project, this would provide a strong basis for potentially continuing the work or pursuing a handoff/collaboration with an interested industrial partner. While the impact can clearly be inferred from the slides, it was surprising to see no reference to outputs (potential publications or patents) as seen with

all other projects. The lack of details in this space—even if the outputs were provisional, in progress, or anticipated—was disappointing.

- The project team has a good collaboration strategy with a reputable catalyst manufacturer, enabling the metal/acid bifunctional catalyst design to be realized in an engineered form. The project has provided good insight into the impact of various reactor loading strategies and the associated modeling for it.

- The approach here is to take the mixed olefin stream out of MTO and to oligomerize that further into SAF-range material, eventually followed by a hydrogenation stabilizing/polishing step. This approach is a generally accepted pathway for methanol-to-jet technology, looking at a supported metal on an acidic surface. The bulk of the work on this project will take place at the national lab. The approach is to do fuel property testing at the university and develop the engineered form of the catalyst along with scale-up manufacturing. A third-party inspection lab verification could also be useful on this project. There was no mention of aromatics potentially showing up in the product stream. The state-of-the-art material and how materials on this project differ were not discussed in any detail. One risk—catalytic deactivation due to the impurities present in the real feed—was mentioned, but no mitigation strategy was proposed to address it. The plan to connect the MTO and oligomerization reactors together should be able to happen in a year. The plan to hire one intern from an underrepresented minority group is a notable goal for 2023 because it is directly related to the project. Additional milestones/goals for DEIP should be included along with a vision for EJ with this technology. They have students from underrepresented minority groups. They hired a student from the Energy and Environment Diversity Internship Program (EEDIP). This is a good outcome.

- The team should highlight any special features of the testing apparatus for carrying out the oligomerization reaction. The co-dimerization C5 product offers interesting opportunities for SAF-range material. The carbon number of the sequential versus hybrid study should be disclosed. Olefins are no good for SAF. The team should recommend the appropriate reactor configuration strategies for the 75% loss of activity within one day on stream. The team should define moderate acidity outside of just numbers and show amine titration results by temperature programmed desorption to understand strength (via surface energy). The sequential reactor gave high yields of SAF-range material for a day on stream. The team should carry out the reactions on much longer time scales and work more closely with the catalyst deactivation team out of ChemCatBio. The project yielded material that demonstrated good SAF properties after hydrogenating the mixed olefin product. There were no details on the hydrogenation step, and there was no insight on the possibility of cofeeding hydrogen into the sequential reactor.

- Renewable methanol from biogenic syngas will continue to be a strong path for the bioenergy industry. The opportunity to upgrade this methanol to a premium fuel commodity such as SAF could have a huge impact. A robust catalyst system capable of performing oligomerization on stream in a stable manner for thousands of hours would also resonate across the industry. The team was able to get a reputable catalyst manufacturer as a collaborator on the project, which points to the significant business potential as a result of this work. In terms of benchmarking, this project has significant kerosene yields relative to other well-known routes (e.g., Fischer–Tropsch [FT], Mobil olefins to gasoline and distillate, Shell middle distillate synthesis), which opens up an opportunity for significant R&D in this pathway moving forward.

- This project aims to develop C2–C5 co-oligomerization catalysts and demonstrate an efficient path to generating SAF from syngas via a mixed olefin intermediate.

- This project targets a low-TRL step in the process of converting syngas to SAF. The R&D activities include the catalyst development, evaluation, and characterization. It has tested two kinds of catalysts and discovered their different ability to catalyze the co-oligomerization of olefin. The team also integrates the R&D activities with DEI activities by recruiting summer interns through PNNL's diversity internship program. The team also combines catalyst development with TEA/LCA to analyze the viability of the process in terms of scale-up and commercialization.

- Despite the short period, the project has illustrated impressive progress that can help achieve the project goal and DOE's mission for SAF and GHG emission reduction. The project has delivered 100 milliliters of finished jet fuel sample from the representative methanol-to-olefin feedstock. It would be very interesting to observe how the process might work with real feedstock. The team is also constructing a new reactor that can handle multiple olefin feeds. The construction of this reactor can help accelerate the R&D, focusing on the scale-up. The team also discovered the distinct performance of metal and zeolite catalysts in oligomerization. I encourage the team to reach out to CCPC to further analyze the science behind this difference. It may lead to a foundation for developing catalysts that can selectively catalyze the co-oligomerization reactions.

- The project is targeting the step with the lowest TRL in a multistep syngas-SAF process. Its success will improve the TRL of the whole process and could lead to a complete syngas-SAF process that has commercialization capacity.

- The olefin oligomerization project is progressing well, with the development of a dual-catalyst system in sequential configuration and commissioning of a new reactor system for performance evaluation. The catalyst system has shown promising activity and stability, which is an important step toward producing SAF from bio-syngas via the MTO route with higher jet fuel yield than other routes. However, further investigation is required to determine the root cause of the hybrid catalyst's quick deactivation. Using a different kind of zeolite could potentially lead to better results.

- Moving forward, it is critical to determine whether this catalyst system can still function as an engineered catalyst under commercial operation conditions. Computational modeling and fundamental understanding of active sites and kinetics should aid in rational catalyst design. The two-catalyst zone design may require dealing with different mass and heat transfer requirements and different deactivation mechanisms. Therefore, hybrid catalysts may still be an option.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for your valuable feedback on the "Syngas-Derived Mixed Olefin Oligomerization for Sustainable Aviation Fuel" project. We appreciate your positive remarks about the progress made and the potential impact of our work in achieving the project's goal of reducing GHG emissions and aligning with DOE's mission for SAF. We are glad to hear that you recognize the collaborative efforts of our research team, which includes PNNL, WSU (fuel property analysis), and Topsoe (engineered catalyst development). The expertise and contributions of WSU in fuel testing have been instrumental in the project's milestones at the end of Year 1 of this project. The development of a catalyst system and the optimization of reaction conditions to achieve C2–C5 co-oligomerization with over 75% selectivity to jet-range products are significant accomplishments. We acknowledge the durability of the catalyst as a key aspect, and we plan to conduct testing for approximately 500 hours to demonstrate its long-term stability by the end of this 3-year project. This project will demonstrate the syngas-to-fuels pathway and provide a better understanding of the process economics by successfully achieving milestone goals set by this project. Moreover, our project is specifically targeting the unit operation with the lowest TRL in a multistep syngas-SAF (via methanol) process. Its success would not only improve the TRL of the whole process, but also pave the way for a complete syngas-SAF process with commercialization capacity. We highly value the reviewers' feedback regarding diversity and inclusion, as well as the significance of establishing a support community to foster collaboration and alleviate individual pressure. Our team shares the same recognition and is actively implementing measures to address these aspects. We have successfully hired a student through the EEDIP, which has allowed us to bring in multiple students to work on various projects within the energy and environment program areas. Furthermore, EEDIP includes a comprehensive mentoring plan and programming to provide dedicated support to these interns, ensuring their success and facilitating their growth throughout the project. We appreciate your emphasis on collaboration and interaction with the deactivation project in ChemCatBio and CCPC. Understanding deactivation mechanisms in the sequential versus hybrid bed catalysts is indeed critical, and we will actively engage with the deactivation project to advance our understanding of the reaction system and increase its efficacy. We apologize for the oversight of not providing sufficient details about potential outputs, such as publications or patents, in our presentation. As this project is in its early stages, having commenced in FY 2023, we currently have limited published journal articles or patents. However, we are actively working on completing two journal articles based on the experimental outcomes of this project, and we anticipate their publication prior to the next Peer Review. Additionally, our project team has already submitted a patent application for the mixed olefin co-oligomerization process derived from our research. We recognize the importance of sharing these outputs and will ensure that we provide updates on publications and patents as they become available. We acknowledge the concerns raised regarding the presence of aromatics in the product stream and the potential catalytic deactivation due to impurities in the real feed. To address these challenges, our Year 3 project plan incorporates longer-time-scale experiments, allowing us to study and mitigate these issues effectively. Furthermore, we are committed to investigating the root cause of the hybrid catalyst's quick deactivation and gaining a deeper understanding of the associated deactivation mechanisms. This knowledge will enable us to refine and optimize the hybrid catalyst system, ensuring enhanced stability and performance. We appreciate your comment regarding the hydrogenation step and the possibility of cofeeding hydrogen into the sequential reactor. In our process, we opted for a commercially available hydrogenation catalyst for this well-studied unit operation. However, we did not consider cofeeding hydrogen to eliminate the hydrogenation of small olefins (feedstock) to maintain process carbon efficiency. Thank you once again for your valuable feedback and suggestions. Your input will help us improve our project and address the mentioned areas of concern. We remain dedicated to the successful implementation of our project and the advancement of SAF technologies.

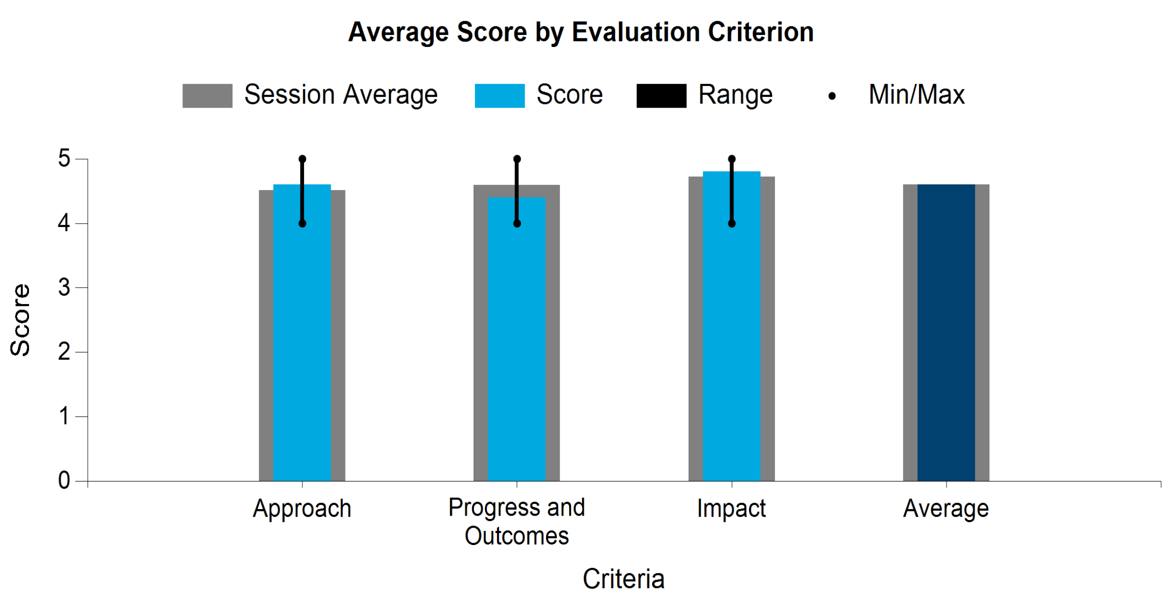
INTENSIFIED BIOGAS CONVERSION TO VALUE-ADDED FUELS AND CHEMICALS

University of South Florida

WBS:	2.3.1.414
Presenter(s):	John Kuhn
Project Start Date:	10/01/2018
Planned Project End Date:	04/30/2023
Total Funding:	$2,296,756.00

PROJECT DESCRIPTION

The overarching goal of this project is to convert biogas obtained from landfills, wastewater treatment plants, or anaerobic digesters to hydrocarbon fuels and chemicals. The specific goal is to develop an intensified process to reduce CapEx and enable a 15% reduction in MFSP relative to SOT. This project also aims to diversify products from biogas conversion and minimize flaring. The project management plan allows each organization to focus on its core capabilities to enable rapid catalyst and process development. The project leverages DOE resources, including ChemCatBio. Development is accelerated by an iterative, multifaceted approach to R&D challenges. Activities focus on critical success factors by addressing the go/no-go criteria and reducing project risks, which has included scale-up and use of real biogas. The approach is to integrate catalysts tuned to specific reactions into the same reactor bed. The project so far has more than tripled the single-pass production nonmethane hydrocarbon products compared to the SOT. Gains are obtained via catalyst development, concurrently to minimize the use of precious metals, and tuning of process conditions. It is anticipated that the inherently improved heat and mass transfer will lower costs, as well as reduce fossil GHG emissions compared to alternatives. The project addresses several BETO barriers, such as increasing yields from catalytic processes, decreasing the time and cost to develop novel industrially relevant catalysts, and improving catalyst lifetime.



COMMENTS

- This project is an excellent fit within the portfolio, and the catalyst characterization work is excellent. This is an amazing pivot. I think this was one of my favorite projects to review.

- The project develops biogas obtained from landfills or anaerobic digesters into liquid hydrocarbon fuels by developing an intensified process with conversion in a single reactor operating at mild conditions to reduce the capital expenses and enable small, modular reactors for distributed production. Currently, the conventional process uses three reactors, operates at high pressure, and has significant methane loss in the reformer. This project had to make an amazing pivot when they lost their original partner (Big Ox Energy), who was supposed to supply their biogas. They were instead able to partner with a local landfill and compress landfill gas (which is really impressive). This project aims to avoid carbon loss and undesirable products as they convert the biogas to chemicals, in line with BETO goals. To do this, they will need to create tailored catalysts with a range of functionality—all while combining process steps into a single reactor. The approach is collaborative; there is a great industry/lab/university partnership.

- This team blew away their 10% target of C_2 hydrocarbons—by achieving 16% hydrocarbon yield on the lab scale using real biogas. That is truly impressive. They have achieved improved catalyst activity by lowering the C-H activation temperature, reduced (maybe eliminated?) platinum with ruthenium and zinc (major cost driver), and demonstrated 100 hours of operation with high carbon efficiency. The characterization work to help determine mechanisms is really impressive. The economic and environmental assessments demonstrated that the capital and operating expenses can be made lower than comparable techniques—and that using landfill gas resulted in net NEGATIVE GHG emissions (huge win!).

- This project demonstrated a new pathway for biofuel production with an underused feedstock and developed a process intensification strategy that creates a low-cost pathway for production. This project is extremely industrially relevant, as it creates a diverse portfolio of products, and the interest from both upstream and downstream companies demonstrates this. This project demonstrates that there are truly cost-competitive pathways to produce valuable products from waste gases that would otherwise simply add to the GHG inventory. This is exceptional work.

- This project is focused on the conversion of biogas to liquid fuels under mild conditions and high carbon efficiency. The project has elements involving both catalyst and process intensification/reactor design. The general topic has a unique niche in the space of projects in the consortium and is clearly a need area for some level of investment. Although mixed hydrocarbon/CO_2 streams may contain less energy content, the opportunity to take such biogas mixtures and leverage them for production of fuels/chemicals of value should certainly be pursued to some degree in parallel with other biomass-to-chemicals platforms. The presentation identifies the challenges in this space well. Moreover, the project brings interesting aspects to the broader portfolio, including considerations of catalyst bed configuration and a separation component relative to catalyst construction and reactor design. There are unique features in these spaces that can add value to the broader ChemCatBio Consortium. Furthermore, the project has forward-looking goals—particularly in developing low-PGM to PGM-free catalysts—that align well with broader consortium efforts. Project roles are generally outlined in the presentation, with one exception. The reactor modeling portions could more clearly be delineated in the slides. The project benefits significantly from ChemCatBio ACSC and thermochemical platform analysis enabling projects. Given the potential complexity involved with overcoat catalysts, it seems that ACSC might offer additional opportunities beyond advanced characterization for the project and should be pursued where appropriate. Risk mitigation was also well identified, with sufficient strategies in place if particular scenarios play out. The go/no-go milestones were clearly achieved, and bifunctional catalysts were prepared with activity, selectivity, and stability profiles that appear promising. The further movement toward non-PGM catalysts and more realistic biogas streams is also notable. The use of precision synthesis in preparation of coated catalysts seems like a real game-changer in the removal of PGMs. The role of ACSC in the project is critical, particularly when it comes to characterization of the mixed metal systems. Reactor-scale modeling, assumed to occur within CCPC, is also a highlight of collaborations across the consortium. The Fe-In catalysts appear promising, given good selectivity despite somewhat reduced activity—however, the lack of atomistic modeling to elucidate what is happening at the active site is a potential missed opportunity and is something that should be considered in the future. This may be an example where a beefed-up emphasis on larger-scale modeling may come at the expense of a better handle on catalyst behavior. The reviewer does recognize that finite resources force these types of prioritization. The process intensification/reactor bed configuration studies also appear to be promising for ensuring that the overall process maximizes efficiency. Furthermore, various components of the system—potential contaminants, promoters—are studied in the context of the system, as one would expect. The move toward realistic feed gas mixtures is commendable and indicates that the technology is moving closer to viability. The economic modeling highlights a strong selling point of the project with potential for a negative carbon footprint. At the same time, coproduct formation and high alkane yield will likely drive economic viability. Continued modeling refinement will be needed to really determine system feasibility. This is a minor note, but more details about the reaction scale would be valuable in framing the current status of the technology for the reviewer. Later slides mention lab-scale studies, but some bars on this magnitude would be useful for the evaluation. Accomplishing the milestone for the formation of C_2 products is a notable outcome that is attracting interest from both downstream and upstream groups associated with biogas utilization. The publication and patent output (five papers and one patent) is also solid.

- The team made great use of characterization tools to help design the encapsulated catalyst concept, as well as supporting Fe-based FT materials. The modeling approaches seem interesting and should continue on the path of verification with experimental data.

- This approach of designing and encapsulating material has always been interesting and promising from a surface reaction engineering standpoint. The team should address the concept of pore restrictions from the external surface. The entire approach is very organized and understood by the team. The state-of-the-art technology is not modular for small-scale processing, needs additional units (e.g., water-gas shift, heat exchangers), and requires more severe conditions (>pressure), and this project solves all of these issues by invoking process intensification within the catalyst pellet. This approach allows for more innovation opportunities at the engineering reactor design scale, which is clear from the loading strategies investigated between the FT synthesis and reforming catalysts. The major tasks outlined for the project appear to be reasonable, with much of the work falling on the university partner. The durations of the tasks weren't mentioned. A project such as this could use a catalyst synthesis scale-up partner or leverage NREL's capability in this area. The actual contributions of the university to the technology readiness task should be explained. The team highlighted a couple of notable risks, namely, a real feed gas contaminant causing catalyst and product issues (solved by treating all gases) and equipment failure threatening process operation uptime (solved by purchasing spare parts and equipment). The DEIP should have been comprehensive because the project is university-led, as should the EJ commentary because landfills have a long history of being near disadvantaged communities. There were no comments on either issue.

- Modeling information was published in 2022 on designing outer core thickness along the axial profile of the reactor. The team made a good case for the impact on training students, releasing information to the public (via presentations and publications), and forming local industrial partnerships. There is an interest in knowing whether larger multinational process technology licensing organizations have inquired about this work yet. This pathway provides a sustainable route to transportation fuels using wasted biogenic carbon, which is worth highlighting.

- The team did an excellent job of characterizing the positive impact of incorporating zinc to a certain level on turnover frequency. The catalysis was clear, confirming the presence of zinc in the bulk crystalline and surface moieties. The TOS for data using dry reforming went out over 150 hours. The dynamic catalysis work using isotopic transient kinetics analysis, *in situ* X-ray photoelectron spectroscopy, and diffuse reflectance infrared Fourier-transform spectroscopy was impressive, as was the work using extended X-ray absorption fine structure and X-ray absorption near edge structure. The conclusions from this work should be clarified a little further, as it looks like different experiments were being presented across a variety of objectives. For the pore restriction work, the team should present the entire product distribution rates, including any wax formation. The effect of indium promotion of iron FT materials was interesting. The dispersion count data seemed to show only up to a certain level of indium concentration. The team was able to show in a compelling way how activated CH_4 spent three times longer on the surface of the indium promoted, supported, dispersed iron surface. The materials spent >70 hours TOS. The team should define the selectivity and if normalized to 100%. Potassium-on-iron materials had a significant effect on C-C bond forming transformations. The team should report where the rest of the mass yield is going for combined bed testing. It looks like an online analyzer output. This project aims to develop an intensified process to reduce CapEx and enable a 15% reduction in MFSP relative to SOT. This is a project led by a university and participated in by the national lab.

- The team focused on tailoring the catalyst activities, designing bed configurations, and developing a zeolite coating that enables an *in situ* separation for reactions. The various R&D activities include catalyst synthesis, validation and reaction testing, materials characterization, design, TEA/LCA, and commercialization exploration with industrial partners. They also set go/no-go objectives to help evaluate the progress of the project. It could be beneficial if they reached out to ACSC to discuss the optimization of their zeolite-coated catalyst preparation and characterization. It could also be beneficial if they reached out to CCPC to analyze how the zeolite coatings may impact the heat and mass transfer.

- The R&D activities have illustrated appropriate progress that helps achieve the project goals. For instance, the team illustrated that their R&D has helped reduce the cost of catalysts by 40% and increase the catalytic activity at low temperatures significantly. It would be beneficial if the team could introduce TEA/LCA efforts into the R&D activities and use them as a tool to help determine the viability of technologies and processes.

- This project demonstrates a new pathway for biofuel production to BETO. If successful, it will enable the industrialization of a process that converts the underused feedstock—biogas—to valuable fuel products. The R&D activities have shown the potential of this process to be commercialized via intensification. The team also leveraged the R&D activities to connect academia, a national lab, and industry. It would be beneficial if the project could leverage the R&D activities more to enhance the DEI and workforce development.

- This study investigated intensified catalytic synthesis for the conversion of biogas into liquid fuels on a small scale to meet the requirements for landfill waste treatment. The research was a significant challenge, but its potential impacts are enormous. The study employed remarkable approaches, such as the tailoring of catalysts, close collaboration, and simulation/computation work. Both mechanistic understanding with many *in situ* techniques and the efforts toward commercialization with real gases and stability testing with impurities are very impressive, leading to numerous outstanding achievements, including satisfactory C_2 hydrocarbons yield and GGE. The stability of reforming/FT catalysts is a crucial factor to consider, as they are expected to operate for several years. Most zeolites exhibit coking and structural stability issues under hydrothermal conditions, despite having good initial activity. Additionally, metal migration from other catalysts could adversely affect zeolites. Therefore, further deactivation studies are recommended.

PI RESPONSE TO REVIEWER COMMENTS

- In addition to the many positive comments, our team appreciates the time and effort of the reviewers. We would like to note that many literature contributions are still in progress. As three Ph.D. students are wrapping up their respective dissertations on these topics, there are a handful of additional papers in the pipeline. Thus, we anticipate further contributions in the literature within the next year. We agree that the doped (e.g., indium) iron carbide catalysts are a great opportunity to delve deeper into structure-functional relationships and mechanisms. A subsequent proposal was written in collaboration with

NREL. The reviewer comments were positive, but the proposal was not awarded. We will look for other opportunities to dive deeper into this topic. We also agree with the reviews that additional examinations of deactivation would be great next steps in this effort. We apologize that at least one reviewer noted a lack clarity in the reactor modeling. We were limited due to time/space limitations. We also note that the collaboration with CPPC is in an early stage. We agree that such a collaboration, especially to leverage expertise in heat transfer effects, would be a great direction. There were some uncertainties about the overall mass balance. Carbon dioxide, carbon monoxide, methane, and condensables, including heavier hydrocarbons, oxygenates, and water, are the primary species in the effluent that are not reported with the TOS gas-phase gas chromatography analysis. For the hydrocarbons, the cutoff point for gas or liquid phase is ~C6/C7, based on the operation of the condenser. Those that are lighter than the cutoff chain length are included in the TOS data for C_{2+} and C_{5+}. The condensable hydrocarbons typically add ~4 mass % to the TOS mass yield. In a hypothetical case of 1:1 methane:carbon dioxide in the feed, ~53% of the feed mass is oxygen atoms, which does not result in the hydrocarbon products. Moreover, only one molecule of CO_2 is reacted per three molecules of methane ($3\ CH_4 + 2\ H_2O + 1\ CO_2 \Rightarrow 8\ H_2 + 4\ CO$) to achieve a hydrogen to CO ratio of 2:1, which is the molecular ratio in targeted hydrocarbons. Thus, there is a substantial amount of CO_2 in the effluent. The experimental studies were on a single pass. In our process simulations, we modeled recycling to increase the overall conversion to C_{2+}. With recycling, the non-condensables (CO_2, CO, and light hydrocarbons) can be used to boost the higher hydrocarbons. However, in any scenario, CO_2 and water will be formed to allow escape of oxygen atoms, which are not desired in the final product. We note that the project was funded under a FOA in which a DEIP was not required. We acknowledge that there are many potential benefits of new processes being applied to the waste industry.

DATA, MODELING, AND ANALYSIS

PROGRAM

CONTENTS

INTRODUCTION

The Data, Modeling, and Analysis (DMA) Technology Area is one of 12 technology areas reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 26 presentations were reviewed in the DMA session by 6 external experts from industry, academia, nonprofit, and other government agencies. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks (https://www.energy.gov/eere/bioenergy/data-modeling-and-analysis-program).

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $33.6 million, which represents approximately 6% of the BETO portfolio reviewed during the 2023 Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Andrea Bailey as the DMA Technology Area review lead, with contractor support from Bryce Finch of BCS, LLC. In this capacity, Andrea Bailey was responsible for all aspects of review planning and implementation.

DATA, MODELING, AND ANALYSIS REVIEW PANEL

Name	Affiliation
Jason Jones*	ICF International
Nikita Pavlenko	International Council on Clean Transportation Fuels Team
Chris Ramig	U.S. Environmental Protection Agency
Sarah Mittlefehldt	Northern Michigan University
Yalin Li	University of Illinois Urbana-Champaign
Steele Lorenz	Farmers Business Network

* Lead Reviewer

DATA, MODELING, AND ANALYSIS REVIEW PANEL SUMMARY REPORT

Prepared by the Data, Modeling, and Analysis Review Panel

INTRODUCTION

The BETO DMA Technology Area continues to provide a vital and strategic portfolio to DOE, the bioeconomy industries, and wider national sustainability objectives. The 2023 Peer Review of the DMA program was conducted over 3 days, from April 3–5, 2023, in Denver, Colorado, featuring 26 principal investigators (PIs) who presented their research to a diverse 6-person review panel that included members from academia, the private sector, research organizations, and other federal agencies. This report consolidates the panel's perspectives on the program, focusing on strategic management, implementation, progress, and the pursuit of program goals. It concludes with three prioritized recommendations for future directions.

During the 2023 Peer Review of the DMA program, reviewers were presented with an array of projects that were shown to significantly contribute to BETO's program goals of decarbonizing the transportation, industrial, and agricultural sectors and developing cost-effective, sustainable biomass and waste utilization technologies. The DMA program's portfolio demonstrates a diverse range of feedstocks and technologies that carefully align with BETO's evolving strategic objectives. Many projects are at the cutting edge of their respective fields, including the Global Change Analysis Model (GCAM) Bioenergy and Land Use Modeling and Directed Research and Development (R&D); Bioeconomy Scenario Analysis and Modeling; Integrated Landscape Management; Life Cycle Analysis of Biofuels and Bioproducts and Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) Development; and the Net-Zero Carbon Fuels Technical Team (NZTT). These initiatives serve as crucial resources for an array of stakeholders in the U.S. bioeconomy and contribute valuable methodological rigor for policy and business applications across local and global scales. The program strategically adapts to the shifting priorities and needs in the bioeconomy, reflecting BETO's focus on low-carbon and net-zero-carbon fuels for the aviation; marine; rail; and heavy-duty, long-haul freight industries.

The review panel commended the DMA program for its innovative and pioneering work in advancing a sustainable bioeconomy while emphasizing the need for strategic alignment with BETO's objectives. The panel also underscored the importance of distributing the analysis portfolio across high-priority biomass use cases and balancing short- and long-term decarbonization strategies. Further, focusing on equity, addressing it early in the program's growth, developing concrete metrics, and ensuring consistency across the portfolio will enhance the DMA program's impact and contribute to a more equitable and sustainable bioeconomy.

STRATEGY

Overall, all reviewers found the DMA program to have a well-defined strategy that aligns with its mission, goals, and technical targets, considering relevant industry and stakeholder input. Reviewers were "impressed by the breadth and depth of BETO-funded projects." The program's ability to quickly adapt to emerging priorities, such as sustainable aviation fuels (SAFs), demonstrates its agility; however, some reviewers felt there is room for growth in ensuring sufficient coverage across relevant sectors, such as rail, marine, plastics, and chemicals. In contrast, another reviewer praised BETO for adequate coverage in these areas.

Reviewers found the DMA program's funding mechanisms, including funding opportunity announcements (FOAs) and annual operating plans, are well suited to the varying technical topics. Reviewers noted that the program should continue to balance near-term decarbonization through first-generation biofuels with long-term solutions involving advanced biofuels. One reviewer suggested, "Funding projects that are readily market competitive—though not aiming at direct production of biofuels or not highly innovative—might present as great opportunities to actualize the bioeconomy." DMA should consider funding projects that are market competitive in the near term while maintaining focus on mid-/long-term goals. One reviewer suggested that supporting non-biofuel markets, such as animal bedding, could alleviate farmers' concerns about the lack of biomass buyers and lead to faster adoption of bioenergy crops. Such a strategy may contribute to the actualization of the bioeconomy and advance the adoption of sustainable practices. To address gaps in the current strategic vision, DMA should prioritize end use applications, incorporate economic considerations, support bioenergy pathways with the greatest potential for deep decarbonization, and lead BETO in developing environmental justice (EJ) and diversity, equity, and inclusion (DEI) efforts for bioenergy R&D.

Several reviewers noted that the DMA program could improve its strategic plan by designing a complementary portfolio of projects that address different aspects of the bioenergy value chain and support technology development and policy design. Increased inter-project communication and consistent approaches, assumptions, and platforms will help create a coherent model ecosystem to support BETO's mission. Ensuring transparency in models and methodologies will also enhance the program's effectiveness.

Last, incorporating social aspects—such as social acceptability, community impact, and EJ—is essential to the DMA program's success. Paty Romero Lankao and Rebecca Efroymson's work serves as an excellent starting point for integrating social considerations into BETO-funded research. To encourage collaboration, BETO should consider inclusion of review criteria that emphasizes iterative communication and collaboration with related projects, advisory boards, and impacted stakeholder groups.

STRATEGY IMPLEMENTATION AND PROGRESS

The Strategy Implementation and Progress section of this review analyzes the effectiveness of the DMA program's project funding and management, with specific attention to their alignment with strategic directions, innovation, progress toward set goals, and beneficial outcomes for both the performer and the government. The review panel assessed all projects on their implementation and development, identifying leading-edge work, evaluating whether goals are achievable, and evaluating how the technology area team is managing these projects.

The DMA program, as part of its strategic direction, is effectively funding various projects. Notably, projects such as the GREET model and GCAM have been highly significant, working at the forefront of their respective fields, and they are expected to make considerable impact. The GCAM Bioenergy and Land Use Modeling and Directed R&D project, for instance, offers a detailed economic and physical model that integrates global trade, energy, agriculture, and consumption, providing valuable insights into terrestrial carbon management practices. Similarly, the GREET project continually evolves its model, incorporating new methodologies, fuel pathways, and technologies, making it a valuable tool for academia, industry, and policymaking.

Projects like the Biofuels National Strategic Benefits Analysis (BNSBA) and the Biofuels Information Center (BIC) align well with BETO's strategic objectives. BIC provides a comprehensive resource for biofuel stakeholders, compiling and organizing information on biofuels and bioenergy-based chemicals and offering effective data visualization. This project has seen wide adoption among industry and policymakers, as reflected in its numerous page visits. One reviewer said, "This project fills an important niche, as the data is extremely challenging to collect and yet it is compiled in one convenient place with excellent organization and data visualization." Also, the BNSBA project focuses on understanding and enhancing the socioeconomic and environmental benefits of biofuels. It has made significant strides since 2021 by improving its existing model to address key interest areas, contributing to decision making and policy design. Despite being well aligned with objectives, reviewer drawbacks of the BNSBA framework included discussion about a lack of market response and land use change (LUC) considerations.

In terms of managing projects, the technology area team actively ensures beneficial outcomes for all involved parties; however, there are areas for improvement, such as enhancing communication, access to models, and harmonization across projects. Also, there is a need for increased focus on version control, flexibility, and robust uncertainty and sensitivity analyses in models like GREET.

Reviewers felt encouraged to see BETO funding projects that incorporate DEI efforts in their scope. Aligning with the DOE Office of Energy Efficiency and Renewable Energy (EERE) mission, the DMA program can further contribute to the creation of a clean energy economy that benefits all Americans by addressing environmental injustices, fostering a diverse science, technology, engineering, and mathematics workforce, and developing robust workforce training opportunities. In the future, it would be beneficial to prioritize such projects and to broaden the focus to various transport sectors and generations of biofuels.

Last, although the program is on track to meet its near-term and midterm goals based on the current project portfolio, there are some gaps that need to be addressed. These include a stronger push toward decarbonization and more focus on the social dimension of projects, which is often overlooked despite its importance in project deployment and EJ. Additionally, one reviewer noted, “Another methodological area for improvement is to ensure that all modeling and analysis projects start to incorporate uncertainty analysis and sensitivity analysis into their approach as a standard practice.” With these improvements, the DMA program can ensure more significant progress toward its strategic goals.

RECOMMENDATIONS

The DMA program has made significant strides in promoting a sustainable bioeconomy, evidenced by their innovative projects and strategic alignment with BETO’s objectives; however, from the collective input of several reviewers and the robust discussions that ensued, the review panel identified three key recommendations to further bolster the portfolio in the near to medium term. These suggestions include enhancing stakeholder engagement, ensuring distribution of the analysis portfolio across high-priority biomass use cases, and placing a greater emphasis on equity.

Recommendation 1: Enhance stakeholder engagement and measure impact.

First, stakeholder engagement and measuring impact is crucial for directing the program and measuring success. The DMA PIs should provide an explanation of how stakeholder feedback will inform the model and research as well as emphasize validation and ground-truthing. This involves translating model data and output into real-world applications, fostering partnerships with other agencies, and improving communication, marketing, accessibility, and usability of tools. Additionally, the program should outline clear goals and designed use cases, ensuring that the portfolio addresses stakeholders’ needs and expectations. Such a design element can be included as a required component of the study by BETO.

Recommendation 2: Align the analysis portfolio with high-priority biomass use cases.

Second, it is essential to distribute the analysis portfolio across high-priority biomass use cases, aligning with the EERE strategic vision and broader federal objectives. This requires clearer plans for distributing funding to cover the necessary scope/objectives, leveraging tools/resources to reduce duplicability, and balancing short- and long-term decarbonization strategies. By doing so, the DMA program can effectively address various aspects of the bioeconomy and accelerate progress toward sustainability goals.

Recommendation 3: Prioritize equity in projects and objectives.

Finally, the DMA program should prioritize equity in its projects and objectives. Recognizing the importance of this issue early in the program’s growth can lead to significant long-term benefits. Instead of biomass projects solely focusing on “supporting rural economies,” the program should develop concrete metrics for equity that can use both qualitative and quantitative data. Developing equity metrics can be achieved by enhancing stakeholder engagement (linking to the first recommendation), ground-truthing, and ensuring that models have the capability to investigate issues related to fairness and justice. By working with BETO’s EJ office and achieving consistency across the portfolio, the DMA program can contribute to a more equitable and sustainable bioeconomy.

DATA, MODELING, AND ANALYSIS PROGRAMMATIC RESPONSE

INTRODUCTION

The DMA program would like to thank the review panel for their time and effort during the review process and their careful review of the portfolio. Feedback on the overall program is especially valuable as DMA works to pivot to address new office and administration goals and priorities. The program also appreciates the comments on increasing the utility of existing models and tools for multiple audiences and recognizes the importance of incorporating better uncertainty and sensitivity analysis into results to the extent possible.

The full set of recommendations from the review panel will be discussed and considered when working on future project selection and program design, as future appropriations allow. Following are the responses to the three key recommendations identified by the review panel.

Recommendation 1: Enhance stakeholder engagement and measure impact.

The DMA team agrees with this recommendation to improve both the practice of engaging stakeholders across the bioenergy supply chain and measuring this impact to ensure that BETO-funded models and tools are reaching the intended audience. Many models presented in this review will finish internal development and scenario testing before the next review, and the DMA team plans to work with these groups to include metrics on engagement and actual model use in the next set of updates. Beginning with the annual Fiscal Year (FY) 2024 call for proposals to the national labs, DMA has also committed to including a metric for the planned publication of all relevant tools and models and tracking views/downloads and other relevant engagement metrics. In addition, for projects that are not working on a specific tool or model, the team is encouraging either stakeholder engagement sessions, where relevant, or partnering with relevant organizations that already specialize in stakeholder engagement, such as land trusts and farmer-led cooperatives. The team is also looking into providing training to lab staff on how to best engage stakeholders such as small landowners who may not be as familiar with all the variables that go into a bioenergy model but would still like to engage with the bioeconomy. By the FY 2025 review, DMA will produce a list of relevant metrics for different project types for reviewers to use as a benchmark for these projects.

Although stakeholder engagement is critical for most DMA-funded models, some economy-wide models are primarily aimed at internal-facing analytical and policy needs for DOE. These models may be good candidates to publish less complex public versions as funding allows. Part of following this recommendation will also be carefully working with PIs to determine the targeted end user of their model and the degree of engagement or tracking that is appropriate.

Summary of actions:

- Work with existing projects to include metrics on engagement and actual model use.
- In future project calls, include a metric for the planned publication of all relevant tools and models and tracking views/downloads and other relevant engagement metrics.
- Work with national laboratory partners to provide staff training for stakeholder engagement.

Recommendation 2: Align the analysis portfolio with high-priority biomass use cases.

The emphasis on decarbonization goals since the 2021 Project Peer Review has resulted in many changes across the DMA and larger BETO portfolio. The DMA team has worked to address as many administration and office goals as possible and to prioritize analyses that cover an appropriate breadth of feedstocks and end use cases while emphasizing the areas in which biomass has the largest role to play in decarbonization.

Some projects that that were selected as part of competitive solicitations that had goals set at the time of publication may have stronger links to past office priorities than to the overall current office goals. Even so, the DMA team is committed to working with them to support these goals as much as possible within their existing work plan. The entire BETO program has also recently engaged in a larger internal portfolio analysis exercise that will attempt to better map how each program has structured its portfolio to address administration goals and the March 2023 Multi-Year Program Plan. As a part of this analysis, the DMA program will create a mapping of analysis projects in other program areas for the 2025 Project Peer Review and show their relationship to areas of strategic priority for the office.

In addition to internal BETO analyses, BETO is committed to working with other EERE offices on analysis related to how biomass can support decarbonization across the chemicals sector and for additional hard-to-decarbonize transportation sectors. Portions of this analysis should be available in more detail in time for the 2025 Project Peer Review. As the analysis related to these different sectors becomes available, the DMA team hopes to enhance the overall understanding of the best use of biomass to maximize the overall decarbonization potential of this resource.

Summary of actions:

- Assess the feasibility of providing an overview of various analysis projects throughout the entire BETO portfolio in terms of the highest-priority biomass use cases.
- Define with other EERE offices the highest-priority biomass use cases with updates available by the 2025 Project Peer Review.

Recommendation 3: Prioritize equity in projects and objectives.

DOE has increased the focus on incorporating DEI priorities into the research and application of technologies since the 2021 Project Peer Review, and BETO is no exception. The DMA team appreciates the reviewers' recognition that this is an important piece of any R&D program, and we will continue to commit to achieving a better understanding of these issues as they relate to bioenergy and prioritizing research that takes equity concerns into account. The DMA team also appreciates the recommendation to robustly use stakeholder engagement, particularly of people and groups from less consulted expertise and backgrounds; ground truth research on social, environmental, and equity considerations of bioenergy; and ensure that the research done in the DMA portfolio can be responsive to equity considerations where relevant. These steps are being enacted in parts of the DMA portfolio, and the team aims to support the expansion of this approach throughout the DMA and BETO portfolio in appropriate, impactful ways.

In the near term, DMA will focus on the research, analytic capabilities, and integration of equity considerations into biorefinery siting. DMA has begun work with different national lab analysts to better understand the sustainability impacts (both social and environmental) of full-scale biorefineries with the intent of promoting more equitable siting decisions for the refineries that will be necessary to reach BETO's long-term goals. In addition to this work, DMA plans to engage with energy equity and siting experts and stakeholders on the best metrics and areas for research for incorporating equity into not only DMA research but also research across the entire BETO portfolio.

Internally, BETO remains connected to larger DOE and EERE-wide efforts related to equity and is committed to contributing data and staff time to those efforts. This has included supporting the development of DEI plans and, more recently, community benefit plan language and requirements in an effort to make the research project process more equitable, and it has included devoting resources to research areas that improve understanding and enabling equity and social and environmental sustainability, such as the biorefinery siting work. Increasing the amount of work in the portfolio specifically funded by BETO is subject to future appropriations, but the DMA team as well as representatives from other BETO technology areas are working to stay current on equity concerns surrounding bioenergy and continue to incorporate equity into existing projects as much as possible. In the near term, BETO aims to have more resources about applying to FOAs and drafting meaningful community benefit plans.

Summary of actions:

- Continue to support research on biorefinery siting, social considerations, and equity implications, and ground truth this research with methods such as engagement with equity experts and stakeholders and case studies.
- Identify two or three high-priority research areas for the bioenergy supply chain in terms of equity implications and social sustainability.
- In future calls, as appropriate, include requirements for projects to identify whether and how their models and analyses have capabilities to measure and examine equity implications and social considerations.

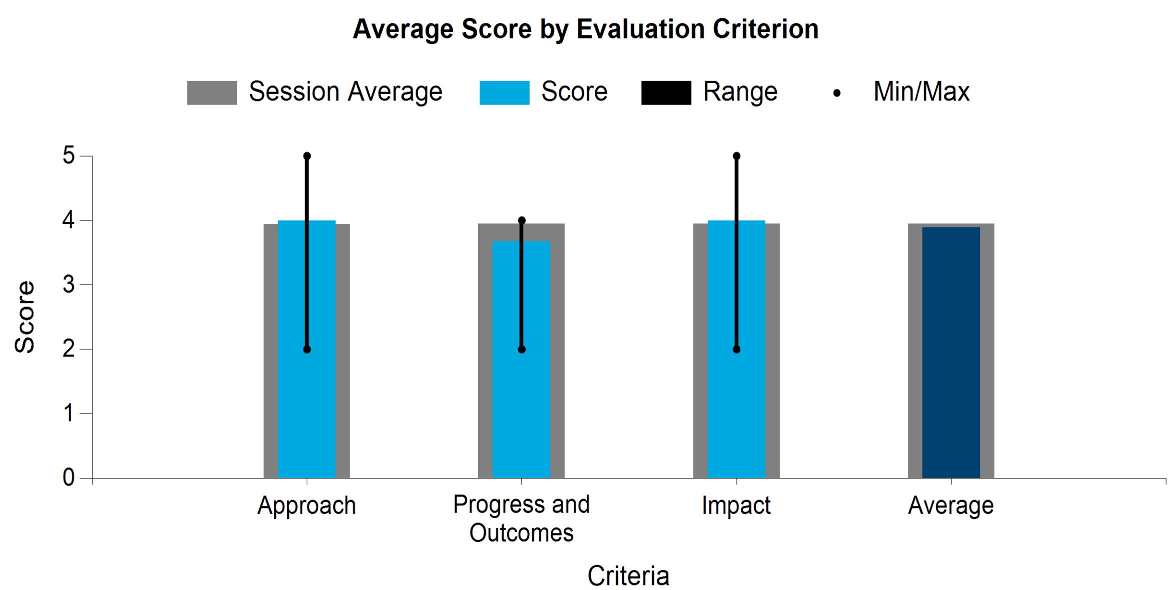
GCAM BIOENERGY AND LAND USE MODELING AND DIRECTED R&D

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	1.1.1.7
Presenter(s):	Marshall Wise
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$525,000

This project provides quantitative analysis of the potential scale and impact of bioenergy and land use in the integrated economic context of energy, agriculture, and carbon. The Pacific Northwest National Laboratory (PNNL) GCAM, a prominent model of long-term global energy and land use, has been widely used for DOE, the U.S. Environmental Protection Agency (EPA), and private industry. Using GCAM, we have published studies for BETO on biofuels, biopower with carbon capture and storage (CCS), resulting land use, and emissions impacts. The biggest challenge is to manage the complexity of modeling detailed bioenergy systems and terrestrial carbon strategies within the larger GCAM structure. For this FY 2022–2024 project, we are partnered with the National Renewable Energy Laboratory (NREL) (WBS 1.1.1.8) to study terrestrial carbon enhancement strategies in agriculture, including their impact on domestic and global land use and emissions. NREL performs biogeochemical modeling of physical parameters, including crop yields and soil carbon. PNNL uses these parameters to create crop practice options in GCAM and analyzes scenarios considering the economics of crop production under carbon incentive strategies. We have completed a study of biochar production and application to cropland, and we are currently developing scenarios for no-till practices and cover crops. In addition to terrestrial carbon, this BETO project is building GCAM capability to study the potential for alternative energy in the agricultural sector as well as the potential for renewable fuels for aviation demand.



COMMENTS

- Overall, this is a great project. GCAM is used by a wide variety of researchers and other stakeholders, demonstrating the value of the approach. I think the areas in which BETO is funding GCAM generally make sense, but I do see room for improvement.

Exploration of terrestrial carbon sequestration methods makes sense in general. But the focus on biochar is somewhat confusing to me. I agree that GCAM is a good approach for exploring the potential of this strategy, but there are other strategies being considered more widely in the near term that could benefit from analysis in GCAM. Examining no-till makes more sense to me, and I support the continuation of that line of research. I would encourage the researchers to consider other practices, such as nutrient management and conservation agriculture, which could yield DEI or sustainability cobenefits.

The work examining agricultural energy consumption is great and should continue. This is an under-researched area and a place where biofuels could play a strong role for decades to come. The forthcoming work on aviation is also very worthwhile. I do, however, think there is not enough emphasis here on the other BETO priority end uses of bioenergy. The use of biofuels for marine, rail, and off-road applications other than agriculture should be part of the scope as well as industrial chemicals and plastics. This is an area of suggested improvement for the project.

- Thank you for the opportunity to review the GCAM Bioenergy and Land Use Modeling and Directed R&D project. I am pleased to say that I believe the project is well aligned with BETO's goals, and I look forward to seeing how SAF is included in the framework and additional DEI metrics. The economic and physical model spanning until 2100 and covering domestic energy, agricultural production, consumption, and trade is an impressive undertaking. As most of the model parameters and assumptions are informed by other BETO research, the model is constantly evolving, and methods/data are somewhat crowdsourced and verified from an active community. The progress and outcomes of the project are also impressive, including completed biochar, current research on no-till and cover crops, and the expansion of the no-till option. I suggest providing more information on how the model decides between practices and the data or mechanism that defines the ultimate share. During the presentation, it was described that this was based on the input cost of the expected rate of return (output*price); however, there are other drivers controlling the share across production technologies/practices that should be included in this explanation. Overall, this is an excellent project that is making great strides toward its goals.

- GCAM is a valuable component of the technology area, providing a capable and publicly accessible open-source model for use by policymakers and researchers. This model balances both accessibility and flexibility to appeal to a wide array of stakeholders working on a variety of topics. This model is already extremely relevant in its current form, but the forthcoming updates to its analytical scope will further improve its usefulness. In particular, the integration of terrestrial carbon management technologies and the aviation sector will expand the range of analyses possible with the model.

  The progress toward incorporating terrestrial carbon management in the model underscores the model's utility as it combines detailed technology and physical data with economics to assess the trade-offs and net impacts of different approaches and policy incentives. The structure of the model also allowed for an evaluation of these management practices beyond a field level and their effects at a global level. It was clear from the presentation that these updates to the model will provide valuable insight on these land management practices and can inform policy.

- This is a very ambitious project. In striving to be a comprehensive model for all types of bioenergy for all regions for so many variables, a lot of important nuances and complexities are obscured. But, of course, that is the case with many models.

  When modeling inputs to agriculture, does the model account for fossil fuel inputs required to maintain certain biofuels, such as corn-based ethanol—greenhouse gas (GHG) emissions created through fertilizer manufacturing, etc.?

Land and water systems are highly vulnerable to current and future climate changes. How does the model account for climate change? Different regions—India, for example—are and will continue to experience different change trajectories. How are these accounted for?

How does the model account for issues of water quantity and water scarcity?

The DEI milestone mentioned hiring one high school student from Washington, D.C. This is a great first step, but more work could be done—if not in the models themselves, possibly in terms of the broader use and application of the model and related project artifacts and outreach activities.

Overall, this project strove to account for a wide range of variables in modeling land use as related to bioenergy, and it has the potential to advance the thoughtful implementation of bioenergy technologies. The project included a clear management plan and implementation strategy. I encourage the team to continue to consider how the project can address diversity and equity issues. The project has made progress toward its stated goals and has the potential to be useful to several different entities.

- While the inclusion of DEI in the internship program is appreciated, this type of modeling naturally lends itself to more informative diversity and EJ topics. EJ factors should be incorporated in future modeling.

  Calibration of the DayCent model is important and can substantially change soil carbon outcomes. Even with a robust literature review, it could be useful to include ground truth data on soil carbon. Adding sensitivity analysis or a range of outcomes to the permanence of sequestration would also likely make both pricing and climate outcomes more robust.

- The project has a broad and impactful goal, but it is unclear how the outcomes of this project have contributed to other BETO efforts. In particular, there do not seem to be many interactions with other models. A lot of previous/existing efforts seem to be on biochar, but this focus on biochar is not sufficiently justified. Admittedly, biochar has the potential for carbon sequestration, but it is not clear if and how biochar can achieve significant market penetration (and if this modeling effort complements other efforts on biochar). On the other hand, one strength of this project is that GCAM is publicly deposited on GitHub with good version control and a decent user basis.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you to the review panel for your constructive and expert comments and suggestions for research directions on this project. Concerning the study on biochar, we put our initial focus there for two main reasons. First, there has been a growing interest for natural climate solutions in the international carbon dioxide removal community. Second, we believe we were well positioned with our GCAM modeling to provide integrated analyses of biochar in agriculture, energy, and carbon management that was missing in the literature; however, we agree that other conservation and terrestrial carbon practices may have more near-term impact and broader relevance, and we are currently performing modeling and analysis of no-till and cover cropping. In terms of the energy system aspects of this BETO project scope, we are planning on directly linking the fossil or other energy required for the agriculture sector in more technological detail. With that, the incremental energy to expand crops for bioenergy or other reasons is explicitly accounted for in some technological detail with feedback to the rest of the energy and agriculture systems. Also under the BETO scope, we are upgrading the GCAM refinery sector model structure and the technologies involved in the production of jet fuels and other liquids. The outcome of this effort will be to enable a robust economic and physical representation of the potential scale and impact of biojet and other low-carbon pathways for aviation energy. For other targeted uses of bioenergy, such as marine and off-road, improving these is not explicitly in our BETO project scope, but these demands are considered in GCAM generally. Finally, in terms of DEI, we were happy to have the chance to use this project as a vehicle for inclusiveness and provide some research experience to a local high school student. This was a small step but hopefully one that makes some impact. In terms of the DEI impacts of terrestrial carbon management or conservation agriculture, those impacts are not something that we currently quantify as part of the economics of our modeling in GCAM. Impacts would have to be inferred using expert judgment, or they could be analyzed by a model that focuses on labor impacts and income distributions.

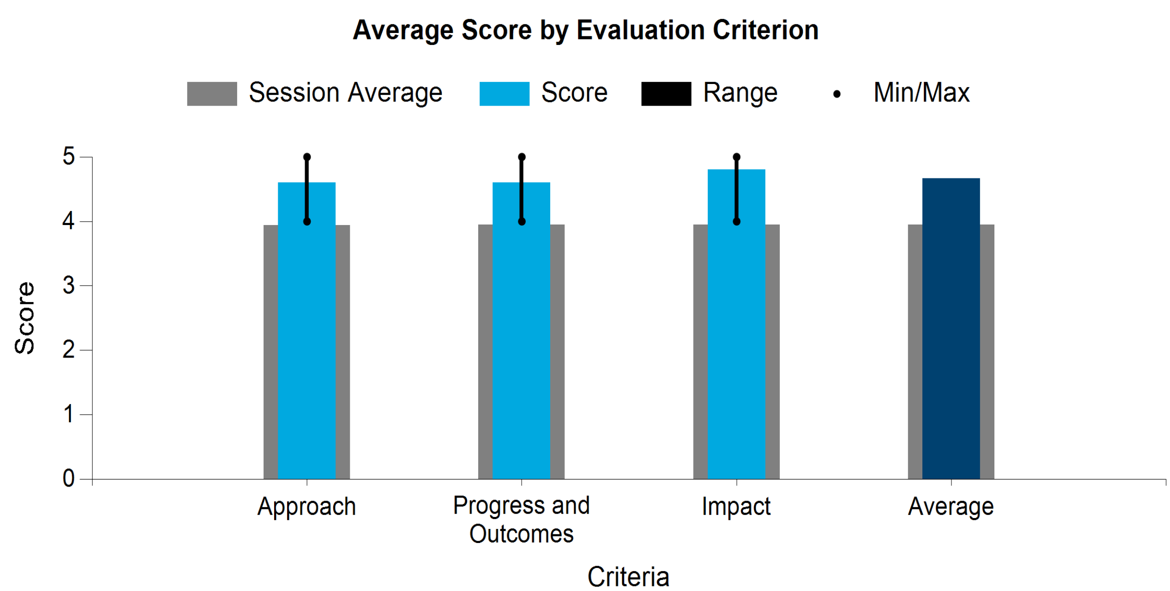
LIFE CYCLE ANALYSIS OF BIOFUELS AND BIOPRODUCTS AND GREET DEVELOPMENT

Argonne National Laboratory

PROJECT DESCRIPTION

WBS:	4.1.1.10
Presenter(s):	Michael Wang
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$4,000,000

Argonne National Laboratory (ANL) has been developing and applying the GREET life cycle analysis (LCA) model to support the three EERE transportation offices, including BETO, for more than 25 years. This project for BETO continues to expand, update, and upgrade GREET to consistently and holistically address energy and environmental effects of bioenergy/bioproduct technologies and identify opportunities to improve their sustainability performance. With holistic LCA modeling of bioenergy technologies, ANL supports BETO R&D efforts across the entire biomass-to-bioenergy supply chain that encompasses terrestrial, aquatic, and waste feedstocks for SAF and road transportation fuel production. It addresses analytical challenges, such as data availability for bioenergy technologies, through national lab collaboration and industry engagement, and it examines important LCA system boundary issues, such as indirect effects of LUC of biofuels. Through this project, ANL releases an updated GREET model annually to benefit the bioeconomy community and the more than 50,000 registered GREET users globally. It dissimilates LCA results of biofuels/bioproducts via peer-reviewed publications and conference/workshop presentations. It provides credible, objective LCA results for R&D and other decision making at the federal, state, and international levels.



COMMENTS

- This is an excellent project with a strong approach and clear impact for stakeholders and the public. This is an excellent modeling framework, so my main area of focus as a reviewer was the selection of specific areas for expansion and analysis. Expanding GREET to include bioplastics and bioproducts is a great new feature. I also look forward to the new marine module, which seems highly valuable. The planned future work to improve this module, develop an aviation module, and identify opportunities for deep decarbonization all seem worthy of pursuit.

- Thank you for the opportunity to review the Life Cycle Analysis of Biofuels and Bioproducts and GREET Development project. The project is well aligned with BETO's goals as it focuses on establishing LCA methodologies, developing reliable data, and maintaining model transparency for biofuel and conventional fuel pathways. The development of a feedstock analysis tool, carbon intensities for SAF pathways, and waste-to-energy conversion are important advancements in BETO's capabilities and are vital for achieving their stated goals. The project's regular communication and discussions with stakeholders and partners to mitigate data collection delays and obtain critical inputs are commendable. Overall, the project is on track, and the well-established tool that is heavily used in regulation and by commercial entities has significant impact. The project's engagement with stakeholders to improve the understanding and use of LCA results and its transparency make it a valuable resource. Kudos to all involved.

- This is a flagship project for BETO and for the technology area, with outsize influence among the policymaking community, academia, and industry. With a relatively small quantity of funding, this model has a tremendous impact and a wide audience. Within BETO, many other projects rely on the LCA estimates developed using the GREET framework. The project team has done an admirable job to continually update the model, with regular updates to improve the data quality referenced in the tool as well as to add additional fuel pathways and technologies to stay relevant, such as the recent addition of SAFs and e-fuels.

  Though the tool very much sets a standard for LCA for policymaking, there are some risks associated with its ubiquity. The increased recent political salience of the model, where significant quantities of policy support and investment may rest on minor assumptions and judgments within the modeling tool, greatly raises the stakes of results generated within the model. This may be particularly important in cases where the model combines attributional and consequential LCA (such as assumptions on induced land use change [ILUC] or counterfactual emissions for some fuel pathways) or for a handful of fuel pathways where long-term emissions assumptions are made based on expected future behavior and permanence (such as for soil carbon in the feedstock calculator). Though these are helpful and useful calculations, particularly for some academic and policy work, there may be issues with enshrining "one" GREET methodology in policy when the model mixes and matches emissions with differing degrees of certainty and verifiability or in cases where the model allows users to pick from different assumptions; thus, it may be helpful to break GREET out into policy-specific modules, as needed.

- The goal of this project is to quantify life cycle energy and environmental impacts of biofuels/bioproducts. GREET has been in development since 1995 and has 50,000 registered users. Clearly, the project has been developing, growing, and being refined for decades, and it has widespread impact. I am curious to know how the model adapted to changes in regulatory standards, such as criteria air pollutant emissions standards and others.

  How does GREET LCA address LUC for conversion to biofuels? Does the supply chain sustainability analysis include changes in labor, such as labor shortages and other social or economic barriers? If so, how are these changes reflected in the model?

  How has feedback from international, national, and state agencies helped to shape this project? Other stakeholders (researchers, industries)?

  One goal of the project was to identify key drivers affecting the sustainability of bioproduct and bioplastic technologies. Does GREET allow for comparison between biomass feedstocks for energy versus other bioproducts?

Another goal of the project is to facilitate discussions among government agencies and the private sector for opening low-carbon-intensity feedstock certification. Clearly, GREET has been used by many different entities, but what is the current status of those discussions? Have the ways in which agencies have used GREET changed over time?

The long and impressive list of project presentations includes ANL's Sept. 19, 2022, Energy Justice Webinar on GREET Bioenergy Life Cycle Analysis. How does GREET address energy equity? They have developed a concurrent mapping tool that shows data by zip code. This sounds like an incredibly helpful tool, and I will be curious to learn more about the linkages between the model and the mapping tool.

- GREET is a leading tool for LCA of a variety of bioenergy and biochemical products. It is transparent, well maintained, and continuously updated with user inputs. It also played a significant role in making policies at the state, federal, and international levels. It has accumulated a large user base, and the project team is consistently looking for ways to engage more users (e.g., through regular workshops). Within this GREET platform, a series of tools are also being developed with different focuses (e.g., Carbon Calculator for Land Use and Land Management [CCLUB], Feedstock Carbon Intensity Calculator [FD-CIC]), and different versions of GREET have been created to support different policies (e.g., CA-GREET). This is overall a very impactful project.

  But at the same time, both of the existing forms of GREET, Excel and .NET, are not built for version control, flexibility, and robust uncertainty and sensitivity analyses. Especially for the still more popular Excel form, it is hard for the users to track what changes have been made and quickly understand the implications of those changes. At the same time, the broad scope of GREET leads to (often necessary) a large number of default assumptions and model simplification. GREET is a great tool to get an out-of-the-box answer, though adjusting assumptions to tailor the answer to the specific application is also needed; therefore, balancing accessibility (on how easily a new user can learn and correctly use GREET) and model accuracy should be considered in future development plans.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for pointing out these important areas in the GREET LCA as related to policies and regulations. Since 2010, GREET, originally built as an attributional LCA model, has been expanded with consequential elements, such as ILUC effects of biofuels, coproduced animal feeds, and counterfactual scenario emissions of waste and residue feedstocks. This approach is similar to those in regulations such as the California Low-Carbon Fuel Standard and the International Civil Aviation Organization (ICAO) Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) program. It is widely recognized that ILUC GHG emissions and soil organic carbon (SOC) changes from different farming practices associated with biofuel feedstock production are important and unique analytical issues in bioenergy LCA. The bioenergy LCA community, including the GREET LCA team, has been adopting the consequential approach to addressing ILUC issues with economic models. The agro-ecological zone emission factor approach (originally developed by the Intergovernmental Panel on Climate Change) and the process-based simulation approach (such as the Century and DayCent models) are both used to address SOC changes. GREET has used both approaches. In particular, for domestic SOC changes, ANL has relied on the Century model, and for international SOC changes, GREET has used the emissions factor approach as used by the California Air Resources Board and the EPA. Despite the inherently greater uncertainty of the consequential LCA approach, data, and assumptions that are considered in addressing these consequential issues, the GREET LCA team has been engaging with the research community, agencies, and feedstock producers in the agricultural and forest sectors, among other stakeholders, to improve the data, assumptions, and modeling approaches in consequential LCA. Both ILUC and SOC issues are subject to great uncertainties in modeling and difficulties in verification. Advances in ILUC modeling have been made in the past 14 years, and ANL has benefited from the advances. There are ongoing efforts in the U.S. Department of Agriculture (USDA) and DOE Advanced

Research Projects Agency–Energy to develop better SOC inventory data and new sensor technologies to potentially economically measure SOC contents. ANL will continue to benefit from these efforts. The treatment of counterfactual scenario emissions reflects the belief of future, as well as current, treatments of wastes and residues. ANL will continue to examine these treatments and their effects on emissions. Further, the GREET model allows users to change the default assumptions and modeling options regarding these issues to reflect alternative approaches and data from the users and/or unique aspects of the user-specific technologies. The comment rightly identifies the difficulty of technical analyses versus policy considerations of fuel technologies, especially biofuel technologies. While the GREET model is developed to address technical/analytic issues as much as we can, policy considerations of energy technologies is different from technical analyses. We will continue to make GREET as comprehensive and flexible as we can so that policy considerations can benefit from the model. Given the unique analytical issues that may be relevant to different technology areas, ANL is currently working on specific modules that provide interactive features so that different technologies can be modeled separately but with a consistent, transparent LCA approach and background data for cross comparison.

LUC emissions have been modeled for GREET biofuel LCA with two key steps: economic modeling of the types and magnitudes of LUC due to biofuel production and changes in GHG emissions, particularly in SOC changes associated with each LUC type, such as grassland conversion to cropland. ANL has relied on Purdue's Global Trade Analysis Project (GTAP) modeling to estimate the types and magnitudes of LUC of a given scale of biofuel production (a "shock"). This is the same approach used by California's Low-Carbon Fuel Standard and the ICAO CORSIA program. For SOC and other GHG emissions, such as N_2O emissions associated with specific LUCs, as stated in a previous response, GREET has relied on the Century model process-based SOC model and California Air Resource Board and EPA emissions factors of different land conversions. The Century model is coupled with U.S. statistics of long-term crop yield records. These two steps are combined organically in the CCLUB module (https://doi.org/10.1111/gcbb.12237; https://doi.org/10.1111/gcbb.12333; https://doi.org/10.5539/sar.v10n1p61) that was developed for GREET to generate LUC GHG emissions for biofuel production. The supply chain sustainability analysis, a significant GREET application task for BETO, does not include changes in labor or other social or economic barriers. It only addresses energy, GHG emissions, criteria air pollutant emissions, and water consumption. Some of these issues, such as economic barriers, are addressed in separate but linked techno-economic analysis (TEA) for BETO. Stakeholder engagement and interactions are an integral part of the GREET project. These activities have dual purposes. First, we want the GREET development to be relevant to the pursuit of energy and environmental sustainability of bioenergy technologies. The inclusion of relevant sustainability metrics and technology options are key to GREET. Second, technology advances are important to consider for addressing the potential of bioenergy technologies. Our engagement with technology developers helps us understand technology options and their advances over time for GREET considerations. We have interacted with agencies such as the ICAO, the International Energy Agency, the International Maritime Organization, U.S. federal agencies (DOE, USDA, U.S. Department of Transportation, and EPA), California, and several other states to ensure that GREET has broad coverage of energy technologies including bioenergy technologies. We have interactions with stakeholders from industry and academia who help us understand the current state of technology (SOT) and the potential directions. One example is the interaction with several chemical companies that helped us refine the steam cracking modeling by providing shares of feedstocks for the steam cracking process to reflect the current U.S. average shares of the production of major chemical building blocks used as the baselines for LCA comparison with bio-based chemicals. While GREET does not directly compare the use of biomass for the production of biofuels and bioproducts, such analyses have been done outside of GREET to determine the best use of biomass for the decarbonization of U.S. economy. Further, biofuels and bioproducts are sometimes coproduced. In such cases, both are evaluated in GREET LCA for their joint energy and environmental benefits. Such analyses are conducted with holistic LCA methodologies and consistent background data in GREET to address their life cycle sustainability effects. For example, GREET simulates integrated biorefineries that produce both biofuels and bioproducts and addresses the synergies and trade-offs of producing biofuels and bioproducts together. Some of the work published in this area includes https://doi.org/10.1002/bbb.1893, and https://doi.org/10.1016/j.jclepro.2021.127653. For the energy justice issue, GREET LCA provides results for the regional use of biomass, regional environmental effects such as criteria air pollutant emissions, and water consumption. These results can shed light on opportunities to improve energy and environmental benefits to disadvantaged communities by promoting bioenergy development and deployment with data and science that are critical for stakeholders to make sound EJ and bioenergy investment decisions.

We appreciate the comment on the need to improve the tractability, enhance user accessibility, and enable more robust/interactive sensitivity/uncertainty analysis of the current GREET model platforms. In FY 2023, with support of the DOE Office of Technology Transitions, ANL began the effort to develop different modules (such as the SAF, marine, clean hydrogen, and battery modules) to make the Excel version of GREET with interactive user interfaces to help users clearly identify key input parameters for changes. Further, ANL will design a new GREET modeling platform to increase the functionality, traceability, expansion, and maintenance of GREET. The latter effort is anticipated to be completed in the next two years. (Related references: https://doi.org/10.1002/bbb.1893, https://doi.org/10.1016/j.jclepro.2021.127653 https://doi.org/10.1016/j.jclepro.2021.127431, https://doi.org/10.1111/gcbb.12237, https://doi.org/10.1111/gcbb.12333.)

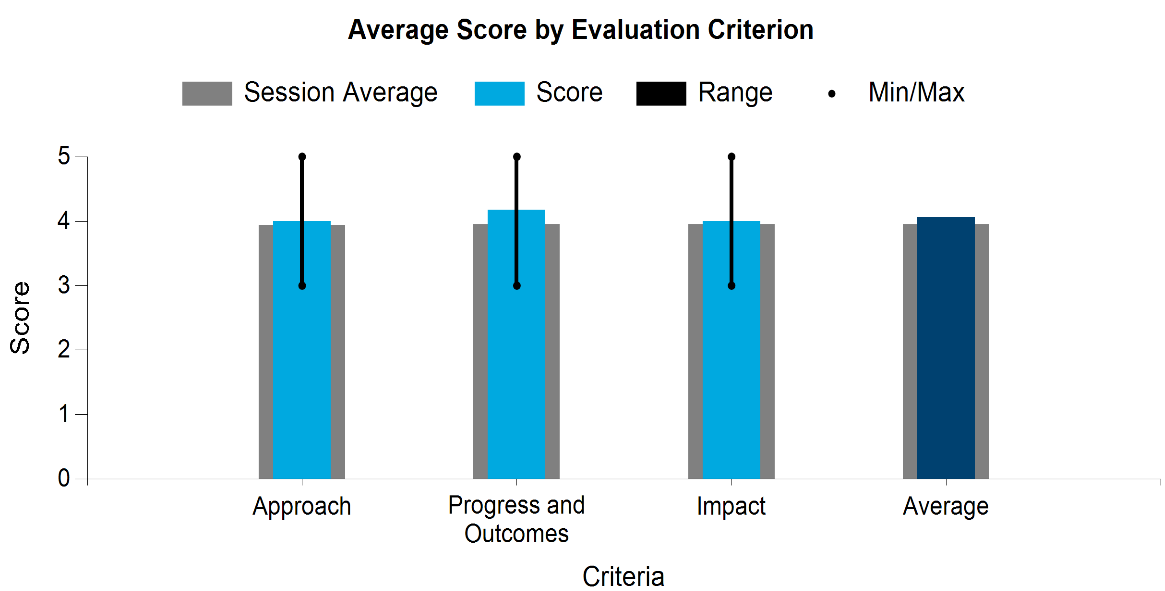
MULTI-INPUT, MULTI-OUTPUT BIOREFINERIES TO REDUCE GREENHOUSE GAS AND AIR POLLUTANT EMISSIONS

University of California, Berkeley

PROJECT DESCRIPTION

WBS:	4.1.1.100
Presenter(s):	Corinne Scown
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2023
Total Funding:	$1,000,000

Lignocellulosic biorefineries can produce renewable liquid fuels vital to the transportation sector, including replacements for gasoline, diesel, aviation fuel, and marine fuel; however, they also have an important potential role to play in manufacturing high-value bioproducts, creating jobs, supplying electricity, and treating waste in rural communities. The goal of this project is to conceptualize, design, and assess the economic and environmental performance of multi-input, multi-output biorefineries that can convert locally produced lignocellulosic biomass, manure, and other wet organic waste into liquid fuels, platform chemicals, and high-value products. The resulting TEA and LCA models will be released as highly customizable, transparent web-based tools for public use. The optimized biorefinery designs will produce a suite of fuels and products that will reduce GHG emissions by at least 70%, reduce fossil energy consumption by 50%, and reduce air pollutant emissions by at least 20%. Challenges include balancing the cost of biogas upgrading to products and increasing the capacity of the on-site anaerobic digester with the environmental benefits of organic waste treatment. The project has resulted in peer-reviewed publications on biogas yields from codigestion as well as cost, energy, and life cycle GHG impacts of biorefinery designs coproducing renewable natural gas (RNG), compostable plastics, and single-cell protein (SCP).



COMMENTS

- This is an excellent project. The environmental impacts of collecting biogas from manure digesters is a highly controversial question for many stakeholders in the bioenergy space. Assessing which livestock systems might be more or less suitable for manure collection and digestion and the potential economic viability of bio-compressed natural gas production from manure digesters are also worthy goals of potential high impact to stakeholders. This project appears to have developed new tools and data and distributed them through an accessible web tool that seems likely to realize much of this impact. I encourage DOE to consider how platforms like the Bioenergy Knowledge Discovery Framework (KDF) could be used to inform potential users of these capabilities. Overall, I find nothing to criticize about this project, and I hope to see BETO continue to fund work like this in the future.

- Thank you for the opportunity to review the Multi-Input, Multi-Output Biorefineries to Reduce Greenhouse Gas and Air Pollutant Emissions project, which is somewhat aligned with BETO achieving their goals. The project is innovative in its approach to designing cost-competitive biorefineries that can process lignocellulosic biomass and organic waste, and the use of integrated models is commendable. The employment of a machine learning methodology is also impressive; however, an opportunity for improvement would be to couple this with more traditional methods to compare outcomes. Such a framework may ensure more confidence among industry. The project has a significant number of publications and has the potential to attract and support industry entrants.

- This project fits well with BETO's mission, and it is a good use of FOA funding to develop a targeted, short-term analysis. The focus on developing a flexible biorefinery that can use multiple inputs is unique across the projects studied, and the focus on identifying the optimal end product offers flexibility and could inform future biorefinery design and investment. The progress and outcomes also had compelling results about the cobenefits of the feedstock selection.

  It is a bit difficult to see how it is integrated with other projects at DMA. It is unclear if this approach to multi-input, multi-output biorefinery design and TEA is going to be incorporated into further analyses or if this is a one-off project.

- The goal of this project was to assess the economic and environmental performance of multi-input, multi-output biorefineries. Specifically, the project explored the question of whether or not lignocellulosic biorefineries could coprocess organic waste in rural communities at comparable or lower costs and environmental impacts relative to a conventional stand-alone design. The team sought to build and demonstrate integrated siting, TEA, and LCA models to simulate designs and explore trade-offs.

  As with all models, especially ambitious ones with many inputs and outputs, there were many forms of uncertainty embodied in this project. For example, the team noted that manure availability was a major source of uncertainty. What determines whether or not manures are collectable? How might the model seek to address those constraints and other uncertainties associated with the logistics of collecting a wide range of wastes, including poultry blood, lactose, sludge, etc.

  Project goals were clear, and activities supported the intended outcome. The team included a small business (Mango Materials) to build a launch-scale facility for lignocellulosic refining and worked with a local wastewater treatment plant. In the future, it would be good to continue to work with other labs and stakeholder groups that may add valuable feedback to the model and analysis. For example, the team plans to publish water and GHG results and post polyhydroxyalkanoate (PHA) and SCP scenarios on a web tool. Who are the intended audiences for these additions on the web tool? How might different groups benefit from these additions?

  I am also curious to see how the team plans to explore potential rural benefits such as improved wastewater treatment in building new biorefineries. This is an understudied area that would be interesting to explore further.

- Overall, the approach of this project is unique and important. The multi-input, multi-output approach allows for a more complex biorefinery to be conceived and a more diverse set of inputs to be consumed and products to be produced. This model also included comprehensive impact analysis in GHG, water quality, and air quality evaluations.

Excellent real-world experimentation with Mango Materials as an implementation partner. Would be great to have more partners documented using the system.

Manure's use as fertilizer is an important method to replace synthetic fertilizer and to decarbonize corn and wheat production. This model has a useful approach of identifying manure-saturated areas for siting using regional watershed loads as a guide for maximum manure applications.

- This project focuses on the biorefinery design with TEA and LCA. Its strengths include the close collaboration with industry partners, the consideration of multiple configurations for different emerging bioproducts (polyhydroxybutyrate [PHB], SCP), the rigor of analyses (sensitivity and uncertainty analyses), and the inclusion of biorefinery designs in web tools. It is a nicely executed project near completion, but it also only focuses on a few select products, and therefore the larger implication on the entire bioeconomy is limited.

PI RESPONSE TO REVIEWER COMMENTS

- We want to extend our thanks to the reviewers for their careful review of our progress, excellent discussion during the Project Peer Review, and thoughtful and encouraging written comments. It is true that this project is nearing completion, so we have limited flexibility to adjust or expand the scope based on the reviewers' comments; however, the feedback is still valuable for us as we finalize and disseminate our results, and it provides great direction as we think about potential follow-on work. The points raised about possible benefits of improved wastewater treatment in rural communities are excellent, and we agree that this is an interesting topic for further study. Manure management and septic waste treatment (which can include brown grease) is a challenge for small, rural, and tribal communities. The EPA has some great resources available on this subject. A key challenge is that it is difficult to collect reliable, comprehensive data on how this waste is managed across the United States, which is critical to prioritizing where diversion to bioenergy facilities can offer the greatest GHG, water quality, and air quality benefits. As noted in our presentation, it has been difficult to obtain manure management plans from some states, but we continue to make progress, and this is an area where follow-up work could be enormously valuable. Regarding the comments about the targeted set of products analyzed in this project—specifically, RNG, PHB, SCP, ethanol, and isoprenol—we hope and expect that our findings can be generalized to other products. In particular, we see great value in further exploring the potential for biorefineries to address the needs of historically underserved communities by providing additional options for treating wet organic waste in a manner that reduces emissions to air and nutrient runoff. Matching the available waste types with the most economically attractive end product(s) is essential to achieving that goal. In terms of integration with other DMA projects, our data and scenarios will be available on Bio-Cradle-to-Grave (BioC2G) (a tool supported through a DMA national lab project). We will continue to disseminate all our data sets in publicly available, web-based platforms so that national labs and universities can use our outputs for their own analyses and publications.

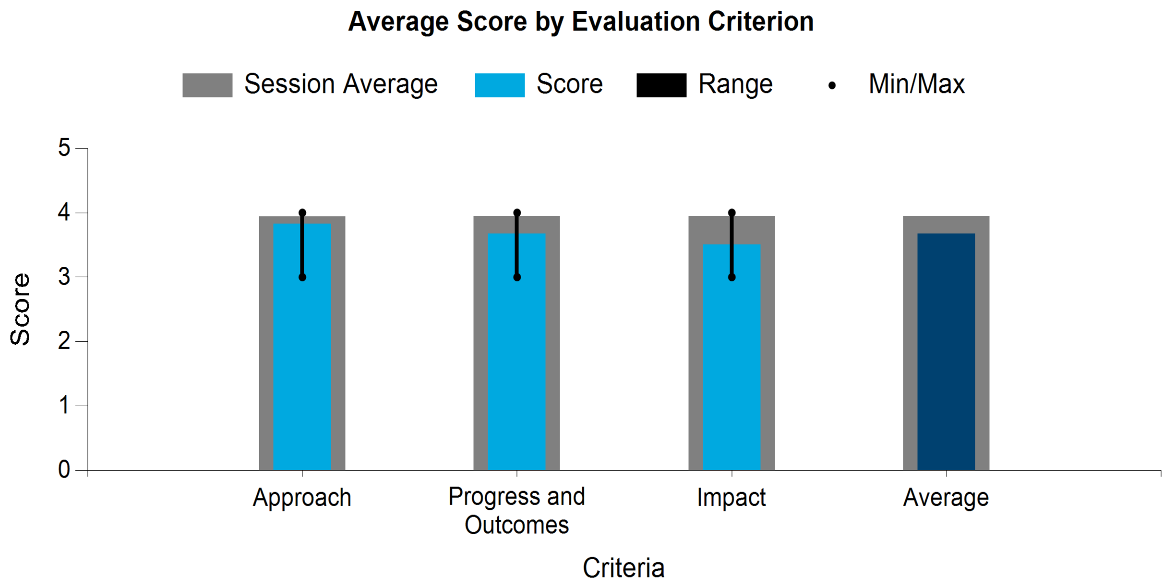
AGENT-BASED MODELING FOR THE MULTI-OBJECTIVE OPTIMIZATION OF ENERGY PRODUCTION PATHWAYS: INTEGRATED TECHNO-ECONOMICS AND LIFE CYCLE ASSESSMENT

Colorado State University

PROJECT DESCRIPTION

WBS:	4.1.1.101
Presenter(s):	Jason Quinn
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2024
Total Funding:	$1,000,000

A changing world is increasingly straining the precarious balance of energy and the environment. This strain has motivated researchers to search for long-term solutions that ensure the proper balance and use of limited resources. Concerns over depleting oil reserves and national security have spurred renewed vigor in developing bio-based products. A variety of feedstocks, conversion technologies, and bio-based refinery concepts have been proposed and are being investigated. The viability of these systems is typically quantified through sustainability assessments. Current work has focused on the assessment of technologies either based on economic viability or environmental impact but typically not concurrently. Further, there has been minimal work in the area of biorefining optimization. The proposed work will develop a unique tool set that is capable of identifying promising production pathways as well as performance targets for bio-based energy and coproduct systems. The foundation of the work is a modular engineering process model that captures the performance of various feedstock production systems, conversion technologies, and end use. This foundation is coupled with TEA, LCA, and resource demand modeling to understand the sustainability of the various production pathways. The work includes the novel coupling of economics and environmental impact through the integration of a social cost of carbon such that a more holistic assessment can be performed. A unique aspect of the work is the use of multi-objective optimization and agent-based modeling to evaluate the various production pathways. The development of foundational modeling work and results will include an external advisory board for feedback and research direction. The work will demonstrate the ability to evaluate new and emerging technologies and provide performance targets for specific pathways to meet sustainability criteria. Advantages of the proposed work include the ability to evaluate multiple production pathways, perform optimization across multiple sustainability metrics, identify areas for strategic investment at a system level and subprocess level, and decrease the risk associated with future technology investments by DOE.



COMMENTS

- I am supportive of BETO including this type of approach in the DMA portfolio. Optimization modeling and agent-based modeling are two potentially valuable techniques that seem underrepresented in the suite of tools attempting to understand biofuel producer decision making. I think the PI demonstrated the potential value of this project in that area.

  Overall, the project seems to be making good progress and appears to be on track to deliver the open-source tool set to DOE. One comment is that the scenario analyses and applications of the tool set to date seem a bit all over the place. I can see how these analyses may be useful for evaluating the potential for SAF production. But what was missing for me in the materials was a clear strategic vision for how all these pieces fit together to do that.

  Regardless, I think this tool set could have some impact. These are underrepresented perspectives in this area of modeling, and including them in the analytical conversations around SAF potential could be valuable. Releasing them as open-source tools should amplify that impact. I'm also encouraged to see that this framework will be capable of estimating particulate matter ($PM_{2.5}$) impacts and other metrics relevant to EJ considerations at a fairly fine spatial resolution.

- Thank you for the opportunity to review Agent-Based Modeling for the Multi-Objective Optimization of Energy Production Pathways: Integrated Techno-Economics and Life Cycle Assessment. I find that the project reasonably aligns with BETO's goals, using multi-objective optimization and agent-based modeling to integrate TEA and LCA. I appreciate the inclusion of equity as an objective and the integration of models to address inconsistencies. The open-source nature of the project, with peer-reviewed papers, can result in a community resource and help inform policy design. A suggestion for improvement would be to clarify the model components completed and those still under development. It is recommended that the model team explores the inconsistencies across the frameworks, understanding that each is solving a fundamentally different problem, and achieving the same results should not necessarily be a goal but rather to understand the differences and in what situations they are the same problem (removing what components from the objective functions). Overall, the project seems to be on schedule, and I wish the team all the best in future endeavors.

- This project is nicely designed and seeks to address one of the core risk areas of the technology area by integrating the results of some different modeling approaches across DOE. The PI was very clear on how they leverage the existing resources of DOE to build out the agent-based modeling approach and how they fit together. The outputs of the model are very clear and serve an important role in evaluating the feasibility of broader policy goals, such as the SAF Grand Challenge, and illustrating the pathways to reach them.

  The multi-objective optimization modeling approach is useful in that it allows the modeler to balance multiple competing priorities for a given agent. In particular, this approach does a good job of identifying potential equity risks with bioenergy policy via its spatial analysis. It may still be relatively early in the project to draw conclusions, but several key findings and progress presented still appear to be theoretical; it would be helpful to provide additional detail on exactly which policy or technology gaps this model can identify.

- The project's goal for a unified and multipurpose bioenergy-based tool set embodies a holistic approach that supports BETO's goals and objectives. The model uses county-level data, which is consistent with BETO's interest in regional data and understanding disparate impacts. For example, this county-level assessment could be useful in looking at equity in the siting of biorefining technologies.

  Like other models, however, some assumptions might be worth exploring a bit more. For example, one of the project goals is to determine land availability and total biomass that can be grown for bioenergy. What factors are used for determining land availability? There is well-developed literature that looks at the social availability, or willingness, of landowners/farmers to grow different crops. The project might benefit from more engagement with that literature to ground truth some model assumptions.

  The project addresses equity issues by including things like exposure to PM in the multi-objective optimization to measure system equity. This is a great start, but other EJ indicator systems have been developed to account for a wider range of variables. Here are a few of the different ways in which agencies have attempted to quantify and model concerns about equity as it relates to energy equity and environmental justice (EEEJ): https://screeningtool.geoplatform.gov/en/#3/33.47/-97.5, https://www.epa.gov/ejscreen. Several states have developed their own EJ mapping tools as well: https://cdphe.colorado.gov/enviroscreen, https://www.michigan.gov/egle/maps-data/miejscreen.

  The agent-based modeling example shows the miscanthus 100-mile radius familiarity expanding in California—is Miscanthus a fire-adapted grass? How is the team quantifying, addressing, and communicating about uncertainties in this model? Overall, the project models risks to the fuel supply chains and seeks to account for dynamic systems. The model could be of potential use to several different user groups and is worthy of funding.

- This project was strong overall but could improve in several key areas. Strengths of the approach include a robust inclusion of familiarity with new crops and agent modeling over time. Practice change in farming often includes a component of time that cannot be accelerated with incentives. The DEI approach was good with the inclusion of the $PM_{2.5}$ impact by county.

  The inclusion of the carbon pricing scenarios and tax incentive scenarios could improve comparisons and understanding of end product price points. It would also be good to document stakeholder use. In particular, including feedback from the Natural Resources Conservation Service (NRCS) and local agronomic nonprofits could help improve the modeling of familiarity. An important understanding extension of the agent model would be to include and model processing locations along with production areas. Often paths to market can limit grower crop selection. Finally, crop insurance is an important factor in the risk of switching crops, and crop failure with and without should be included both in financial and adoption curves.

- This project clearly identifies the gap in the current modeling efforts, and the goals of this project align well with BETO's priorities. The team uses multiple layers of modeling (TEA, LCA, geographic information system, multi-objective optimization, agent-based modeling) to consider land availability, spatial variation, multiple feedstocks, and fuel production pathways as well as the implications of stakeholder priorities (i.e., objectives). This approach also enables the explicit consideration of EJ and DEI in the optimization objectives. This is an impressive modeling undertaking with great impacts. Although this amount of modeling involves a great level of uncertainty that should be carefully evaluated, the project team acknowledges the existence of such uncertainties and has plans to characterize them. The team is also making the tool publicly available, and this transparency should help to address this issue (i.e., the users would be able to know/adjust the underlying assumptions); however, the agent-based modeling approach used in this project is purely based on rational decisions without actual inputs from agents (e.g., farmers, landowners), which may lead to significant deviation from reality and invalidate conclusions generated by the modeling system.

PI RESPONSE TO REVIEWER COMMENTS

- The project team is grateful for the positive feedback on our approach to date. We will make sure to clarify the strategic vision of the work to ensure that all components align toward evaluating SAF potential in the United States moving forward.

  At present, the process modeling and biofuel feedstocks are complete. This work was recently published in the *Journal of Cleaner Production*. Ongoing work is being done to finalize the geographic information system modeling and get accurate results for the total SAF production potential of the United States. It is expected that this work will be submitted for review during the summer. Multi-objective optimization and agent-based modeling work is ongoing, but publications related to each plan will be submitted during the fall. We will clarify the current progress of the work in future presentations/communications. The technology gaps that this model can identify are the large-scale resources required to meet DOE goals (SAF Grand Challenge, Renewable Fuel Standard [RFS], etc.), the geographically resolved deployment of technologies to meet the goals while optimizing for economics or environmental impact, and highlighting the impact of technology advances on achieving DOE goals such that DOE can focus its resources on critical pathways/technologies. We will review the referenced EEEJ work and ensure that our work aligns with previous work. In terms of land area under consideration, we have included nondeveloped marginal land classifications that are not protected according to the U.S. Geological Survey's Protected Areas Database of the United States 2.1 and Key Biodiversity Areas. Each feedstock has a limit on the maximum slope on which they can be cultivated, and each has a minimum yield required to ensure biofuel prices less than $20. This work uses the Parameter-elevation Regressions on Independent Slopes Model Environmental Limitation Model (PRISM-ELM) data set of predicted rain-fed yields of various bioenergy crops across the United States. The PRISM-ELM data set includes climate and soil data as inputs to their model, so our work has put no constraints on climate regions or soil quality required for biomass growth. Moving forward, we will be sure to include carbon pricing/tax scenarios in our simulations and evaluate the impact of crop insurance in financial and adoption analyses. As mentioned, there are uncertainties with all the inputs to the modeling effort. This tool set will be publicly available, so end users can adjust inputs and assumptions with new values as they become available. The project team will work to better understand the decision making of agents (farmers, landowners, biorefinery operators, etc.) through published survey data, journal articles, and interviews.

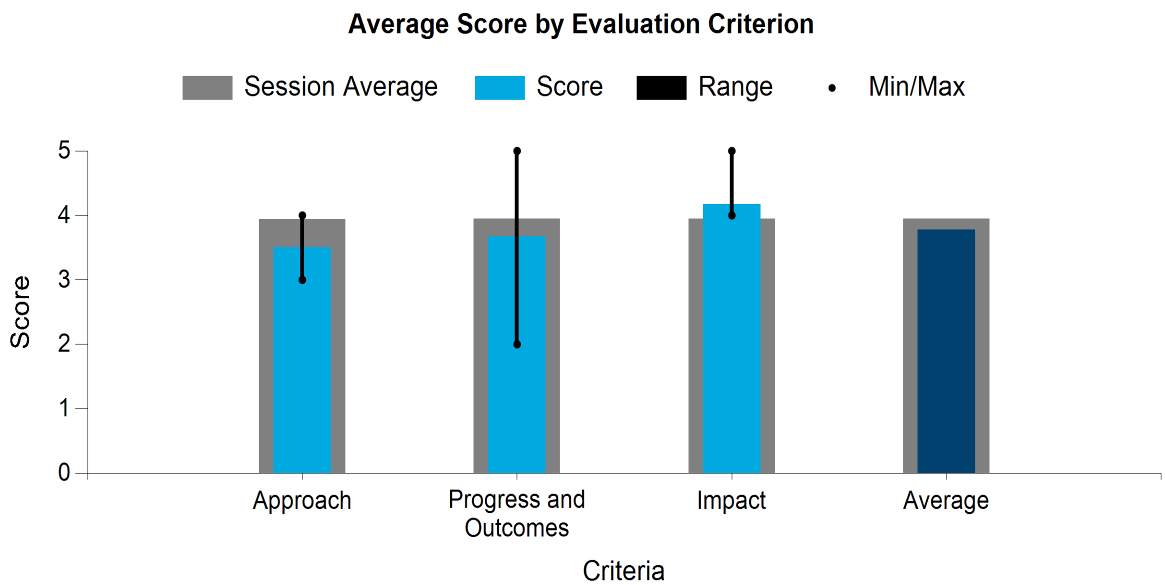
STRATEGIC ANALYSIS SUPPORT

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	4.1.1.30
Presenter(s):	Ling Tao
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,000,000

The objective of the NREL strategic support project is to provide sound, unbiased, and consistent analyses to inform the strategic direction of BETO. This project addresses key technological questions, provides critical data needed to inform strategy, and highlights barriers, gaps, and data needs in support of BETO's mission to improve the affordability of bio-based fuels and products. This task employs various tools and analysis capabilities (TEA, Gauging Reaction Effectiveness for the eNvironmental Sustainability of Chemistries with a Multi-Objective Process Evaluator [GREENSCOPE]-process sustainability analysis, refinery integration and bioeconomy optimization, job analysis, EEEJ) to allow for direct comparisons of biomass conversion technologies across a wide slate of processing platforms, products, and impact categories. The project is tasked with evaluating drivers that support the growing bioeconomy. This project team supports the federal government goals of 3 billion gallons of SAF by 2030 and 35 billion gallons by 2050, and it has specifically supported the SAF Grand Challenge with pathway strategies and analysis insights. Critical to the success of this project is the development of defensible methodologies, analyses, and tools that are publicly available to support stakeholders and bioeconomy growth. To develop such high-quality analyses, the biggest challenge to this project, as with most analysis-focused projects, is the availability and reliability of the underlying data; therefore, the project team works extensively with key stakeholders (e.g., policymakers, bioenergy technology developers, and investors) in developing, validating, and reviewing the results of these analyses to overcome this challenge. Any remaining uncertainties associated with the analysis efforts are clearly defined and quantified.



COMMENTS

- This is a project with many different elements. Each of the six major tasks seems like a worthwhile scope for BETO to be funding. And most of these tasks seem to be well scoped and showing good progress. I do, however, have some specific areas of criticism regarding some tasks.

The sustainability scope seems to be missing or underrepresenting some critical factors. Impacts on water quality do not appear to be considered directly. Possibly some of this impact is captured in the ecotoxicity metric, but that seems incomplete in a way that a broader measure of water quality would not be. LUC, particularly indirect LUC, is also conspicuously missing from the sustainability metrics. This is not simply an emissions metric. The impact of LUC on both terrestrial and aquatic species must also be considered. Finally, as a general methodological matter, it does not appear that the sustainability analysis includes any consequential LCA. The recent National Academy of Sciences study on biofuel LCA makes it clear that program-level impacts analysis of the type being conducted under this project are most appropriately conducted with consequential modeling rather than attributional modeling. This National Academy of Sciences study was only recently published, but future work under this project should heed its findings.

The sustainability scope appears to narrowly focus on processing plant sustainability. While this is an important subcomponent of biofuel sustainability, it is incomplete. Assessments of biofuel environmental, energy, economic, and efficiency impacts need to consider the full life cycle of the fuel, not just the processing plant. This appears to be a significant gap in the scope of the project and the overall assessment it is trying to achieve. The types of assessment being visualized on slide 18 are highly valuable, but the data going into them need to be more complete.

Finally, the focus of this project on corn alcohol to jet (ATJ) is out of step with most of BETO's feedstock analysis portfolio. This work needs to allow itself to be informed by other projects in the portfolio. BETO-funded work has already demonstrated the limited emissions benefits of corn ATJ barring substantial advances in carbon capture, utilization, and storage (CCUS). And the general focus of BETO seems to be on low-emissions feedstocks with substantial potential for knock-on ecosystem benefits. It would seem more in-line with this work to focus on pathways where the potential for sustainability benefits seems greater.

- Thank you for the opportunity to review the Strategic Analysis Support project. I am pleased to report that this project is well aligned with BETO's goals through developing and applying various analyses to support BETO's strategic direction and inform collaborations across EERE. I am particularly impressed with the project's use of a "meta-model"; however, the project could benefit from advancing the state-of-the-art (SOA) analysis in indirect economic impact analysis in other sectors, particularly with regard to jobs and indirect impacts. I don't believe the input-output approach applied should be referenced as SOA, as mentioned in the presentation. Overall, the project appears to be progressing well toward its goals, including identifying scenarios for achieving net-zero SAF and investigating farming practices with biochar options. The impact of the project, including the 11 peer-reviewed papers and book chapters and 7 conference and invited talks, is significant, and the project appears to be on schedule.

- This project is highly relevant and necessary to the portfolio by coordinating across multiple modeling teams and assessing a wide array of data and expertise to inform and respond to BETO's long-term goals. Particularly impressive is this group's ability to coordinate across BETO to iterate and improve different, disconnected modeling tools to contribute to broader strategic visions, particularly the recent focus on SAFs as part of the SAF Grand Challenge. The consolidation of the TEA database to the KDF was also a critical point of progress because it helps to improve transparency, access to, and relevance of BETO's analysis. There is a high degree of coordination with DOE and with other parts of government as well as industry, indicating high impact.

  In terms of strategic direction, the multidimensional analysis appears to undercut other priorities of BETO and the administration. For example, this presentation appears to emphasize existing or near-term biomass resources (e.g., the focus on hydroprocessed esters and fatty acids [HEFA] and corn ATJ) rather than those emphasized in most other presentations, as well as an emphasis on using existing refinery infrastructure.

This project also emphasizes Justice40 and equity goals while potentially undermining those goals with its recommendations. Specifically, this project emphasizes the importance of retrofitting existing refineries. This is a current flash point in the policy space in California, where the low-carbon fuel standard (LCFS) is prolonging the life of some refineries against the wishes of those located in nearby communities who have disproportionately borne the burden of the pollution; therefore, recommendations on refinery retrofits from this work group should take special care to consider this type of recommendation with respect to DOE and the administration's equity priorities.

- The goal of this project is to develop analyses that go beyond traditional biorefinery-focused TEA/LCA to identify both technical and nontechnical barriers, mitigation strategies, and R&D needs. One of the great strengths of this project is that it investigates EJ factors involved in biorefinery development. The project partners acknowledge that there is a lack of tools for understanding the socioeconomic impact of bioenergy technologies, and this project aims to fill that gap.

  To capture EJ impacts, they used NREL's Feedstock Production Emissions to Air Model (FPEAM). They note that most BETO models have native geospatial resolutions that are not sufficient to meet Justice40 requirements, which is census tract level. Downscaling is the process of estimating high-resolution values from low-resolution data and enables community-level analysis without alteration to existing models; however, downscaling introduces additional and unavoidable uncertainty. This is an important direction given Justice40 goals of 40% of the benefits of federal investments going to disadvantaged communities, but how will some of the uncertainties associated with downscaling be mitigated (changing census track data over time, alignment with air quality data, etc.)

  For the renewable chemical analysis, the project team narrowed 30 chemicals down to 15 to focus on energy intensity and GHG emissions connected to those 15 chemicals—what criteria were used in this narrowing selection process?

  For the SAF regionalization case study of O'Hare, the project examined the SAF potential of the surrounding region. It sounds like this study occurred before the EJ factors were developed, but this kind of regionalization study will be particularly useful in thinking about Justice40 and disparate impacts on communities.

  The project reached out to many stakeholders, including agencies outside BETO, such as the EPA, EERE Strategic Analysis, the Vehicle Technologies Office, the Fuel Cell Technologies Office, and several others. Were any EJ groups consulted? Or even the EPA's Office of Environmental Justice and External Civil Rights in the development of the new EJ analysis? This would be useful as the project continues tdevelop the EJ portion.

  The project goal is to understand and address rapidly changing externalities.

  Another important direction for developing socioeconomic indicators would be job analysis. This could be especially compelling for potential investors and local policymakers in decisions about the siting of biorefineries and other bioenergy technologies.

  It is fantastic that BETO is trying to find ways to integrate equity into analyses, and this spatial approach could be very helpful for understanding issues of distributive justice. That said, the analyses presented here do not necessarily get at issues of procedural justice: Who is involved with decision making? Who controls land and other forms of capital? This is an important next step, and working with other BETO-funded researchers to develop more sophisticated indicators on equity and justice would be an important direction forward for this team.

- This program performed very well in terms of engagement and accessibility. The model is published on KDF and has been cited in more than 50 publications. The model is also being used in complex industry partnerships, notably O'Hare and the Port Authority of New York.

  The updating of the model annually is an appropriate cadence and will help keep the model relevant and useful.

  The inclusion of farm-specific practices such as variable-rate N is an important inclusion. The model should also include opportunities to differentiate the type of fertilizer and allow for those types produced using renewable energy to be appropriately credited.

- This project takes a meta-model framework for TEA/LCA with job and EJ analyses. It also considers the integration of bio-feedstock/bio-derived crude products into existing chemical refineries throughout the analyses. The general approach is sound, and it is encouraging to see social factors being considered in the analyses, but the differentiation between this project and the U.S. Driving Research and Innovation for Vehicle Efficiency and Energy Sustainability (DRIVE) project is unclear. It seems there are opportunities for the multiple pathways considered in the U.S. DRIVE project to be included here, and there are opportunities for the job and EJ analyses performed in this project to be included in other studies.

  Additionally, it is great that this project supports the SAF report, but the underlying Aspen model has not been released on NREL's Biorefinery Analysis Process Models page (https://www.nrel.gov/extranet/biorefinery/aspen-models/; the page has not been updated since 2018, but it is indeed challenging to keep the website current, and the team has made good efforts in setting up this page).

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' recognition of the contribution of this NREL's strategic support to the BETO program and key accomplishments for this project over the last two years. We especially thank the reviewers for their helpful feedback and comments, which are helpful in shaping our analysis direction and ensuring we provide high-quality and timely strategic analysis support to the program in the future. Going forward, we will continue to publish TEA data via a KDF database so that valuable analysis research data are publicly accessible. Our goal for all our analyses is to develop defensible studies and tools in support of the strategic direction of BETO.

  In response to the reviewer's comments on the project being more focused on near-term pathways, we would like to clarify that we did include comprehensive biomass pathway strategies, including both near-term (e.g., HEFA and corn ATJ, as included in the presentation) and long-term opportunities (a variety of biomass carbon conversion as well as waste carbon utilization via electrochemical, biological, and thermochemical conversions). Due to time constraints, we presented only a few examples in the Project Peer Review, but our peer-reviewed publications provide more examples on our analysis covering as many carbon conversion pathways as possible. Also, U.S. DRIVE analysis is included in this strategic analysis support project as Task 7. Based on high interest from our funding agents, stakeholders, and industry collaborators, in addition to the significant amount of work and associated content, U.S. DRIVE analysis was presented as a separate project in the Project Peer Review.

  Thank you for the insightful question on the scope of our sustainability analysis and for suggesting additional critical factors to consider, such as impacts from direct and/or indirect LUC and water quality. Our sustainability analysis focuses on the process level and is complementary to other sustainability analyses funded by BETO, such as water analysis, GREET, and LUC analysis. It is important to integrate sustainability into process design early in the development stage and not at the end. By considering multiple metrics for evaluation when comparing technologies and design modifications, we can make more informed decisions by looking at the design more holistically. We implemented the GREENSCOPE methodology, which is an effective tool for biomass-to-fuels/chemicals process sustainability evaluation and design. GREENSCOPE is able to capture the multidimensional aspect of the process design because making any design change to improve one aspect of the process sustainability may likely impact other aspects. Further, the GREENSCOPE gate-to-gate process sustainability assessment is not about replacing any effective frameworks (e.g., TEA and LCA) but complementing them. It synergistically associates with environmental LCA, and the combination of the two enables a more sustainable design and the development of bioenergy supply chains. Improving the sustainability of the biorefinery will also enhance the life cycle environmental impacts, which can be assessed through LCA. We hope that this explanation clarifies our approach to the sustainability analysis in our project.

Regarding the comments related to refinery integration, the scope of the refinery analysis within the Strategic Analysis Support task was originally developed to evaluate cost and operational efficiency benefits for biofuels production through the utilization of existing refining and ancillary infrastructure. The team has recently begun integrating carbon intensity calculations to enable both cost and decarbonization optimizations in response to DOE and industry needs. The team will continue to seek opportunities to further develop analysis approaches to meet the evolving priorities of DOE and society with specific considerations for justice and DEI.

We would also like to thank the reviewer for the comments about the input-output approach for the job analysis and indirect impacts. While the input-output model is not the only approach to estimate economic impacts from a change in demand for a given product, it is still one of the most commonly used methods by governmental agencies (e.g., U.S. Bureau of Economic Analysis, EPA, U.S. Bureau of Labor Statistics), academia, and consulting industry to quantify direct and indirect benefits or costs, such as impacts on jobs. We agree with the reviewer that this project could benefit from advancing the SOA analysis on indirect impact analysis. For example, using computable general equilibrium models could help quantify the nonlinear impacts on other sectors due to the change in demand for biofuels by a given policy. Because modifying and running computable general equilibrium models and partial equilibrium models requires significant efforts, our project will need a significant funding increase to advance such analysis. Going forward, we will work to adopt suggestions to advance our analysis by seeking opportunities to integrate with other DOE-funded (BETO or other offices) computable general equilibrium models.

We appreciate reviewers' comments on the Justice40 and EJ-related topics. It is critical to recognize the lived experience of residents surrounding biorefineries and how the perpetuation of their activities, and commitment air emissions, can affect them. While the current project does not explicitly address this issue, we have proposed to address this in future work.

We thank the reviewer for the recognition of the importance of EJ to the future success of the bioeconomy and in particular the model downscaling to spatial resolutions compatible with Justice40 evaluation. It is important to note in the context of the suggestions for the future direction of this component of the project—which were all valuable—that the funding level supporting this component is a small fraction of the total project funding, and thus there are significant limitations to how far and fast we can progress. Through other funded work, we are aware of the significant challenges to the durability of Justice40 evaluations owing to changes in census tract boundaries, population demographics, and Justice40 constituent metric scores that can then affect Justice40 designation (e.g., disadvantaged community status). We have looked at this in the context of California, and we are eager to expand our analysis nationally, should there be funding support, and consider implications of how model downscaling uncertainty interacts with underlying census variability. Indeed, the O'Hare regionalization case study occurred before the EJ component was completed but would be an interesting follow-on application of the model downscaling work should funds be available. The purpose of the model downscaling effort, especially in the context of the funding made available to it, was to preliminarily explore quantitative approaches to transforming BETO-supported models to Justice40-appropriate resolutions. A natural step after this exploration would be to socialize the approach with DOE's and the EPA's EJ offices and EJ groups. We are actively looking for opportunities in the future to carry it forward.

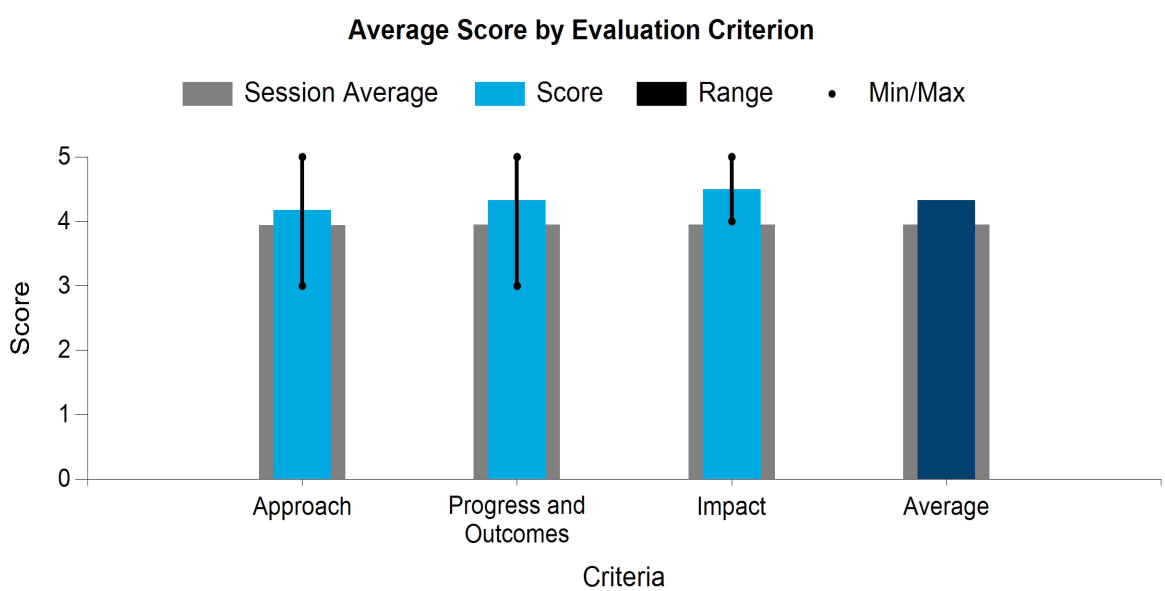
A FRAMEWORK FOR EVALUATING JUSTICE AND EQUITY IN THE TRANSITION TO RENEWABLES: THE BIOENERGY CASE

Oak Ridge National Laboratory, National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	4.1.1.40
Presenter(s):	Patti Romero Lankao; Rebecca Efroymson
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2023
Total Funding:	$500,000

This project provides BETO with tools to analyze and address equity (justice) in the energy transition. The project has three tasks: (1) development of equity indicators for measuring or modeling progress, (2) inventory of current BETO activities that support equity, and (3) options and best practices for community engagement. A framework was adopted that includes distributional, procedural, and recognition justice. A diverse stakeholder advisory committee was assembled to codevelop distributional and procedural justice indicators to be used and modified by communities for bioenergy facility siting processes. Committee members are from industry; a historically Black college; a labor union; environmental, agricultural, and energy nonprofits; the U.S. Forest Service (USFS); a utility; and a state EJ department. Distributional justice indicators include social, economic, and environmental metrics. Procedural justice indicators are a significant advancement over the SOA. A review of justice tasks in the BETO portfolio identifies research gaps. A review of best practices for community engagement and energy equity is under development. Energy transitions can perpetuate, aggravate, or mitigate historic inequities. The project is responsive to Justice40 (requirement that 40% of the benefits of clean energy flow to disadvantaged communities) and executive orders related to energy and racial equity, underserved communities, and well-paying union jobs.



COMMENTS

- This project is an excellent addition to BETO's portfolio. I find nothing significant to criticize in the approach, current progress, or impact. The list of new research directions on Slide 20 is excellent, and I look forward to seeing progress in some of these areas.

- Thank you for the opportunity to review A Framework for Evaluating Justice and Equity in the Transition to Renewables: The Bioenergy Case. This project is well aligned with BETO achieving its goals, particularly those surrounding DEI. The tools proposed to evaluate equity and diversity in BETO R&D are thorough, and the portfolio analysis identifies gaps and tasks that need attention. The project's focus on incorporating impact on underserved communities is commendable. Additionally, the effort put forth on both the literature review and the construction of the expert panel shows the significant progress on this project. One opportunity for improvement could be to engage with BETO projects and teams at the design phase. Overall, this project has the potential to significantly impact the bioenergy industry's transition to renewables in an equitable manner.

- It is great to see this project added to DMA based on feedback from the last Project Peer Review and the administration's increased focus on equity issues. This project fills a clear role, and the managers have developed a well-structured plan to develop DEI metrics and evaluate opportunities to assess BETO's work with an equity lens. The gathering of a group of outside stakeholders is also helpful to add perspectives from outside BETO. Because this process is still in its early stages, it is difficult to evaluate, but at this stage, I think that this fits well within the DMA Technology Area and would align well with many of the projects here. The development of indicators can be a critical piece of tools that optimize scenarios based on multiple metrics. In particular, it is extremely helpful to make sure that projects with a broader scope do not offer recommendations that exacerbate existing historical inequities (see refinery retrofits) or offer opportunities to redress those wrongs.

- The goal of this project was to develop metrics to assess DEI, conduct an inventory of BETO R&D that supports DEI, and make suggestions for how DEI could be incorporated into existing work or new activities at BETO that could improve DEI.

  This is very exciting to see a BETO-funded project that focuses squarely on evaluating justice and equity in the context of bioenergy. There is a dearth of work in this area in terms of both research and, until recently, policy. Many of the projects reviewed are attempting to incorporate energy equity into their analyses, which is great, but it seems many engineers, scientists, and modelers do not have the language or examples of how to do this kind of work. This project will help address the gap between the urgent need for addressing historical inequalities in the shift to the low-carbon economy and the ability of modelers and researchers to account for these often hidden, complex human dynamics.

  The project partners explain that distributive and procedural justice are likely to be the easiest factors to measure, while recognition justice is more difficult because it deals with understanding how the past shapes the present. I understand the relative ease of distributive justice, but what examples and metrics have been used to account for procedural justice? Are there any examples of recognition justice?

  For distributive justice, the project partners discuss ways in which BETO-funded researchers have started to account for disparate impacts in terms of air quality data (often focused on PM) or siting issues. There is an exciting array of composite EJ health indicators developed by other entities, like the EPA's Environmental Justice Screening and Mapping Tool (EJScreen), the Climate and Economic Justice Screening Tool (CEJST), and many states now have tools such as Michigan's EJ screening tool that will help understand distributive justice factors. These tools allow researchers to focus on different aspects of EJ. Are there particular EJ issues around bioenergy development that require greater attention in terms of distributive justice? This might be an interesting and important line of further research.

  In terms of procedural justice, the project team worked with an advisory group to come up with key metrics, including the percentage of key organizations and communities providing input and the percentage of decisions on which stakeholders feel they had real input. I like the effort to break this down into tangible metrics, but how would this data be gathered? By emphasizing percentage, that implies you can determine total number of people providing input or total number of decisions?

It appears indicators for distributive (bioenergy) siting and procedural justice (good practices for community engagement in energy projects) are coming along nicely, but what to do about recognition (or restorative) justice? That is, what kinds of indicators can be developed to understand how the past shapes the present?

In the strategic literature search, project partners used terms such as *engagement*, *energy equity*, *transitions*, *social acceptance*. One thing I am currently exploring is the relationship between social acceptance and EJ in the context of bioenergy development. I think these things are slightly different, as famously revealed in the 1984 Cerrill report on waste-to-energy siting in California. Both concepts may be useful in planning and siting of bioenergy technologies, but there are some important nuances that need to be carefully examined.

The project team's collaborative work was impressive, including the cultivation of a stakeholder advisory committee and work with EERE, the DOE Office of Economic Impact and Diversity, the Energy Futures Initiative, Resources for the Future, the Sloan Foundation, the Deep South Center for Environmental Justice, the University of Michigan Energy Equity Project, and the Initiative for Energy Justice. This kind of collaborative approach can serve as a model for other BETO-funded projects looking to authentically address equity and diversity issues.

One particularly interesting finding was that engagement does not necessarily improve equity. Understanding the nuances of what forms of engagement lend themselves to equity outcomes is an important direction for researchers.

Also, moving forward, the project will provide and implement ways to measure the progress of research portfolios toward Justice40, and it will work to develop a community of practice for BETO justice-focused projects with bimonthly meetings. This project is essential to achieving the goals of the Justice40 initiative—and, more fundamentally, to ensuring that the path to a lower-carbon economy does not reproduce the inequalities established in the era of fossil fuels. Keep up the excellent work.

- This is a crucial part of the BETO portfolio and should be perennially funded. Progress in the first year has been impressive and the literature review and stakeholders convened substantial.

  Providing BETO methods and metrics to measure the progress of the research portfolio toward Justice40 is one of the most important next steps, and the project is wise to focus on that as one of its top priorities.

  It was not clear from the presentation how indigenous lands and peoples are being included in this work. If they are not, please include this perspective in future efforts.

- This is a very important and impactful project on DEI and EJ. The review of existing literature and the profiling of BETO projects delineates the current status of EEEJ and points to future priorities. The development of bioenergy justice indicators would also assist the integration of social considerations in BETO's modeling work. It would be very beneficial to disseminate the outcomes of this study to the public and leverage this project to develop a DEI guideline for future BETO FOAs (e.g., example tasks PIs can integrate into their projects to promote DEI).

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their valuable and enthusiastic comments that suggest the project is headed in the right direction to meet needs of BETO, underserved communities, and industry. We also agree with the reviewers that much work remains to be done. Reviewers recommended that we "engage with BETO projects and teams at the design phase"; we will work to learn more about new projects at BETO and their potential equity or justice implications. One reviewer suggested that future work be designed to help redress past wrongs. We plan to pay special attention to recognize justice in all activities, including any case studies where industrial facilities are repurposed for renewable energy. This project direction also responds to a separate reviewer recommendation to develop indicators that help convey how the past shapes the present. Regarding the question about which metrics are used for procedural justice, we have worked with the stakeholder advisory committee to develop a broad first cut at candidate metrics that can be modified by communities where bioenergy projects may be sited. We will soon submit a manuscript for publication that includes these indicators. We will also submit a review paper examining the nature and links between energy equity and community engagement—an essential means to operationalize procedural justice. As recommended, we will consider forms of engagement that are associated with improvements in equity outcomes. Finally, we will try to incorporate indigenous perspectives into future work, as recommended by a reviewer.

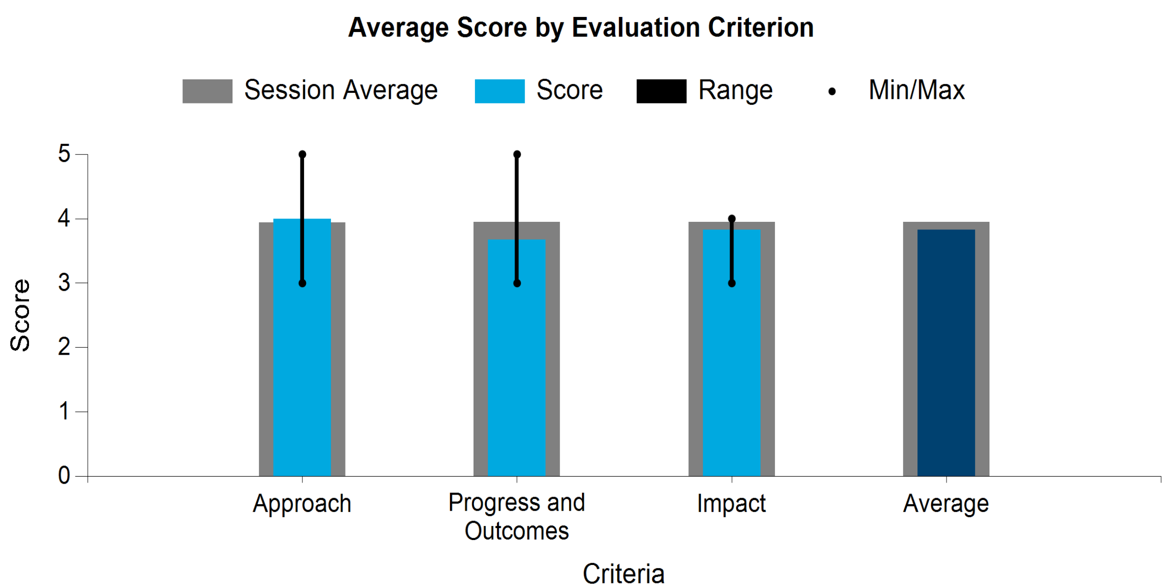
SUSTAINABLE BIOMASS THROUGH FOREST RESTORATION

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	4.1.1.52
Presenter(s):	Mark Wigmosta; Zhuoran Duan
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$750,000

In 2022, 68,988 wildfires burned more than 7.5 million acres, with 6 fires each requiring more than $90,000,000 in suppression costs alone. Climate change and poor forest management practices contributed to the severity of the wildfires. Sustainable biomass from forest restoration to reduce high fuel loads and fire risk is a potentially significant source of bioenergy with numerous potential environmental benefits; however, additional planning and decision support tools are needed to ensure economic and environmental sustainability. A multiagency collaboration between DOE and the USFS is using high-resolution spatial vegetation characteristics data to develop accurate estimates of sustainable forest biomass along with distributed hydrological and wildfire risk modeling in a multi-objective analysis framework. We are initially focused on high-fire-risk areas in the Pacific Northwest at the subbasin to regional scale using data, models, and analysis techniques that can be applied nationally. We have developed a decision support tool and used it in a 100-year simulation of the Wenatchee basin (historical climate) for multi-objective trade-off analysis considering vegetation regrowth, biomass, carbon, wildfire and smoke emissions, snowpack/streamflow, and economics. This work has resulted in significant two-way knowledge and technology transfer through follow-on federal and state funding for six projects.



COMMENTS

- In general, this is a well-developed project. Developing tools to aid targeted forest restoration and fire mitigation is a scope that is both timely and likely to be of strong interest to stakeholders. The modeling approaches appear sound, and progress to date shows a lot of promise for this work to benefit decision making. I also appreciate the plans to consider the impacts of climate change on these physical systems. This is an area where more work is generally needed.

One area of project weakness is in the scenario design. To date, all the scenarios assume the use of sustainable harvest practices. While these are excellent scenarios, to fully quantify the impact of these practices, the modelers must also produce scenarios where the model solution is not constrained in this way. It is certainly possible that harvesters in the real world will not fully adhere to sustainable practices. Part of the value of this work will be to articulate the economic and ecosystem benefits of sticking to those practices. To do that, a counterfactual scenario set where sustainable harvest constraints are relaxed is needed. The project team should incorporate these scenarios into their future research plan.

- Thank you for the opportunity to review the Sustainable Biomass Through Forest Restoration project. I believe the project is reasonably aligned with BETO achieving their goals. The project has made great use of spatial and biophysical models to prioritize and target forest restoration to address multiple objectives, and I appreciate the good use of LANDIS-II, the presented visual representations, and the use of different general circulation models. While there are opportunities for improvement in clarifying how follow-on tasks mentioned in the presentation are related to project goals, I'm pleased to see that progress is being made toward the goals and the project is on schedule. The significance of impact is noteworthy, and the continued engagement with Blue Forest is encouraging for potential commercialization. Additional commendation for the five publications.

- The opportunity to implement forest management practices that would reduce wildfire risk, generate a stream of sustainable biomass, and other cobenefits is very promising. The scope of the project and its plan appear very clear and well defined, though one important question to determine is how well integrated and consistent the approach here on management practices is with forest biomass updates to the integrated landscape management tool. The analytical tool appears robust and nicely incorporates a mix of ecological functioning, community needs, and economic viability to inform the model recommendations. Further, the collaboration with multiple outside groups—nonprofit, Native American communities, industry, and local government—illustrates the impact of the project.

- This project simulates vegetation regrowth to better estimate long-term biomass supply and impacts to wildfire intensity and streamflow. The project partners aim to estimate the scale of spatially explicit, time-dependent forest treatments required (over decades) to stabilize landscapes, their carbon, burned area, smoke emissions, water resources, and biomass.

  One main assumption of the project is that they only consider biomass for energy associated with commercial activities. Are there sufficient markets to sustain biomass for energy?

  What does the Roundtable on Sustainable Biomaterials (RSB) think about forest residuals being used for energy as opposed to other biomaterials?

  The goal of this project seems to be to improve USFS decision-making software to target forest restoration in fire-prone areas in Washington. What kinds of outreach activities have been done to other academic researchers, agencies, industry, and (especially) policymakers?

  There is a lot going on with this project, and while the goals support BETO's primary objectives, it is not always clear how all the pieces fit together.

- The partnership with LanzaTech, collaboration with the USFS, and the inclusion of indigenous tribes make this program clearly relevant to and inclusive of many diverse stakeholders.

  One project goal for the future is continued outreach to the science, policy, and industry communities. It would be helpful to quantify this with both measurable outcomes and timelines.

- This project focuses on forest restoration through sustainable management strategies. The project team developed the LANDIS-II model to simulate the impacts of different events on the ecosystem. The team has regular communications with collaborators and stakeholders, and this project has led to multiple follow-up projects. But it would be good if the team could explore and discuss the broader implications of this project. For example, the team mentioned that they are engaging with private equity on a pilot project—what are the investors attitudes toward the management strategies considered in the project? Are these strategies financially viable or are incentives required? Addressing questions like these would help the project move to the next stage.

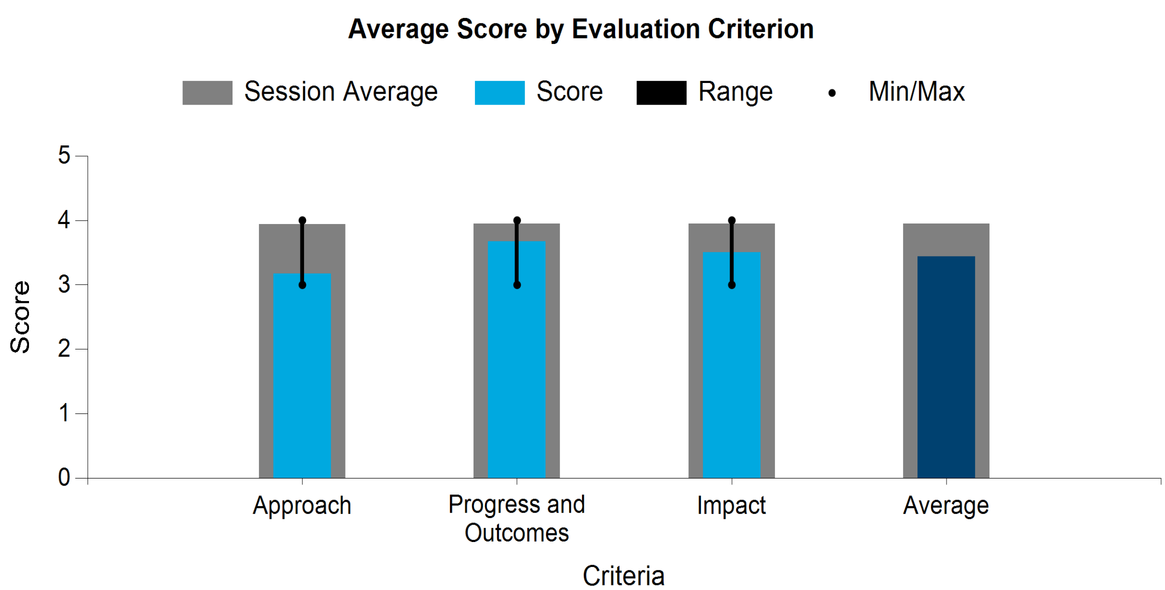
PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their valuable and encouraging input. The project team is encouraged by all the positive comments made by the panel. Forest restoration is being used to reduce wildfire risk and has been identified as a potentially significant source of bioenergy; however, additional planning and decision support tools are needed to access economic and environmental sustainability. As noted by the reviewers, developing tools to aid targeted forest restoration and fire mitigation is a scope that is both timely and likely to be of strong interest to stakeholders as wildfires pose greater threats to society and are being exacerbated by climate change. A decision support tool is vital for weighing the trade-offs of biomass harvests for wildfire reduction. Our management scenarios currently span a range from minimal intervention to full intervention through varying levels of prescribed fire, wildland fire use, restorative thinning, and commercial thinning. We appreciate the comment that we should simulate a more intensive harvest. Although it may not have been clear in our presentation, the current scenarios do just that. We are applying heavy commercial harvest in parts of the landscape where this is likely to occur. We are also actively working with stakeholders on the management side (federal, state, and tribal) to develop scenarios that align with their anticipated management activities (in terms of treatment type and treatment rate). Given the computational resources required to run the model, we are not able to run scenarios that are too far departed from reality. We currently assume that biomass for energy is only associated with commercial activities; however, as increased public funding is being directed toward fuel reduction programs to mitigate the risk of extreme wildfires, there will likely be opportunities for additional biomass for energy beyond commercial activities. For example, the USFS Central Washington Initiative, encompassing most of the project study area, is an all-hands, all-lands effort to implement the national Wildfire Crisis Strategy, the Bipartisan Infrastructure Law, and Washington House Bill 1168 to promote resilient landscapes and resilient communities that are adapted to changing wildfire conditions through targeted fuels reduction. A significant portion of our outreach has been through close collaboration with academic researchers, nongovernmental organizations (NGOs), and local, state, and federal agencies (including policymakers) through follow-on funding external to BETO. These collaborations provide not only provide a means of technology transfer from our BETO project to application but also important information on the needs and constraints of a broad range of land managers, stakeholders, and policymakers to develop scenarios that align with their anticipated management activities. Our recently funded collaboration with LanzaTech will provide a valuable industry perspective as well. As part of our BETO annual operating plan, we specify priority outreach activities for the upcoming year and provide outcomes in our quarterly progress reports. Our engagement with Blue Forest continues as they grow their Forest Resilience Bond footprint in eastern Washington state. The Forest Resilience Bond funds the upfront costs of restoration that are covered by returns from fiber recovery. The strategies we are advised (by Blue Forest) are financially viable because the avoided costs outweigh the restoration costs. As the total forest biomass calculations and trade-offs are better understood, our work with a range of stakeholders will continue to incorporate these values and improve our understanding of how these values trade off with others in management scenarios via the decision support models. Already, we have begun developing management-grade tools from the research findings that can be incorporated into land management planning and decision making. A first such investment by the Washington state Department of Natural Resources has already occurred, and we have an expectation of continued interest and support in this area.

MAXIMIZING CO-BENEFITS OF CARBON REMOVAL AND SUSTAINABLE AVIATION FUELS PRODUCTION

Lawrence Livermore National Laboratory

WBS:	4.1.1.80
Presenter(s):	Wenqin Li
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$450,000



COMMENTS

- Based on the initial TEA and LCA, the researchers have identified bioenergy CO_2 capture technology that seems to work well theoretically. The next step of conducting more detailed process design and modeling makes sense generally. And the project is focused on SAF, giving it a chance to deliver insights of significant impact.

  The critical element that seems to be missing from the current approach is consideration of the practical technical and economic barriers. This project has demonstrated on paper that carbon-neutral corn ethanol should be economical under currently available incentives. But, as discussed in the Q&A, significant technological risk remains in areas such as carbon supply chain logistics, retrofitting downtime, and the availability of RNG. I have no doubt that the researchers can model a process design that should work out from a theoretical TEA and LCA perspective in this next phase. But what will be just as valuable, if not more so, is if they can model the technological risks of project failure that a plant constructor would face, quantify those technical risks and the associated economic risks, and compare that to what investors might be willing to bear.

  This and other projects have demonstrated that ethanol with carbon capture should be feasible from a technical perspective and that it should be possible economically. But, to date, that has not occurred, and there are real technological and financial difficulties that have prevented it. What is sorely needed along with process modeling, TEA modeling, and LCA modeling is an understanding of these risks and an assessment of where they are greatest. This type of assessment does not appear in the current description of the research plan.

- Thank you for the opportunity to review the project Maximizing Co-Benefits of Carbon Removal and Sustainable Aviation Fuels Production. The project is well aligned with BETO achieving their goals given its focus on SAF. The project showcases the advance of science and innovation through multi-pathway research and the incorporation of uncertainty, which is commendable. I appreciate that policies and their interactions were investigated, and costs were incorporated in the analysis. The project's risk identification and mitigation strategies are well outlined, and the advisory board and DEI were well considered. Despite some issues with the suitability of strategies given the small economies of scale, the project shows great ambition and progress toward its goals. Two publications and collaborations with other research groups also indicate significant impact. Discussions with industry could also help in identifying a feasible project size.

- With an increased focus on net-zero targets, this project is both timely and relevant. This seems to be very close to the design of the NZTT project but with a greater emphasis on negative carbon intensity pathways and a spatially explicit analysis. Because the two projects are coordinating, there is less risk of redundancy. This project also draws on other models in the portfolio to develop TEA and LCA expertise to inform the project design and model emissions reductions. There is immediate policy relevance, as indicated by the potential value of LCFS and 45Q tax credits.

  I have concerns similar to those for the NZTT project. In contrast to most other projects in this technology area, this work appears to be largely focused on incremental changes and benefits for existing, commercialized technologies (at least based on the initial progress) rather than the wastes or cellulosic energy crops emphasized in BETO's mission; however, this project manages that risk by focusing on a small-scale biomass gasification project, which would align with many feedstocks emphasized in other DMA projects.

- This project seeks to quantify the technical and economic potential of multiple, diverse bioeconomy pathways that draw down carbon dioxide from the atmosphere. The project partners acknowledge that CO_2, biopolymer, wood products, and biochar have different projected end states and wide bounds of uncertainty, and some of this uncertainty seems worth exploring in greater detail.

  For example, they argue that corn ethanol could be considered carbon-negative, but does the model account for LUC for conversion for the expansion of corn ethanol and the increased inputs/fertilizer of that converted land?

  I am very curious to see if their plans to see if a small-scale biorefinery with carbon capture could be both economically and practically feasible. Presently, it is not entirely clear what small-scale biorefining could look like and what the implications would be. This project's focus on distributed, decentralized, small-scale production is an interesting approach. I wonder how small they consider small-scale. Can bioenergy with CCS or biomass carbon removal and storage work on a small scale?

- The focus of this project is excellent as much near-term progress can be made on decarbonizing Tier 1 biofuels. Please include industry feedback on these decisions and evaluations.

  Reducing carbon intensity in feedstock production through the adoption of low-carbon and regenerative practices is an important potential path toward net-neutral corn ethanol production and should be considered in future modeling.

It is currently unclear how engaged industry is in adopting these outlined opportunities. It would be helpful to document industry conversations and evaluate the interest in each aspect of decarbonization outlined. For example, how many ethanol facilities are currently under contract for CCS given the current price points of both the Inflation Reduction Act incentive and LCFS.

- This project is unique in the sense that it is looking at more readily implementable strategies for decarbonization. Although this project does not involve innovative technologies, it has the potential for substantial impacts in the near future. For example, given the large number of 1G corn ethanol biorefineries in the United States, switching to oxyfuel boiler (a mature technology) might be more easily accepted by the industry. Similarly, analyzing the economics of a small-scale biorefinery-based CCS system, while not having the economies of scale as a 2,000-tons-per-day (TPD) cellulosic ethanol plant, could be more relevant to near-term deployment. The team solicited certain inputs from industry, but more efforts can be made (e.g., are current corn ethanol plants on board to switch to oxyfuel boiler? If not, what needs to be done to get them on board?).

  One limitation of the presented results is that uncertainties are completely missing in the results (a few scenarios are considered, but they are far from enough), and the presenter acknowledged that assumptions were made in the analyses that might be debatable. Future work should address the main sources and the level of uncertainties.

PI RESPONSE TO REVIEWER COMMENTS

- Assessing the risks associated with integrating carbon capture with fermentation to ethanol plants may not perfectly align with the scope of our current project; however, we recognize the importance of understanding industry concerns and risks, and we have plans to continue interacting with more biorefineries to gather further insights. By engaging with biorefineries and incorporating their concerns and risks into our modeling design and writings, we are ensuring that our research remains relevant and valuable to the industry. This iterative approach of learning from industry stakeholders and incorporating their feedback will contribute to provide a more comprehensive and practical understanding of the challenges and opportunities associated with carbon capture integration in biorefineries. A 2,000-TPD-scale biorefinery is great to achieve higher economic viability; however, it is important to consider the potential challenges associated with selecting refinery locations, such as biomass density, logistics, and traffic considerations. In light of these factors, we propose two representative scenarios with smaller-scale biorefineries: 1,000 TPD and 500 TPD on a wet basis. These choices were made in consultation with companies in the gasification field considering practical considerations and the ability to maintain economic value. By focusing on these smaller-scale refinery scenarios, our research aims to address the challenges of biomass logistics and other constraints while still ensuring economic feasibility.

  Our project aims to conduct an in-depth design and analysis specifically targeting the integration of carbon capture and sequestration in a small-scale gasification-to-SAF refinery. By focusing on this specific context, we aim to maximize the potential for carbon removal by capturing both post-combustion flue gas and high-purity CO_2 from syngas cleanup. One significant aspect of our research is recognizing that the integration of carbon capture on biorefineries is often assumed to follow the design and cost estimation of large-scale power plant capture systems; however, we have identified that at smaller scales, the design and costs of the capture systems could significantly differ from those at larger scales. Therefore, our project proposes a bottom-up study approach to estimate the costs associated with carbon capture in small-scale refineries accounting for the unique considerations and potential differences compared to large-scale capture systems. Note that while the previous project focused on maximizing carbon removal potential in the existing corn ethanol industry (which concluded at the beginning of this fiscal year), our new proposed project (commencing this fiscal year) will shift its focus to the gasification-to-SAF system. This shift allows for the utilization of a wide variety of cellulosic biomass, aligning with the emphasis on such biomass in BETO's mission.

We appreciate your clarification on the consideration of LUC emissions for corn feedstock in our LCA. It is indeed a critical factor that affects the carbon neutrality of corn ethanol as the significant LUC emissions impose a penalty on its overall carbon footprint. In light of this, our research proposes the integration of carbon capture technologies, including high-purity CO_2 capture during fermentation and low-concentration, post-combustion capture. Additionally, we explore the synergistic effects of renewable electricity and RNG integration. Theoretically, these measures have the potential to reduce the carbon intensity of the process to achieve net-zero or even negative emissions. Regarding the small-scale refinery aspect, we have proactively engaged with various biorefinery industry stakeholders to determine a feasible and practical size for small-scale operations. Through our outreach efforts, we identified two representative scenarios: a biorefinery scale of 1,000 TPD and 500 TPD on a wet basis. These scale choices were determined after consulting companies in the gasification field. While it is common for TEA studies to primarily focus on larger scales, such as 2,000 TPD, due to the economic advantages of scale, we acknowledge the challenges associated with large-scale biorefineries, such as biomass logistics and high risks of capital investment; therefore, we believe that investigating the business potential of smaller-scale biorefineries holds significant value.

We deeply appreciate the insightful feedback received from industry stakeholders, and we are actively engaged in ongoing dialogues with them. These discussions provide us with a comprehensive understanding of their challenges, practical concerns, and ideas for potential collaborations aimed at accelerating the deployment of the bioeconomy. We believe that the proposed study on small-scale biorefinery capture is a compelling demonstration of our commitment to conducting research that directly benefits the industry. Given the limited number of large-scale biorefineries currently in operation—primarily due to practical challenges in the biomass supply chain, substantial financial investments, and uncertainties surrounding incentives—we have recognized the increasing trend of smaller-scale refinery startups in the field; therefore, our research aims to assess the technical feasibility of integrating carbon capture and sequestration systems into these smaller-scale refineries. By doing so, we hope to provide our industry partners with valuable insights into the economic investment and potential returns associated with carbon removal in their small-scale refineries. Regarding the uncertainties surrounding the analysis, we have conducted an in-depth investigation of various key parameters and have included a sensitivity study in the published paper. We have taken note of your suggestion and will continue to incorporate uncertainty quantifications throughout our system analysis. By doing so, we aim to provide a comprehensive assessment that accounts for the potential variations and uncertainties associated with the studied variables.

ECOSYSTEM SERVICES ENTREPRENEURSHIP TECHNICAL ASSISTANCE

Argonne National Laboratory

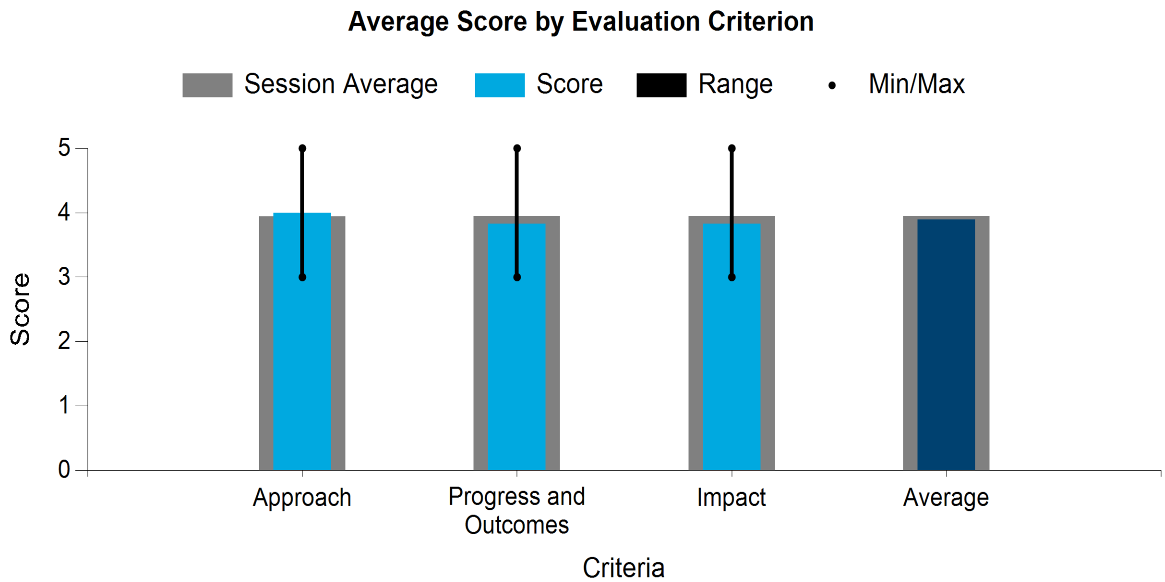
PROJECT DESCRIPTION

WBS:	4.1.2.11
Presenter(s):	John Quinn
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,350,000

As a significant outreach effort, ANL and our nonprofit partner, American Farmland Trust (AFT), are collaborating to provide technical assistance to farmers in matters related to bioenergy crops. Specifically, we are reaching out to farmers/landowners through surveys, listening sessions, public events, and the formation of the Midwest Bioenergy Crop Coalition. We are educating participants on perennial bioenergy crops (crop types, equipment needs, and the ecosystem services they provide, including carbon sequestration) and on approaches for using biomass to generate on-farm energy needs in place of propane in off-grid locations. In addition, we are demonstrating our Scaling Up PERennial Bioenergy Economics and Ecosystem Services Tool (SUPERBEEST) and its use assisting in decision making for the optimal placement of perennials in marginal farmland subfields and the net economic estimate of strategically located perennials in place of row crops.

The connections that AFT has with Illinois farmers have been invaluable in reaching a large number of stakeholders through our outreach events. Women landowners were the invitees to one listening session because women are generally receptive to matters related to conservation agriculture. In addition to farmers, we have specifically met with members of the Association of Illinois Soil and Water Conservation Districts and with industry representatives (e.g., wood chip, carbon credits, biochar, biofuels).

Response to the technical assistance project has been strongly favorable, including comments on SUPERBEEST. Suggestions for changes or additions to SUPERBEEST are added to our list of intended refinements. With AFT, we will continue to work toward offering technical assistance, gathering input on the attractiveness of or barriers against perennials, and informing BETO of our findings. Altogether, this project’s diverse team and partnership aims to explore avenues for the adoption of perennials for biomass, reducing the cost to produce biofuels while assisting underserved rural communities and improving environmental conditions.



COMMENTS

- This is an excellent project. Direct outreach to potential growers of biomass crops is critical, as is documenting their perspectives and preferences. This project is doing that important work. The use of SUPERBEEST to assist decision making in crop planting also appears highly promising. I hope to see this project continue and expand beyond Illinois.

- Thank you for the opportunity to review the Ecosystem Services Entrepreneurship Technical Assistance project for farmers in Illinois. The project is well aligned with BETO's goals and has the potential to support disadvantaged rural communities. The efforts promoting and disseminating the SUPERBEEST framework are also commendable. It seems the project has made good progress toward its goals and has received positive feedback both for the modeling tool and with community outreach. It would be helpful to explore ways to target disadvantaged individuals directly rather than just reaching out to landowners. Also, obtaining characteristics of survey respondents—such as finance, farm size, type, age, ownership, and land characteristics—can aid in understanding the heterogeneity in decision making. Last, there may be benefits of collaborating with additional partner agencies or groups that engage with Illinois farmers to gain a broader perspective.

- Projects like this are critical to the success of BETO's wider mission because it is important to translate the theoretical benefits demonstrated by TEAs and LCAs into practical action. Because the uptake of some feedstocks and cropping practices has struggled in practice, it is very important to solicit perspectives from industry and farmers to understand the disconnect between theory and practice. This project could go further to understand farmers' perspectives and develop a more comprehensive assessment of their opinions. For example, the surveys conducted so far have not yet reached very many farmers, and it is insufficient to break down into meaningful subgroups. Further, some questions/answers are vague (e.g., on-farm energy) and may not be giving meaningful results. I suggest expanding the surveys to reach a wider audience of farmers and, if possible, additional research to measure and observe farming practices to better understand stated versus revealed preferences in these groups.

- The goal of this project was to provide farm holders—in particular, disadvantaged ones—the opportunity to be valued stakeholders in a bioeconomy that leverages marginal land for the creation of biomass and ecosystem services. The project team provided technical assistance for switchgrass varieties, miscanthus, mixed prairie grasses, energy sorghum, and short-rotation woody crops, particularly on economically and/or environmentally marginal farmland. A related goal was to provide on-farm energy independence.

I was very curious to know more about how the concept of marginality was defined and used by different groups. It looks like the scale of cumulative marginalities (slide 5) focused on biophysical factors, but there was also a survey of landowners that indicated that 54% of respondents identified having marginal lands on their farms. How do farmer perceptions of marginal lands match with biophysical characteristics? How do particular land use legacies affect marginality? Is there a way to account for the past when modeling current and future conditions?

It sounds like the project team is considering a related topic for future research. They ask: Do lower income levels in some rural areas relate to the prevalence of marginal soil and therefore an optimal place for perennials and a biorefinery? This would be an interesting direction for future research to look at how land use histories shape current conditions both in terms of degraded/marginal land and the socioeconomic status of the farmers on those lands. How did land become degraded or marginal?

The project team is well positioned to put SUPERBEEST to use. They collaborated with AFT and the University of Illinois Urbana-Champaign Extension on an outreach plan for a wide range of stakeholders. This included listening sessions with diverse groups that resulted in useful feedback that the project then incorporated in its project direction. This is an excellent example of an iterative approach to stakeholder engagement in bioenergy R&D.

One important thing the team learned from their outreach and engagement efforts is that farmers consider a lack of biomass buyers to be a primary barrier to the adoption of bioenergy crops. What can be learned from SUPERBEEST about how to develop markets for biofuels?

Farmers were curious about how payments for ecosystem services and nutrient trading schemes may develop. How does the model account for these and other regulatory changes?

How does the project team define disadvantaged farming groups? I like the direction SUPERBEEST is going by adding biorefinery locations and spatial EJ information.

- This is an absolutely crucial program for DOE. Funding for technical assistance not only allows growers to connect modeled outcomes and practice recommendations but also creates a unique feedback opportunity to improve models through capturing implementation challenges.

  The survey associated with this program was a great start but could improve. It is interesting to know that growers perceive they have marginal acres, but this would have been made much stronger if the results were compared to marginal acres identified by SUPERBEEST. This would add insight to either the accuracy or the perceived accuracy of the model—both of which are important to grower practice change. It would be nice to have a summary of all engagement across partnerships, etc.

  I recommend the exploration of USDA partnership for several reasons. First, NRCS offices regularly interact with growers who are seeking information on how to improve marginal land. They are well positioned to use the model and recommend improvements to growers. Second, Conservation Reserve Program applications not funded by the NRCS could potentially be good candidates for planting perennial bioenergy crops on land that did not score high enough to win Conservation Reserve Program money. Finally, an understanding of how crop insurance could reinforce the adoption of perennial crops would be an important inclusion in outreach efforts.

- This is a unique project because it is akin to an extension effort with the main scope providing technical assistance to farmers (on perennial grasses, energy independence, and the use of SUPERBEEST). The project team partnered with a nonprofit organization, a university extension, and ANL to solicit inputs from farmers on bioenergy issues. The listening sessions and surveys organized by the project team offer valuable insights on topics including farmers' attitudes toward energy independence and concerns over the adoption of bioenergy crops. To a degree, this project seems to be farmers providing assistance to the project team/BETO on how they should prioritize future R&D, demonstration, and deployment efforts to actualize the bioeconomy (e.g., how can we alleviate farmers' concerns over bioenergy feedstock adoption?), which, although different from the stated goal, nonetheless provides helpful insight that should be reviewed by BETO, and such efforts should be encouraged in the future.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the panelists for their attentiveness, their numerous positive comments, and their helpful suggestions on this outreach project. As summarized in the comments, the project focuses on providing a variety of information to—and receiving feedback from—farmers, landowners, and industry representatives on perennial bioenergy crops, on-farm energy independence, and the use SUPERBEEST. This project greatly benefits from our main collaborator, AFT, a nonprofit organization specializing in conservation agriculture with a strong influence in Illinois and throughout the United States. Through our outreach efforts, we are receiving valuable information regarding farmers' perspectives on the topic areas. We are also learning, as noted in the comments, how to recast the questionnaire content to broaden our reach and obtain more detailed, accurate information. As noted in the presentation, we have collaborated with various relevant organizations (University of Illinois Urbana-Champaign Extension, Association of Illinois Soil and Water Conservation Districts, Savannah Institute, Illinois Stewardship Alliance, Sierraview Systems), and we will continue to connect with others to broaden our outreach and obtain numerous perspectives. This will include the USDA NRCS and disadvantaged rural communities identified jointly with AFT. We will target disadvantaged communities coinciding with the marginal lands identified by SUPERBEEST that could have the greatest potential to benefit from bioenergy crop production. We have upcoming events to provide direct technical assistance to farmers, and these will be opportunities for us to gather information on how farmers' perceptions of their own marginal land compares with the results from SUPERBEEST. Preliminary conversations have shown that some farmers may focus solely on crop productivity. SUPERBEEST uses crop productivity in its analysis as well as six other marginalities dealing with soil health and environmental factors. The feedback received from the surveys, individual meetings, webinars, workshops, etc., that have taken place during the last several months has shaped how we will go about providing technical assistance to farmers. They have provided information regarding producers' knowledge of perennial bioenergy crops and on-farm energy production systems as well as what information/guidance producers would like to have before considering the adoption of perennial crops. With this information, we have already started to develop grower guides and personalized production plans to transition into a more applied direction. This includes considerations such as the size, shape, and location of perennial areas within a larger field, a topic that has already been discussed in listening sessions. We are also completing a market analysis to help us understand and eventually incorporate some current policies and market opportunities into SUPERBEEST and other educational materials.

  SUPERBEEST technical development continues under WBS 4.2.2.12, Scaling Up Decarbonization and Sustainability. Insights from this outreach project provide a basis for changes in SUPERBEEST capabilities. As planned, we are adding biorefinery locations to SUPERBEEST to identify potential biomass buyers to drive the conversion of marginal cropland to perennials and overcome a barrier to their adoption. As noted in the comment responses to WBS 4.2.2.12, SUPERBEEST will need to be continually updated in response to changing economic factors pertaining to biomass value and payments for ecosystem services, including aspects such as water quality trading schemes, carbon sequestration, and GHG emissions reductions. The ever-changing governmental and corporate incentives for these key ecosystem services are of great importance to SUPERBEEST's future relevance and usage. Incorporating the presumably favorable crop insurance aspect is a good suggestion for inclusion to complete the economic analysis for farmers. Incorporating spatial EEEJ information in SUPERBEEST will assist in the project's goal of providing an economically viable, environmentally friendly, and socially equitable alternative to traditional row crops in regions with underperforming farmland and associated relatively low farm income.

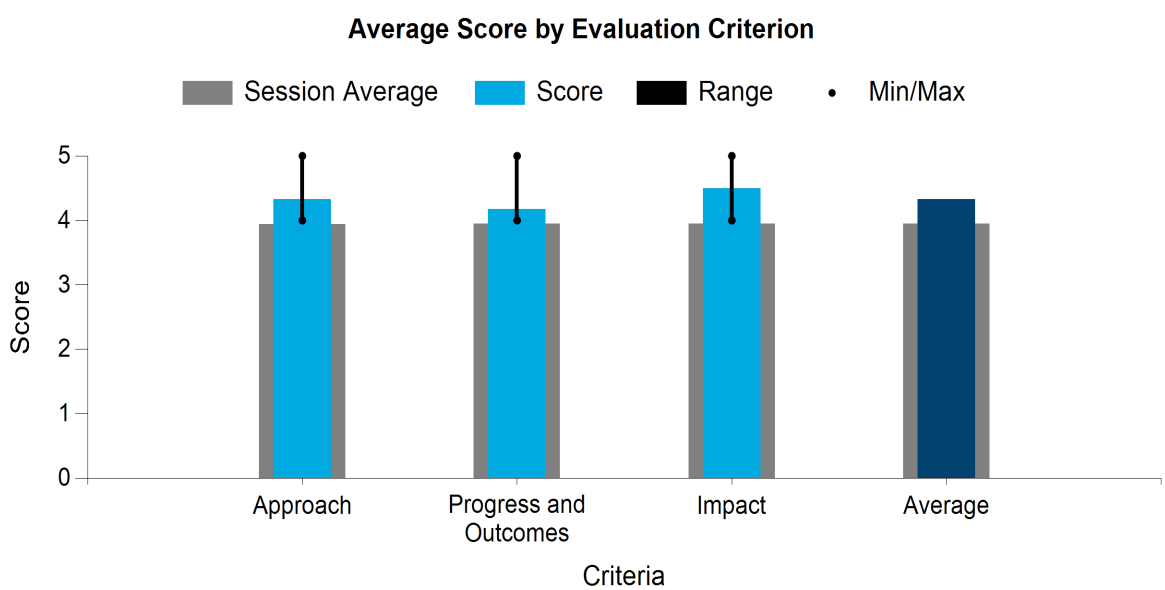
BIOECONOMY SCENARIO ANALYSIS AND MODELING

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	4.1.2.32
Presenter(s):	Emily Newes
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,505,000

The Bioeconomy Scenario Analysis project uses systems thinking and analysis to assess current and/or prospective techno-economics, R&D, deployment strategies, policy, and market conditions and their impact on the potential development trajectories of the bioenergy industry. Results from this project include the identification of opportunities and constraints to industrial development and the quantification of multiple metrics (energy, economic, environmental) to inform researchers, decision makers, and industry of the steps needed for a sustainable, nationwide biofuels industry. Analyses from this project enable the creation of a bioenergy industry by (1) inciting policymakers to explore scenarios for nationwide biofuels production by identifying policy actions; (2) improving the industry's understanding of the industry's growth potential under different conditions, better targeting their development efforts; and (3) providing universities and other interested stakeholders with tools and analyses that can be adapted to meet research and teaching objectives, connecting students with careers that build the industry. One tool used in this project, the Biomass Scenario Model (BSM), is a publicly available, unique, validated, SOA, award-winning, fourth-generation model of the domestic biofuel supply chain that explicitly focuses on how and under what conditions biofuel technologies might be deployed to contribute to the U.S. transportation energy sector.



COMMENTS

- Great project. It provides a rigorous systems modeling approach that makes unique contributions to biofuel modeling. The project has clearly had a strong impact as well. The fact that it is frequently used in policy-relevant contexts speaks to this. The project team has done an excellent job of finding use cases for this tool, and I hope to see that continue.

In terms of recent progress, I particularly applaud the linkage with GCAM. This seems to take advantage of the resolution of each framework in complementary ways. I would encourage both modeling teams to use this collaboration as a platform for future work. One significant weakness of BSM when it comes to analyzing SAF is the lack of detailed trade representation. This will be critical to looking at popular near-term SAF feedstocks, such as canola oil. It is understandable that BSM has been domestically focused to date, and I do not see this as a flaw in progress so far. But this is an area where near-term future work should make improvements. Linking to other models like GCAM that already have detailed commodity trade representation could be an elegant solution.

- Thank you for the opportunity to review the Bioeconomy Scenario Analysis and Modeling project. Based on the information provided, the project is well aligned with BETO achieving their goals. I am impressed by the use of system dynamics and the incorporation of inputs from seven BETO models to create a comprehensive model. The plan to include reduced-form representation and a repository of recreatable results is also a positive step forward. While the project lacks economic relationships and the ability to incorporate inventive policies, it has contributed to the EPA's *Third Triennial Report to Congress* and supported analysis of proposed policies in Congress, which demonstrates its real-world impact and impact. Overall, this project is on schedule and has the potential to support stakeholders in identifying bottlenecks and designing bioeconomy strategies.

- BSM is a long-standing DOE tool that has been extensively used and is publicly available. The project addresses a clear need by assessing biomass supply and associated risks across different scenarios and has a well-documented history of use by policymakers. It has newfound relevance with the SAF Grand Challenge and DOE's recent focus on aviation, illustrating how long-term SAF targets could theoretically be met with biomass. In terms of integration with other tools and research areas within DOE, the presentation very clearly communicated the project's purpose and role and how it interacts with other models to avoid redundancy.

  The project does a good job of communicating its risks and the steps taken to stay focused on the core project objectives and identify and fill data gaps when necessary. The model is also regularly validated against historical data to build confidence in the approach. To stay relevant, there is a good track record of adding TEAs of new fuel pathways to match the aims of broader policy goals.

  My primary recommendation would be to demonstrate, or perhaps to more clearly communicate, how the BSM approach aligns with ground truth data on aspects of the bioeconomy on the availability of wastes and residues as well as on expected yields for energy crops. Can this information go through a validation process as well?

- This project aims to encourage the bioenergy industry by providing data-based scenarios that can help guide decision making. The project team has worked with different stakeholder groups, and they have actively worked to contribute to policy formation. The PIs might look to European examples to see how different carbon pricing tools have influenced different types of biofuels overseas. The project has made progress toward addressing the project goals because the integrated assessment model shows the different commercialization potential of different policy choices. This work could be of great use to industry, investors, and policymakers.

- BSM has been a successful and useful model for many years and is highly accurate in forecasting markets with robust historical information. Modeling with data for markets that do not yet exist or have limited performance, such as carbon markets, poses several challenges that can make it difficult to create accurate and reliable models. One main difficulty is the lack of historical data on which to train the model, which is essential for ensuring the model's accuracy. Additionally, without existing markets, it can be challenging to identify the relevant variables to include in the model because the factors that will drive market behavior are not yet known.

To mitigate these challenges, holding stakeholder workshops can be a valuable tool. Eliciting feedback from industry experts and policymakers can help to identify potential market trends and relevant variables that should be considered in the model. These workshops can also help to identify potential biases or assumptions that may need to be challenged in the model development process. Documenting the breadth and depth of these workshops would also be an important measure in communicating the extent to which this mitigating step has been deployed.

- This project is clearly impactful through its collaboration with/support for multiple other modeling efforts and contributions to BETO's missions. The team is forthcoming with the potential limitations of the approach and takes proactive measures to mitigate the risks. The team also places a big emphasis on increasing the accessibility of the models. The model is publicly available and evolves with the current and future needs, the team leverages a variety of data deposit services to keep good records of the data/assumptions used for each analysis, and the team makes efforts to increase the accessibility of the models through visualization, etc. The team is also planning to move to platforms such as R or Python to increase the adoptability of the model. A regional version of the model (Regional BioEconomy Model [RBEM]) has also been developed for a targeted industry or a local area. One suggestion is to tie the scenarios considered in this project to the specific policy decisions it contributes to.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for the insightful comments on the Bioeconomy Scenario Analysis and Modeling project. We were encouraged by the comments relating to the strengths of the project, and we appreciate the thoughtful suggestions regarding future directions for the project. Here, we respond to those suggestions.

  GCAM, canola, trade, SAF: We are delighted with, and share your enthusiasm for, continued collaboration with the GCAM team, particularly as we create a reduced-form version of BSM. We envision that this reduced-form model will be easier to integrate with models such as GCAM. It will enable us to improve our representation of trade issues around fuels and feedstocks. We are in communication with PNNL and believe that this will make a useful future case study.

  Economic relationships, policies, real-world impact: Thank you for the comments relating to the real-world contribution of this project to policy analysis, including the EPA's *Third Triennial Report to Congress* and analysis of proposed policies for Congress. While the model contains simplified logic of economic drivers and incentives associated with the agricultural system, with bioenergy conversion investments and operations, and with "downstream" operations, the peer review of the model is an opportunity to revisit those relationships. We plan to use a portion of a workshop, planned for August 2023, to review key economic relationships in BSM.

  Alignment of BSM with ground truth data for wastes, residues, and yields: BSM uses data from multiple sources to populate its supply structures for wastes and residues. These sources include inputs from the Policy Analysis Systems Model (POLYSYS) from Oak Ridge National Laboratory (ORNL) (crop residues, forest residues, dedicated energy crop yields), the Biomass Logistics Model from Idaho National Laboratory (INL) (logistics), and available wet waste information from NREL and PNNL. We plan to revisit these data sources and to cross-check the data used in BSM against other sources as part of our FY 2023 scheduled public update to the model.

  Biofuel policy in the United States and European Union: Because the focus of BSM has been on the contiguous United States, we have not directly incorporated international policies. That said, we recognize the importance of international policies and the increased efforts being placed on global decarbonization. This is an area of potential future exploration that we will consider going forward. As for specific policy in the United States, BSM already has representations of many policies either implemented or considered by Congress, and we are currently working on a journal article that will present a review of these policies and how they may influence biofuel production.

Workshops: We agree that workshops are essential as a mechanism to vet and improve model data, model assumptions, and model logic. We have held many workshops during the past 15 years (in 2022, 2016, 2014, 2012, 2010) with varying degrees of public documentation. We are encouraged to hear that workshop documentation will be helpful, and we will be sure to release results from our workshop that will be held in August 2023.

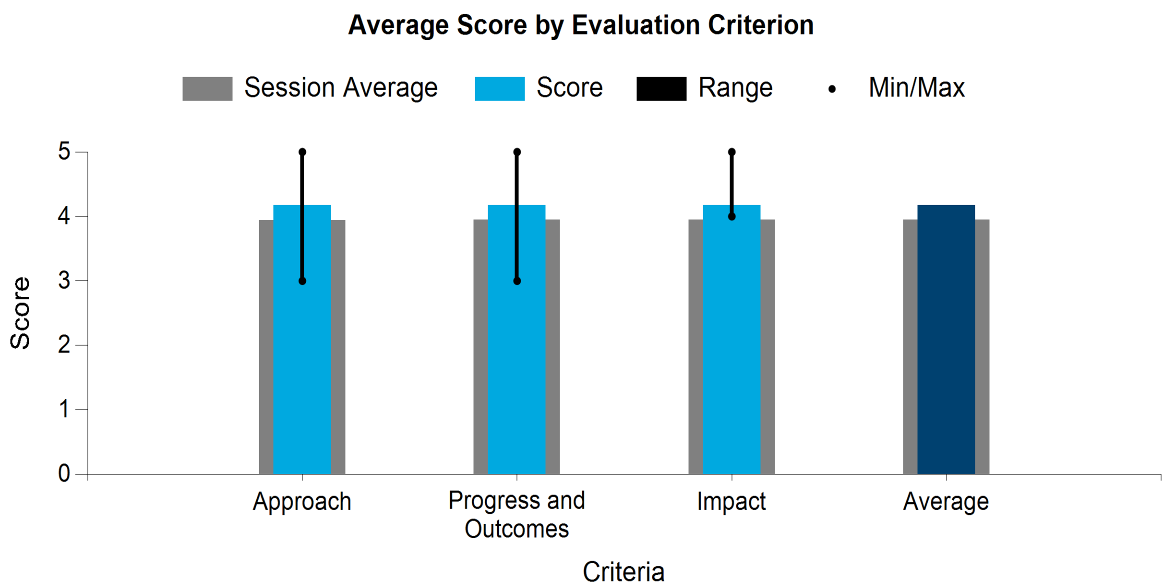
ALTERNATIVE MARINE FUEL PRICING, SUPPLY, AND DEMAND

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	4.1.2.33
Presenter(s):	Emily Newes
Project Start Date:	10/01/2020
Planned Project End Date:	09/03/2023
Total Funding:	$750,000

The International Maritime Organization low-sulfur fuel rules and GHG-reduction strategy may significantly perturb global refinery operations, impacting the volumes and prices of marine fuel globally and within the United States and incentivizing the transition to alternative fuel use. The goals of this project are to (1) enhance the understanding of how very low-sulfur fuel—primarily fuel oil and diesel—and low-carbon fuel requirements and promising biofuel processes will affect the marine fuel supply chain; (2) explore how these perturbations interact with and impact indicators, such as pricing, number of trips, and demand behavior, along with the potential to meet low-sulfur and low-carbon fuel demand with biofuel supply chains; and (3) merge innovative thinking in the area of marine fuels within the research centers of DOE (NREL) and the U.S. Department of Transportation (The John A. Volpe National Transportation Systems Center (Volpe Center)). These goals will be accomplished through the combination of detailed refinery, marine fuel burn, system dynamics, and geospatially explicit linear programming models.



COMMENTS

- This is an exciting project with substantial potential value for stakeholders. The marine sector is understudied in the bioenergy space. This project fills a significant gap by helping to quantify the financial and environmental impacts that bioenergy could have in this sector. The initial progress on logistical modeling, refinery modeling, and supply chain modeling were all well selected, and progress appears to be solid.

  In general, I think this project is on a good track. But I do have two recommendations: First, the project should integrate vessel idling and hoteling loads into the fuel burn modeling. This will make the tool more valuable to federal, state, and local environmental organizations and communities. Second, the supply chain modeling tool should be expanded to support the estimation of cosolutions for multiple ports within a given region. For example, the logistical network displayed on slide 17 should ideally also be able to incorporate the needs of other regional ports in the northwest (Tacoma, Portland, etc.).

- Thank you for the opportunity to review the Alternative Marine Fuel Pricing, Supply, and Demand project. This project is well aligned with BETO's goals to develop sustainable and renewable energy sources for marine fuels. The use of a collaborative modeling framework and proprietary data access in the first-of-its-kind analysis with the Volpe Center is impressive. The progress toward goals is impressive, and the project is on schedule. The significance of impact is high (interactions with Maersk Mc-Kinney Moller); however, the potential for the commercialization of this work is low due to the data confidentiality and nature of the research partner. Additional outreach to industry stakeholders, particularly for more fuel use data for additional ports, could be beneficial for the project's future success.

- This project fills a growing need to evaluate biofuels in the marine context as there is growing pressure to address maritime emissions but insufficient understanding of which biofuels to use and where to deploy them. This project nicely addresses those questions by developing a regional analysis for biofuel deployment in the marine sector, focusing on the needs of an individual port and the supply chains necessary to provide it with advanced biofuels. This project used resources from BETO on biomass supply and economics in conjunction with marine sector expertise from the U.S. Department of Transportation on fuel burn and logistics, and the project team showed good coordination and project design to ensure that the results were relevant to key stakeholders, such as the Maritime Administration.

  The progress so far suggests that the analysis is novel—giving the really valuable granular analysis that is necessary to understand how the Port of Seattle could be supplied with regional biomass suitable for coprocessing. One note of caution, however, is that while the data are granular enough to allow for equity impact analysis, the project does seem to imply that that local existing refineries will be used, so this recommendation must be taken with care to ensure that equity concerns are addressed.

- The goal of this project is to develop a tool for decision makers to assess scenarios for marine biofuels.

  The RBEM shows how different variables produce regional impacts, but what about the ways in which particular regions (i.e., particular landscapes and particular communities) impact biofuel production? If the goal is to understand which conditions are necessary and sufficient for investment, it seems that a better understanding of social acceptability and biofuel availability would be relevant. A regional-level analysis, such as the Port of Seattle example, has great potential to examine local socioeconomic and environmental variability.

  The project emphasizes the need for collaboration. The project partners have done a nice job collaborating with other agencies and entities working in this relatively new marine space. How has feedback from different groups been incorporated into the analysis? Specifically, it sounds like feedback from industry representatives indicated that regulatory uncertainty was the biggest barrier to development—how does the model take this into account?

  The project's preliminary results show that 100% of the projected 2040 marine fuel demand at the ports of Seattle and Tacoma could be satisfied with regionally produced biofuels, largely derived from wood residues. Does the model consider competition for feedstocks for other forms of bioenergy (biopower) or other bioproducts (cross-laminated/mass timber, traditional forest products, paper/pulp, etc.)?

  The project proposes eight new biorefineries for the Seattle area. An important next step for this project could be to incorporate EJ mapping tools to assess how these new biorefineries might contribute to or help address energy equity issues. EJ tools could include CEJST or the EPA's EJ tools.

- The intention of this project is strong and clearly impactful with ports and regions like Seattle that have available data to contribute. The focus on marine needs and uses of biofuels is of substantial importance to BETO's mission and requires separate modeling and infrastructure than SAF or even traditional biofuels required.

  There are substantial challenges to scale beyond ports where data on fuel consumption are available, which may limit the applicability of the project if this continues to be an issue.

- This project looks at the hard-to-decarbonize marine sector with specific focuses on select areas. The collaboration between NREL and the Volpe Center has been smooth, and the team has clearly identified potential risks and made plans to mitigate them. Aside from conducting a first-of-its-kind analysis, another impactful outcome from this project is the collaboration with partners on the feasibility study of a green corridor from Seattle to South Korea.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments and enthusiasm for our project. We hope that the following responses address the major comments raised during the review.

  Fuel burn model: We agree that there are various additions to the model that would greatly enhance its value to stakeholders. An updated version of the fuel burn model will include the characterization of ship operating mode, including accounting for differences in the calculation of fuel burn that occur at berth as well as at anchorage, following the EPA's Port Emissions Inventory Guidance. These modeling improvements will impact fuel usage for future work on auxiliary engines and boilers.

  The Freight and Fuel Transportation Optimization Tool (FTOT): The FTOT modeling tool can easily handle additional ports up to the national scale. When provided with this additional demand data, the tool will adjust its routing solution to maximize the demand fulfilled across all ports in the region while minimizing transportation costs; however, the initial case study focused on the Port of Seattle due to the availability of data on fuel demand at the port; future iterations of the modeling scenarios may include additional ports in the region if fuel demand data can be acquired or if fuel demand at ports can be estimated from the fuel burn model component of this project. We would like additional data from ports on fuel demand that can be used to expand the FTOT supply chain analyses. Proposed future work will address additional ports as well as work more closely with industry and port partners.

  External release of information and engagement: Although the Volpe Center cannot release the data behind the fuel burn model, we can use aggregated data and share the source code used for converting vessel movement and characteristic data into fuel burn. The FTOT model is publicly available. In addition, we can share much of the information from the refinery modeling with the public, but they would need to have a license to the Aspen PIMS software to run the model. There will be published technical reports and journal articles on both topics to disseminate information to a broader audience. In summary, some of the knowledge gained and nonspecific data can be shared with the public. We have already received some feedback on aspects of our project as the fuel burn model approach was discussed with various groups (EPA, Maritime Administration), and their feedback was incorporated into the methodology to align with existing analyses, such as the EPA's National Emissions Inventory Guidance and Port Emissions Inventory Guidance. Future work is intended to address additional ports and to work more closely with industry partners (e.g., refinery owners and port authorities).

  Equity analysis/energy justice: The fuel burn model component is anticipated to support equity analysis. The first step is to complete an inventory of emissions related to current fuel usage, then build scenarios of alternative fuel usage, and finally incorporate dispersion modeling. In terms of FTOT, we can, at a minimum, overlay an equity metric on the outputs of the FTOT scenario runs once finalized to look at how proposed sites and transportation routes intersect with equity emphasis areas/EJ communities as represented in tools such as CEJST and EJScreen. NREL leads a project for BETO on local air quality and EJ impacts of biorefineries. This project has explored emissions from different conversion processes and could assess changes in emissions with coprocessing and related air quality and EJ impacts. We plan to collaborate with them to assess the potential benefits from refinery coprocessing.

Modeling topics: The analysis to date using the Volpe Center's FTOT focuses on available feedstocks that could be leveraged to supply alternative fuels to the Port of Seattle and the associated transportation costs and emissions with a supply chain based on those feedstocks. Complementary work under this project using NREL's RBEM will take policy constraints and opportunities further into account to assess the potential for deployment in the region. Regulatory uncertainty will be addressed by running a sensitivity analysis around policy timing, duration, and magnitude. Feedstock competition with other possible end uses is not addressed in our current analysis. The currently defined scenarios focus on waste materials not used for primary bioproduct production, but they do not consider potential future competition with other end uses outside of biofuels. FTOT is a scenario exploration and analysis tool, so subsequent analyses representing different levels of competition with other forms of bioenergy can be modeled. In addition, what was presented at the BETO Project Peer Review was an interim analysis; we do not expect the final analysis with techno-economic alignment to propose the same number of biorefineries as was presented. There is a definite risk to modeling because marine data are sparse. Having a fuel demand value at the port is important to define the supply chain; however, if those data are not available, we may be able to estimate a first-order approximation of fuel demand at specific ports from the fuel burn model to facilitate continued expansion of the analyses across different ports and regions.

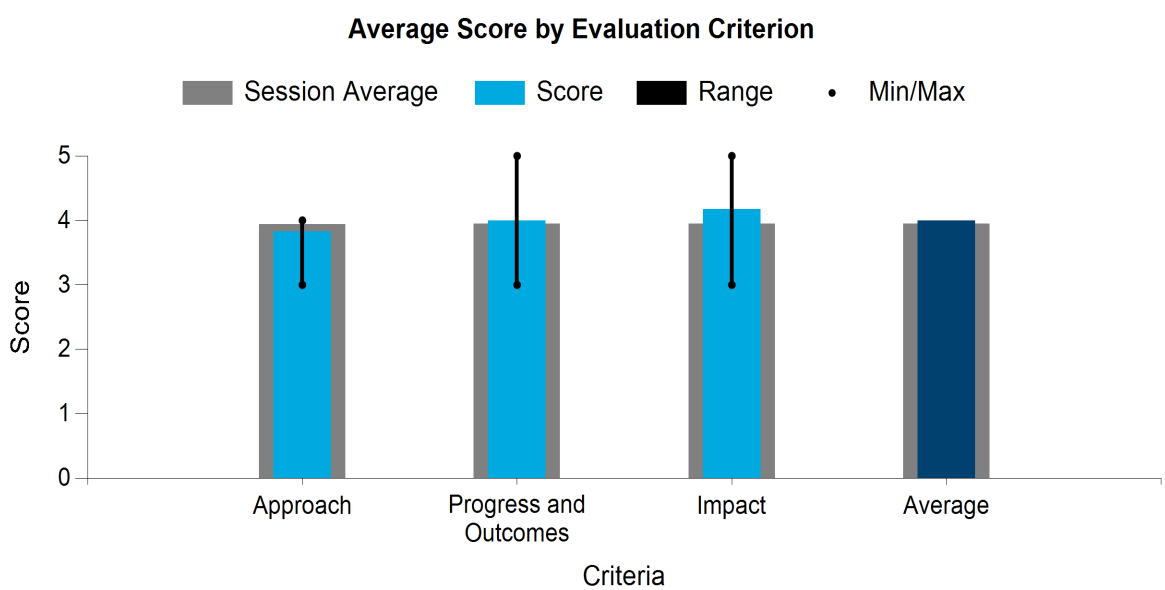
BIOFUELS NATIONAL STRATEGIC BENEFITS ANALYSIS

Oak Ridge National Laboratory

PROJECT DESCRIPTION

WBS:	4.1.2.41
Presenter(s):	Rocio Uria-Martinez
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$750,000

This project contributes to understanding and enhancing the socioeconomic and environmental benefits of bioenergy through economic and policy analysis/modeling of the effect of prices and policy incentives on fuel markets for hard-to-decarbonize transportation sectors, particularly aviation and marine. The analysis pays attention to potential synergies or competition for the use of biomass among different transportation segments while modeling the competition from incumbent petroleum-based fuels. The technical approach builds on the Biofuels National Strategic Benefit Analysis project previously funded by BETO. The market equilibrium model developed for that project (BioTrans) has been expanded and revised to depict the aviation and marine transportation fuel segments. New model features include (1) a new set of feedstocks, conversion pathways, and biofuels; (2) tracking the life cycle GHG emissions for each fuel depicted; and (3) finer spatial disaggregation. Additionally, the analysis approach includes an exploration of the economic equity of model results by linking them to socioeconomic and demographic data. FY 2022 work focused on adding those features and gathering insights from an initial no-policy baseline set of cases. In FY 2023, the policies and incentives affecting the use of biofuels in the aviation and marine sectors will be included in the model. The FY 2024 objective will be to publish the model and results and disseminate them among the target audiences.



COMMENTS

- This is an excellent methodological approach with significant potential to assist stakeholder decision making. I think that the areas of model development in year one of the project were generally well chosen. Overall, this is a worthwhile project, and I look forward to seeing it progress further.

  I do have some specific directions for future development and a couple notes on the results presented to the reviewers.

First, to realize the potential of the model, it will need to endogenously include legacy petroleum systems. Improving energy sector representation in this way would lead to more credible economic and GHG emissions estimates for bioenergy. It would also enable EJ analysis to include impacts on petroleum refining.

Second, biodiesel from waste fats, oils, and greases needs to be included, at least as some kind of aggregate pathway. A substantial share of historical and near-future biodiesel production comes from this pathway, and including it will better reflect the historical baseline.

Finally, a note on the results: The 2020 production volume estimates shown on slides 9 and 10 seem to underestimate the volumes of HEFA-RD and vegetable oil-based fuels in general. It is one thing for a scenario to not find growth from this historical baseline over time. But these fuels seem to simply be missing in the volumes they are currently produced.

- Thank you for the opportunity to review the Biofuels National Strategic Benefits Analysis project. I am pleased to report that this project is well aligned with BETO's goals. The project's approach to understanding and enhancing the socioeconomic and environmental benefits of biofuels is commendable, particularly with regard to modeling the effect of prices and policy incentives on fuel markets for hard-to-decarbonize transportation sectors. The project's progress toward its goals is commendable, including the work on policy and incentives and its state-level supply aggregation from BT16. The impact of the project, including the public DOE BETO Biofuels TEA Database and outreach to industry, is also significant. The project appears to be on schedule, and appropriate risk strategies, such as collaboration and check-ins with PIs and advanced analyses R&D, have been employed. Understanding the constraints of relying on BT16 inputs should be explored, particularly with scenarios that are likely to have large price signals or cause LUC, extensification/intensification, or incentivize the adoption of conservation practices.
- This project very nicely expanded and improved upon an existing model to improve its relevance and focus on specific interest areas for BETO. Particularly given some 2021 feedback that this project did not have a clear target audience, I think that the progress since 2021 has addressed those concerns. The updates make the model well suited to evaluate the SAF Grand Challenge, its impact on SAF production, and the associated economic and equity impacts. In particular, the updated BioTrans can assess the policy implications of SAF deployment in response to different policy designs, but, critically, it can inform the economic and equity implications of SAF deployment. Though the key output of this project is a model, it is not clear if the model will be publicly available, despite its obvious utility.
- I also think it is important to highlight that this project is unique in tackling the cross-sectoral pressures of competing biomass demand for transportation, which is critical for policy design but was not addressed much in the other projects. Particularly given the technology changes across sectors (e.g., electrification in light-duty vehicles), sector-specific policies (e.g., sulfur limits in marine), blending limits, and resource-constrained sources of biomass, assessing how these different transport sectors interact is critical for informing policy design.
- The goal of this project is to understand and enhance the socioeconomic and environmental benefits of biofuels through modeling the effect of prices and policy incentives on fuel markets for hard-to-decarbonize transportation sectors. It is good that this project is now working to account for socioeconomic as well as environmental benefits, and it is also good to consider the distribution of socioeconomic and environmental burdens. This focus on potential burdens as well as potential benefits will be a more nuanced and potentially comprehensive way to think about equity issues.

  That said, the project partners state that land allocation decisions are exogenous to the model. That is a major limitation when thinking about equity issues.

Also, to get at these equity issues, the project team decided to change the spatial units from census divisions to states. Most equity analyses try to get as granular as the data will allow, and census track level-data are becoming more common for this type of analysis. Breaking the data down even further in this way could be an important next step for this project. It appears that a past reviewer suggested scaling up as a means for national-level policy analysis, but for the new equity indicators, scaling up would obscure important nuances. Is there a way to do both?

The project found that 37% of herbaceous energy crops come from economically disadvantaged communities. What are the policy implications of this? What does the model tell us about how to incentivize the benefits of bioenergy development without creating burdens? The project seeks to find which communities could especially benefit from workforce development/financial incentives to participate in the SAF industry as biomass feedstock providers. Are these the same communities that will endure the burden of biorefineries? Who is involved in making these decisions? How do these models address issues of procedural justice? That is, how do the models account for complex decision-making processes?

One goal of the project is to produce maps to visualize disadvantaged counties with potential, economic feedstock supplies. How will they be used? To what extent were representatives of those disadvantaged groups involved in the process of developing this analysis or in discussions of potential uses of the project outputs?

Four states (Texas, Nebraska, Illinois, Iowa) provide 45% of the total biomass feedstock dedicated to biofuel supply in the high oil price with aviation emissions limit scenario in 2050. What are the socioeconomic implications of concentrating production in these four states?

The project identifies other sensitivities, such as biomass use for non-transportation purposes (biopower, bioproducts). This seems to an issue across most bioenergy models, especially for wood-based biofuels. What is the best use of forest residuals and other forms of woody biomass? Does the model account for potential competing uses of feedstocks?

- This project enables granular evaluations of the impact of biofuel policy at the county level. A great example of the usefulness was the evaluation of the potential of herbaceous energy crop production to overlap with disadvantaged communities. A nice step further would be to include other EJ and equity components in that kind of evaluation.

  The spatial distribution of soybean production did not align with current production nor with the supply shed that will feed the new processing capacity coming online in the next 5 years to serve renewable diesel demand. On a related note, the growing seasons and ranges of products are forecasted to change over the next 30 years as a result of climate change. An example is the soybeans being planted farther north in North Dakota every year. The model should consider forecast climate volatility changes in feedstock production, yield, and crop mix if they are not already included.

- The project aims to understand the socioeconomic and environmental implications of biofuels for the hard-to-decarbonize transportation sectors through the BioTrans model, with emphasis on the effects of prices and policy incentives; however, some approaches can be improved. For example, the team shows that there is great potential for disadvantaged communities to grow bioenergy feedstocks for economic growth, but the uncertainty in the profitability from bioenergy feedstock (there is no existing market) may hurt these communities. Future research should consider the opportunity cost of the land and other market factors in the analyses.

  Additionally, the project team is migrating the model to Julia, but the optimization part remains on the General Algebraic Modeling System (GAMS) (commercial software) due to the uncertainty of the open-source solver's performance. The team is encouraged to work with other labs to identify the optimal language and potentially leverage existing work (e.g., Sandia National Laboratories developed the optimization package Pyomo in Python, http://www.pyomo.org/).

Finally, this project is heavily focused on SAF, but alternative clean fuel sources, such as H_2, should also be considered (if within the scope of BETO).

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their helpful comments. Some suggestions involve expanding the model scope (e.g., including an endogenous representation of petroleum refineries and an endogenous representation of land allocation decisions). We are exploring the possibility of collaborating with NREL on refinery modeling. For land allocation, building a representation of the U.S. agricultural sector is outside the scope of this project; however, some biomass feedstock supply response to biofuel policy incentives can be captured using *Billion-Ton Report* supply data for various biomass price assumptions. Two reviewers pointed out divergences between the simulated and actual activity levels and locations for soybean-based biodiesel production in 2020. The presented simulated results are from a no-policy baseline scenario; therefore, the biodiesel tax credit is not included, which partly explains the lower volume of biodiesel production. Several comments point to the importance of accounting for competing uses of feedstocks. We confirm that the model currently accounts for non-biofuel biomass uses by treating them as exogenous demands based on data from the USDA and U.S. Energy Information Administration. The effect of variations in the volume of these exogenous demands will be considered through scenario analysis. As for the public availability of the model, the goal is to make it public by the end of FY 2024. We appreciate the suggestion to continue exploring open-source solver options to enable users who do not have access to the commercial solver we are currently using to also run BioTrans. We appreciate the feedback regarding the approach developed to discuss EJ implications of biomass supply activities in the BioTrans model runs. We consider that the maps showing the overlap between biomass feedstock supply and economically disadvantaged communities provide useful information, but we also acknowledge that they need to be complemented by analyses of both potential economic and environmental benefits and burdens from activities along the entire biofuel supply chain. Much of that work requires more spatial granularity than what the BioTrans model provides.

OPTIMIZING BIO-JET FUEL BLENDS WITH THE FEEDSTOCK TO FUNCTION TOOL

Lawrence Berkeley National Laboratory

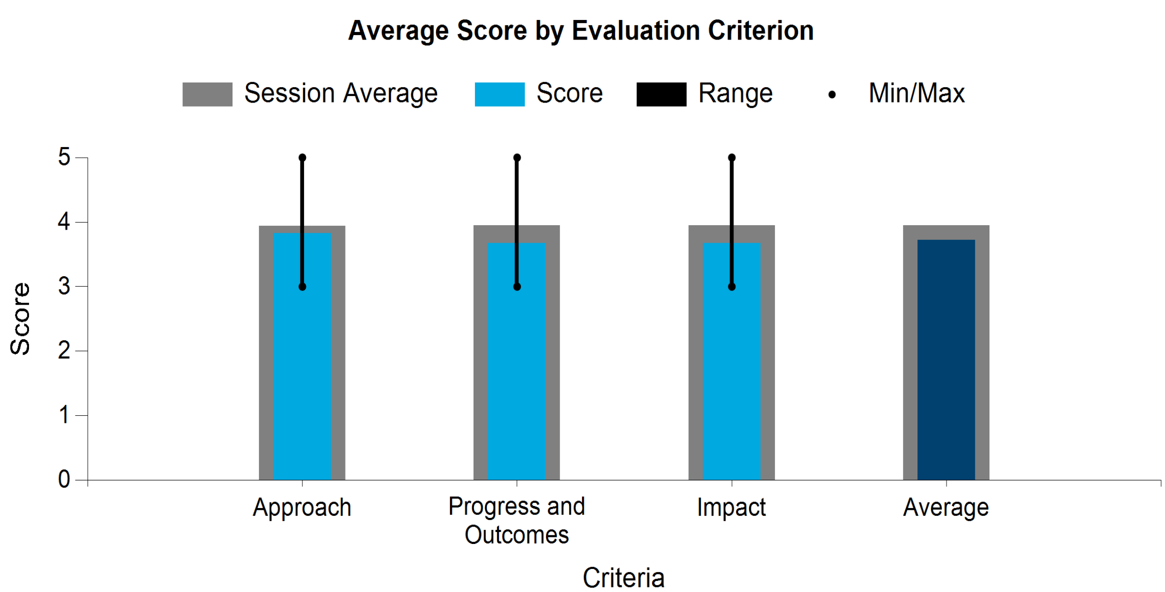
PROJECT DESCRIPTION

WBS:	4.1.3.60
Presenter(s):	Vi Rapp
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,275,000

Biological routes offer unparalleled flexibility when developing novel molecules tailored for high-performance applications (e.g., fuels and products). Due to high costs or high-volume requirements, experimental property testing of these molecules is usually conducted years after initial bench-scale experiments are completed. Kinetic models may be used to compute properties if experimental methods are unavailable, but these models take a significant amount of time to develop and require domain expertise. Regardless, neglecting to conduct property testing early in the development cycle can lead to investments spent on scaling up the production of biofuels and bioproducts that do not perform as well as expected.

Feedstock to Function is the first comprehensive web tool that enables scientists and companies to explore viable bio-based fuels and products without spending time and money testing in the lab (feedstock-to-function.lbl.gov). The web tool leverages machine learning and experimental data to predict high-throughput aviation fuel properties of more than 10,000 molecules, and it links to a separate tool for cost and emissions estimates. By predicting properties, costs, benefits, and risks of promising biomass-derived molecules, this open-source tool will facilitate faster, less expensive bioprocess optimization and the scale-up of SAF.

The goal of this project is to support the optimization and deployment of SAF by expanding Feedstock to Function's capabilities for fuel blends. The new capabilities will include (1) a fuel-blend property prediction model that includes fossil-based jet fuels blended with bio-derived molecules and (2) a fuel-blend design feature that enables users to identify bio-based blends within targeted aviation property values.



COMMENTS

- This project has a well-defined and logical approach, it seems to be exceeding progress benchmarks, and it could have significant impact for stakeholders. I find very little to criticize about this work. I look forward to seeing it progress further.

  One small suggestion: This project seems well placed to develop several EJ-relevant metrics for various fuel blends that could be useful to researchers and other stakeholders. These include estimating the ecotoxicity, sulfur content, and PM emissions associated with different blends. Such information could aid the selection of specific blends in the future.

- Thank you for the opportunity to review the Optimizing Bio-Jet Fuel Blends with the Feedstock to Function Tool project. I am pleased to report that this project is well aligned with BETO's goals given the SAF focus. The project's approach to developing the first comprehensive web tool that predicts promising molecule properties and evaluates the costs, benefits, and risks for bioprocess optimization, certification, and scale-up is impressive. The project's use of a machine learning approach and diverse optimization methods is also innovative. The project has made good progress toward its goals, including surpassing the fuel-blend property prediction model's ability to predict properties of fuel blends at different blend ratios to within 15% of published experimental values. The project appears to be on schedule and could benefit from improved model access and impact metrics. As with the other LBNL tools, the reviewers were unable to access and assess the tools directly. Additionally, there was no available information on who or how many users have been utilizing the tool. Future efforts to gauge the effectiveness of the outreach activities would be helpful in gauging the project impact.

- Due to the relatively narrow scope of this project and its focus on predicting molecules, it is difficult to compare it to the bulk of the projects within this technology area. This is very much at the frontier of feedstock selection, long before the implications of developing LCAs and TEAs or modeling the broader bioeconomy come into play. This project appears to be well designed and managed and is making meaningful progress relative to its goal. The web tool format should be very accessible and easy to use for its end audience, and it could be a good candidate for posting on KDF or another easily accessible portal. The audience and potential impact of this tool are readily apparent, and it clearly addresses a stakeholder need by de-risking R&D for SAF.

- This project acknowledges that the development of SAFs is limited by significant technical, social, and regulatory barriers. To address these issues, the project team developed the first comprehensive web tool, Feedstock to Function, that predicts promising molecule properties and evaluates the costs, benefits, and risks for faster, less expensive bioprocess optimization, certification, and scale-up.

- This seems to have great impact as a potential tool that could be of use to a range of users. Who has been the primary audience for this web tool—industry, investors, researchers? What kind of feedback has been received from users, and how has that feedback been incorporated into more recent iterations of the web tool?

- The availability, accessibility, and accuracy of this tool allows for experimentation, R&D, and innovation for biofuel blends. The project has successfully surpassed its error target and appears to be further than expected in accuracy. Having a free, responsive web tool strongly achieves the goal of availability. It is difficult to judge the accessibility because measurements on users and use is not presented. If they are not being collected, it is important to understand the number of unique users, page views, user queries, or other quantifiable actions, user demographics, and customer satisfaction scores.

  Because information dissemination is a stated goal of the project, it is also important to set measurable goals on what it would mean to achieve this bar.

- This is a straightforward project that aims to develop a machine learning-based model to predict the properties for fuel blends. It also interacts with the BioC2G model and is available on the web. The accuracy of the model is high, although comparisons to alternative methods (e.g., weighted average of individual pure compounds) would be able to further support this. Because this is a machine learning model, the integration of mechanistic insights could be helpful in understanding and improving the trained model.

  Additionally, it would be good to have experimental data for validation (could just validate for the most promising blends) and also work with industry partners on how this can be used in developing fuels that comply with ASTM standards.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you so much for the feedback and comments from all the reviewers. We, too, are excited about the prospects and potential of this tool. We agree about the potential for developing EJ-relevant metrics, and we will explore options for predicting additional metrics, such as ecotoxicity, sulfur content, and PM emissions associated with different blends. We also agree about tracking the tool use to better understand outreach effectiveness and impact. We have recorded the number of users and just started tracking how frequently they use the tool. We really appreciate the suggestion to post the tool on KDF or another easily accessible portal, and we will look into this option. Also, to clarify, the tool predicts properties of individual molecules and blends of molecules. It is also connected to a lightweight LCA/TEA tool to support initial feedstock selection and explore scale-up options. The primary audiences for this web tool are industry and researchers. So far, the feedback has been positive, and it has helped guide user interface and property predictions. For example, researchers have requested that we expand property prediction to include viscosity and density, so we identified reliable experimental data sources for these properties and developed new models. Additionally, we received a request to search for molecules using specific property ranges instead of molecule name or Chemical Abstracts Service number, and the tool was updated accordingly. We also expect to solicit feedback for the blend design tool after the first release to better meet users' needs. We do collect information about the number of unique users, and we have just started logging page views, time on pages, and queries. Demographics are inferred by email address. Adding a satisfaction score and feedback form is a great suggestion, and we will explore options for adding this to the tool. We will also consider reasonable metrics and goals to use with the satisfaction and feedback data. Experimental data are used for developing the blend prediction tool and validating the predictions. We also plan to collect more experimental data for further validation. Additionally, we aim to integrate mechanistic insights and model overviews after we have finalized the models and looked more at how the Fourier transform infrared spectra features are weighted for property prediction. We appreciate the suggestion about working with industry and exploring how this tool could be used to support fuel development to comply with ASTM standards.

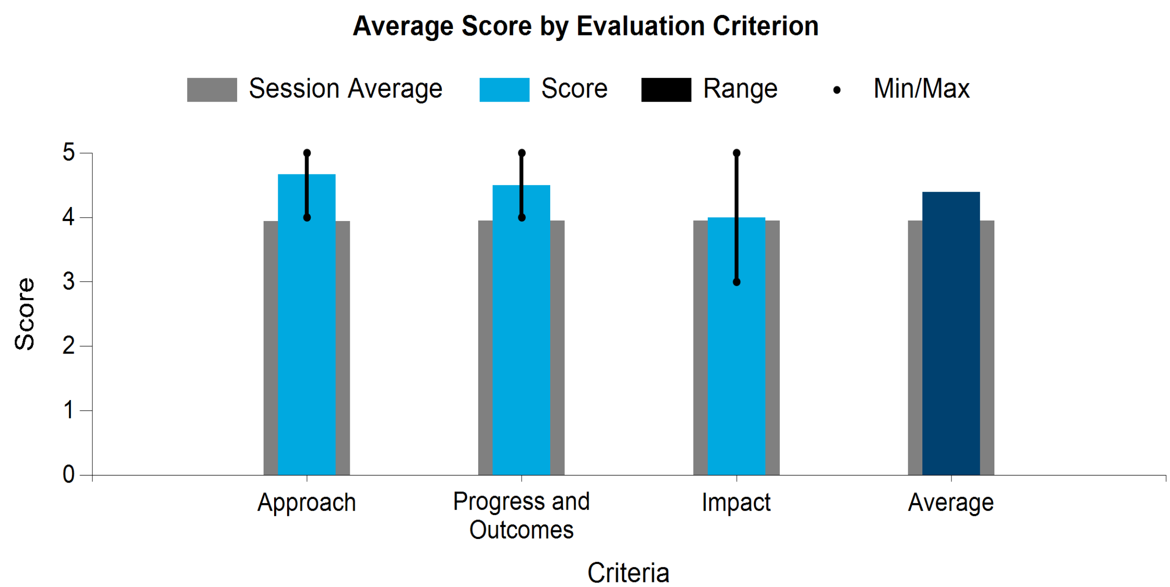
BIOC2G MODEL FOR RAPID, AGILE ASSESSMENT OF BIOFUEL AND CO-PRODUCT ROUTES

Lawrence Berkeley National Laboratory

PROJECT DESCRIPTION

WBS:	4.1.3.61
Presenter(s):	Corinne Scown
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,200,000

The objective of this project is to make rigorous TEA and LCA of biorefinery technologies accessible, flexible, and transparent to a wide range of researchers and industry decision makers. The current project substantially expands the scope and capabilities of BioC2G in response to an increasing emphasis on biojet fuels, net carbon-negative bioenergy, the utilization of waste feedstocks, and EJ. The web-based model has three primary components: (1) a geospatial biorefinery siting and resource filtering tool that leverages a combination of county-level biomass availability projections with location-specific and fine-resolution satellite data to provide detailed feedstock availability across the entire United States; (2) a Python-based process model that enables users to adjust a wide variety of feedstock, scale, and operating conditions to produce customized cost, mass, and energy balance results for different bio-based diesel and jet fuel blendstocks; and (3) a physical units-based input-output model for translating feedstock inputs and biorefinery mass/energy balances into cradle-to-gate environmental metrics, including life cycle GHG emissions. Users to date have included researchers, consultants, bioenergy production companies, venture capitalists seeking to evaluate new projects, and startups seeking basic information on key cost and emissions drivers. The model is publicly available at lead.jbei.org.



COMMENTS

- I found this to be an excellent project. The goal of democratizing both the data and assessment capabilities for biofuel economic analysis and LCA is an outstanding one, and I am happy to see BETO supporting this work. Progress to date appears very strong, and the potential impact of the tool is quite large given the significant potential user base.

One suggestion I have for an area of future work would be to develop methods for characterizing the uncertainty in results. Both LCA and TEA carry inherent uncertainty that nonexperts in particular may not be aware of. Because this tool is designed to be public-facing, it is all the more important to characterize what is uncertain. I strongly encourage the project team to consider how this information can be communicated to users through data visualizations and other means.

- Thank you for the opportunity to review the Bio-C2G Model for Rapid, Agile Assessment of Biofuel and Co-Product Routes. This project is well aligned with BETO achieving its goals. The democratization of feedstock/site assessment, TEA, and LCA through web-based tools is a highlight of this project, and the downscaled results leveraging satellite data are impressive. The project has employed risk identification and mitigation strategies well and has integrated local impacts and disadvantaged community indicators, demonstrating a commitment to DEI. Although the model is deterministic and does not incorporate parameter uncertainty, the project is on track, and the progress toward the goals is commendable. The commercialization potential of the integrated web tool, along with the good outreach to industry, is significant and shows impact. Also, the flexibility in the tool will broaden its usefulness. Overall, this is an excellent project, and I commend the team's efforts.

  Disclaimer: I have still not gained access to verify the tool's features and performance (after the time period stated on the website). The presentation and the website stresses its accessibility, and I have found the opposite to be the case. During the next review, the team must create a working log-in for reviewers to access and assess the tool if it is claimed to be available.

- This project is an exciting addition to the technology area that draws upon a lot of existing expertise and previous work and makes significant progress in making that work accessible for researchers and the public. Further, it is a very flexible tool that allows users to input their own assumptions to develop analyses that fit their own needs. This project looks to be well run and designed, and it could have a lot of impact for a relatively low level of spending.

  The current, in-progress version of the tool already illustrates the potential of this project, and it offers a robust set of parameters to adjust. It will be helpful to evaluate at a later date when more pathways, particularly those with fewer major uncertainties in their TEAs and that are further from commercialization, are incorporated. To ensure the project's success, it would be helpful to develop a plan to make the tool easier for users to access (for example, could it be prominently featured on the KDF?) and to keep it regularly updated.

- The goal of this project is to democratize feedstock/site assessment, TEA, and LCA through web-based tools to help researchers and startups prioritize efforts and speed up the time to deployment for biofuels and bioproducts. Democratizing information and data in this way is essential in meeting BETO's goals and the deployment of different types of bioenergy technologies.

  The project has harmonized with others where appropriate (*Billion-Ton Report*, GREET, NREL grid scenarios), and a bit more information on what that looked like would make an even stronger case for the collaborative nature of this work.

  The project partners acknowledge that one of the risks involved is that availability does not match on-the-ground experience. To account for this risk, the team proposes to leverage deep-dive feedstock availability analyses in this and complementary projects. What does that feedstock availability analysis look like, and how is that incorporated in the model?

  Slide 7 is very helpful to show different types of feedstocks, end uses, and how they are modeled.

  The model is in a new phase that now includes EJ indicators; this is a very exciting and important direction. But it was not totally clear which variables are included in defining disadvantaged community status. The project partners are working to see if the EPA's Justice40 indicators of disadvantaged/not disadvantaged work for this application. Are there factors that shape disadvantages that are specific to bioenergy and land/use? The project team is working with other groups to determine what works best for this project.

Will these EJ factors be as accessible to users as the feedstock data? As a tool to help guide the siting of different types of bioenergy facilities, this model could be helpful. It is great to have this on an easily accessible public platform.

County-level data will allow for a granular analysis that will be useful for assessing both feedstock data and EJ indicators.

The project team says that their next steps are to work closely with key stakeholders to design tools and resources that de-risk deployment and ensure that facilities are good neighbors. The team plans to add location-specific information for bioenergy siting on preexisting environmental/health burdens and preexisting resource constraints (e.g., water). This is an excellent direction that attempts to consider how inequities from the past shape current conditions. This future research may shed light on how new bioenergy technologies interact with existing land use and socioeconomic histories. This is a very exciting next step.

As the project team may have already discovered, different EJ indicators and different ways of thinking about EJ can have very different outcomes, so it is good that they are considering which specific considerations might apply to bioenergy siting in this context.

- The approach of this project is excellent. The user interface is readily available and easy to use in a way that creates access to bioenergy data for non-power users of LCA/TEA models. The inclusion of EJ components are valuable and insightful.

  The road map for including location-specific parameters and local impacts will be useful in evaluating and understanding siting externalities.

  A couple of components would improve the impact of this project. Automating user account creation will speed access and usability. The PI should also measure and set goals for tool engagement, including page visits, account creations, tool use, and user demographic information. It is also important to implement user feedback mechanisms and a methodology for collecting a net promoter score to determine the overall satisfaction users have.

  This project should be awarded resources to fully fund the computational requirements for a growing user base with standard requests. While being scrappy is laudable, the tool will likely not achieve much use without standard uptime and responsiveness.

- The project team has done stellar work in making the BETO models more accessible to the public. The web tool is constantly being updated and clearly attracting interest, although the registration process can be made more straightforward (the project team cited security concerns). The team is encouraged to publicize the tool and further broaden its user base as well as collect more experimental data to validate/support the separation strategy tool.

PI RESPONSE TO REVIEWER COMMENTS

- We extend our thanks to the reviewers for their excellent questions during the review as well as the encouraging and constructive written comments. We agree that BioC2G offers unique flexibility and democratized access to feedstock and process simulation data that users can leverage to answer questions about feedstock availability, conversion costs, life cycle GHG emissions, and water use without having deep modeling expertise. Several comments centered around accessibility—namely, that the site requires new users to create an account before proceeding to use the tool. It has historically been our understanding that this was a cybersecurity requirement based on how we were hosting the site. While creating an account is free and should be fast, we recognize that this is an extra hurdle for new users. In addition to creating guest accounts to avoid future issues in the very near term, we are excited to say that we are planning to eliminate the account creation requirement, ideally within days or weeks. This will ensure accessibility and further expand our impact. In parallel, we will expand the set of user engagement metrics to track, and we will also communicate with BETO management about the possibility of linking to BioC2G from the KDF. Another important point raised by reviewers is the need to continually update feedstock availability in the bioenergy siting portion of the tool. One example of how this might look in the near term is the incorporation of updated manure availability based on a complementary deep-dive analysis that is ongoing at the University of California Berkeley. Another example is the potential inclusion of updated data from the forthcoming updated *Billion-Ton Report* and the *Roads to Removal* report. In all these cases, feedstock availability is either tied to a specific facility (e.g., a confined animal feeding operation or a materials recovery facility) or assigned to a county, at which point we can use satellite land cover data to approximate where it is located within that county (e.g., for crop residues such as corn stover or wheat straw). We provide a detailed table citing all the sources for our feedstock data on the website, with links to the original reports or data sets. Finally, we are glad to hear that the reviewers see value in our planned efforts to incorporate EJ. This is an exciting new direction for us, and we look forward to receiving feedback as these features and data sets become publicly available.

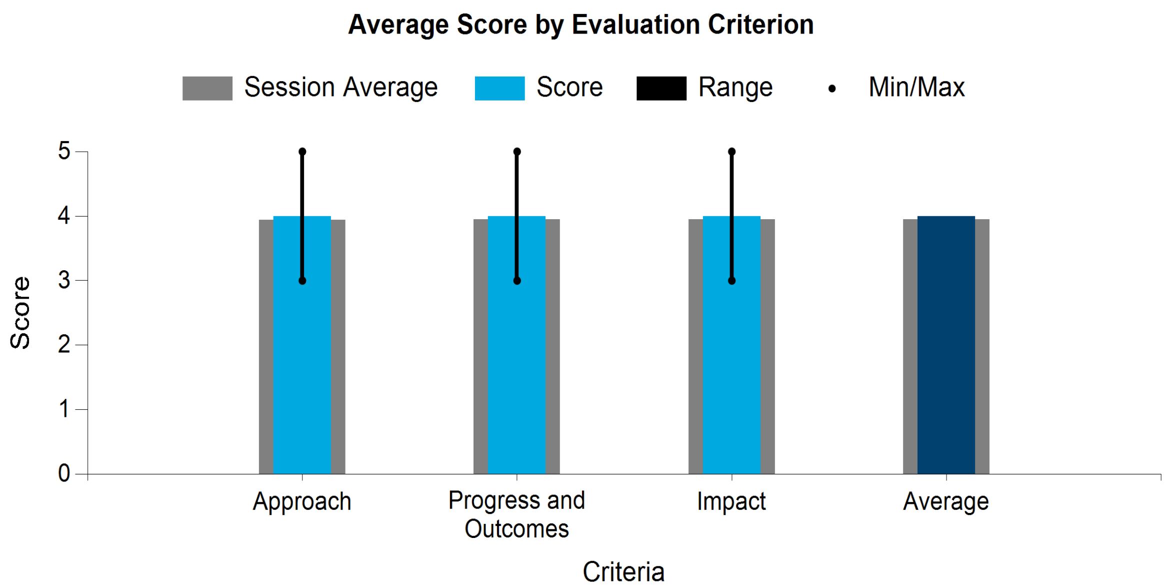
VALUATION AND VISUALIZATION OF WATER SUSTAINABILITY

Argonne National Laboratory

PROJECT DESCRIPTION

WBS:	4.2.1.10
Presenter(s):	May Wu
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,450,000

This project aims to develop science-based tools and metrics to understand the relationships between bioenergy production and water intensity, regional freshwater availability, water quality, carbon, the implication of alternative water use, and trade-offs. We develop models to characterize the interactions of carbon and water quality at the watershed scale; survey practices of water reuse in the United States; and identify gaps and opportunities of reclaimed water for bioenergy. The project delivers a set of analyses and data inventory to illustrate the impacts of water use and availability under future bioenergy scenarios using the spatially explicit Water Analysis Tool for Energy Resources (WATER) model. This work develops a new capability of the Soil and Water Assessment Tool – Carbon (SWAT-C) modeling, and a watershed LCA framework builds on SWAT-C, the FD-CIC tool, and GREET. The project's milestones and outcomes address EERE's decarbonization pillars in transportation and agriculture by identifying opportunities to reduce freshwater use and improve nutrient efficiency in low-carbon fuel production through enhanced conservation practices and the use of nontraditional water resources.



COMMENTS

- The approach of this project is well planned and excellent overall. The attention paid to building a strong network of collaborators is especially laudable. The project team appears to be making excellent use of the expertise of partners. The core aim of this work to create tools for integrating water quantity and quality into the LCA of bioenergy crops is an important research question deserving of support. This work could become critical to fully understanding the environmental impacts of bioenergy. This project has strong potential for policy impact. The results to date appear valuable to the regions that have been analyzed.

I am confused about why the capabilities being developed under this project are not being used in the current *Billion-Ton Report* update work. Water sustainability is firmly within the scope of the 2023 *Billion-Ton Report*, and this would seem like a significant missed opportunity. These capabilities seem well suited to evaluating where water sustainability constraints may bind biomass production potential as well as where there may be substantial cobenefits. I would encourage ANL and DOE to consider making use of these capabilities in the context of the 2023 *Billion-Ton Report*.

- Thank you for allowing me to review the Valuation and Visualization of Water Sustainability project. I believe this project is somewhat aligned with BETO's goals. I am impressed by the innovative approach of leveraging geospatial and other data sources to address the issues of nutrient, carbon, hydrology, and climate. Your investigation of operational changes for municipal water users given changes in water quality is very important. The progress toward goals is impressive, and the SWAT-C model seems to be performing well. The project's schedule is on track, and the team has completed several surveys and assessments. The findings on the impact of three conservation practices on SOC change, nutrient release, and GHG emissions are of significant value to bioenergy stakeholders; however, I recommend providing more information on the infrastructure investment required to use reclaimed water. The significance of the project is high in areas with a water deficit; however, I see the commercialization potential as low. I suggest packaging and providing management data sets from the project to stakeholders and reaching out to other water-interested agencies (EPA Office of Water) for possible collaborations/data.

- This project stands out from the rest of the projects in the technology area for its world-leading, extensive modeling of the water cycle and watersheds. The team's analysis of the water footprint and water availability appears to be well regarded and used by partners in government agencies, academia, and NGOs, particularly those concerned with water reuse. The team has also made meaningful progress across multiple fronts since 2021, particularly on water reuse and soil carbon. This project could also take on additional salience in the future as it is a key resource for DOE and BETO to evaluate the role of water impacts in equity concerns in some regions and identify strategies to mitigate those impacts. I was also impressed with the team's efforts to calibrate and validate the modeled findings with real-world data.

  One note of caution, however: From the presentation, I was concerned about the potential for scope creep and an expansion of the modeling capability from a dedicated water cycle tool to greater work on soil carbon flux, and it was not necessarily clear to this peer reviewer how SWAT-C was a natural extension of the modeling capabilities in SWAT. This could be expanded upon or better explained to make the connection, and better explain why this aspect of the analysis fits within this project.

- This project explores how to produce bioenergy in a manner that reduces impacts on regional water stress and water quality. The project connects to the decarbonization of the agricultural industry and feedstock production while also addressing an important aspect of any land-based energy system: water quality and quantity.

  In a case study of three land use practices in the Raccoon River Watershed-no-till, riparian buffer, and stover harvest with cover crops, the project team found that stover harvests at a 30% rate would lead to a decrease in SOC, and this reduction could be up to 12% in this watershed, but growing cover crops could recover SOC to a certain degree. These kinds of nuanced results are essential to understanding the full picture of the ecosystem dynamics involved in different kinds of bioenergy feedstocks.

  The next step for the project is to develop another SWAT-C analysis of another watershed. This will be helpful to compare the model outputs and functionality.

  The project also assessed the potential of using untapped reclaimed municipal water for bioenergy feedstock and agricultural crops in six states at the county level. The project seemed to incorporate information from large-scale survey work with municipal water treatment plants, but it could have been a bit clearer where this data came from and how it was integrated.

Modeling land, feedstock, water resource, and climate in a single framework is an ambitious goal, but what is obscured in this big picture approach? Case studies such as the Raccoon River Watershed allow for researchers to consider place-based dynamics that can contribute to various types of uncertainty embodied in abstract models.

The project involved strong stakeholder engagement through collaboration with water and agriculture agencies, public and private sectors, NGOs, and academia. Continuing this collaborative approach will help ensure the utility of this work.

- The research question is excellent. Understanding and minimizing the water stress and water quality implications of biofuels are key to the feedstock's usefulness and long-term availability.

  The link to Des Moines Water Works on an economic understanding of water impacts is a useful component of this program.

  Modeling SOC permanence has been somewhat difficult. The model could be improved with consistent ground truth data over time. While likely already partially addressed by the model, a deep exploration of cover crop impacts on water and carbon would greatly benefit growers, watersheds, and supply chains as they make decisions about practice changes.

- This project investigates the important but often overlooked water resource issue for the bioeconomy. It is exciting to see that the project team considers the water needed for the entire value chain, is working with a lot of water/wastewater utilities, and makes the models/tools accessible. But existing work still seems very much focused on traditional feedstocks, such as corn and soybean, and water constraints developed from this project do not seem to be incorporated in the upcoming *Billion-Ton Report*. The team should start exploring work for new feedstocks, such as perennial grasses, and BETO should consider water resource limitations when presenting the potential feedstock availability.

PI RESPONSE TO REVIEWER COMMENTS

- We express our gratitude to the reviewers for their positive comments and words of encouragement. We are delighted to learn that our project's approach, particularly the establishment of a network of collaborators, has yielded positive outcomes. We fully agree with the reviewer that conducting a water sustainability assessment for the 2023 *Billion-Ton Report* falls within the purview of sustainable feedstock resource development. Moving forward, we remain committed to enhancing our modeling and analysis capabilities and to actively seeking feedback from industry and federal agency partners. Our aim is to effectively address crucial water resource challenges, contribute to policy studies, and facilitate decision-making processes in the field of bioenergy and bioproducts. We acknowledge the importance of including information on the infrastructure investment required for utilizing reclaimed water. In fact, we have dedicated a subtask within our project specifically aimed at analyzing the transport logistics of water resources considering the potential challenges associated with supplying reclaimed water for biofuels. Further, we fully recognize the significance of effective communication with stakeholders and the necessity of collaborating with the EPA Office of Water. We understand that their expertise and involvement are vital to the success of implementing reclaimed water applications in the field of bioenergy. To ensure the broad dissemination of our study and to engage with a wider audience in the water sector, we plan to release our findings through a water reuse symposium platform, thereby reaching various stakeholders in the water industry.

  Note that our current engagement with the EPA's National Water Reuse Action Plan lays a solid foundation for fostering increased collaboration. By sharing the synthesized information from our project, we believe that our work can effectively benefit the ongoing efforts of the EPA's National Water Reuse Action Plan initiative and support their endeavors in promoting water reuse. Again, we appreciate the reviewer's valuable feedback, and we are committed to incorporating these suggestions into our project to enhance its overall impact and success. It brings us great satisfaction to know that our analysis and modeling work has made a meaningful contribution to the field of water sustainability in bioenergy development and has reached a wide range of audiences and stakeholders. We fully concur with your perspective that the water analysis capacity developed through this project is well equipped to explore the role of water impacts in equity concerns within specific regions. Further, we recognize the importance of identifying strategies to mitigate these impacts in the context of bioenergy production. We remain committed to advancing our understanding in these areas and working toward sustainable solutions.

The reviewer's comment regarding the inclusion of SWAT-C as a natural extension of the modeling capabilities in SWAT and its alignment with the project is highly insightful. SWAT is a process-based watershed model that effectively considers nitrogen, phosphorus, and hydrological cycles to characterize land, water, land covers (such as crops, grasslands, and forests), and urban areas within a watershed. While SWAT already incorporates carbon elements in plant growth and N_2O emissions, the carbon cycle was not exclusively simulated because the primary purpose of the SWAT model was nutrient loss modeling in agriculture; however, recognizing the significance of carbon in plant growth and the potential implications of land use for feedstock production on the life cycle carbon intensity of biofuels, researchers have increasingly acknowledged the need to integrate carbon dynamics into models that assess carbon, nutrient, sediment, and water interactions at the watershed scale. Unfortunately, such comprehensive models with extensive U.S. agricultural data were previously unavailable. In recent years, the USDA has expanded the capabilities of SWAT by incorporating the carbon cycle, thus enabling the model to account for carbon, nitrogen, phosphorus, water, and soil loss in the context of bioenergy and agricultural crops. By utilizing SWAT-C, the project aims to provide BETO with a comprehensive understanding of the impact of bioenergy at the watershed scale, thereby adding a new capability to BETO's portfolio. The information generated through the examination of various management practices and landscape designs will offer valuable insights to support decision-making processes for growers, regional watershed management, and conservation groups. While the inclusion of soil carbon and GHG emissions analysis represents additional benefits to BETO, it is important to emphasize that the project's primary focus remains on water quality and water resource assessment. The integration of carbon capacity into the watershed modeling framework serves as a complementary aspect that enriches the project's overall scope and objectives.

We acknowledge that strong engagement with stakeholders throughout this project has been instrumental in grounding our assumptions and research plan in practical experiences. We appreciate the opportunity to provide clarification on the data sources and integration process for the water reuse survey. It was indeed a complex undertaking due to the variations in data collection practices among wastewater districts and individual facilities, both at the state level and within each state. Because there is no comprehensive county-level database available for the entire United States, we approached each party individually, considering the availability and storage methods of their data. Additionally, during further analysis, volumes of stormwater direct reuse were excluded from the reuse data because these volumes are not part of publicly owned treatment works effluent. The annual facility reuse data were aggregated at the county level. By subtracting the reuse flow from the total publicly owned treatment works effluent flow, we obtained the net available reclaimed water flow for a specific year and county. The resulting flow data from recent years (2019–2021) were used for the bioenergy analysis. We hope this clarification provides a better understanding of the data collection and integration process for the water reuse survey. The water framework primarily focuses on environmental and land management factors, which are interconnected (e.g., climate, soil, water, land covers, land use, and practices) because it is essential to consider these factors holistically. Assessing one factor without considering the others would not provide an accurate understanding; however, the framework does not emphasize economics and social factors because several other projects within BETO address these aspects. Note that social and economic factors are influenced by environmental factors and land use practices; therefore, the outputs from this project provide highly relevant information for the work undertaken by BETO and other stakeholders in these areas.

With regard to the comments on model uncertainty, we completely agree that all models, regardless of the scale, contain uncertainties. To address this, the SWAT-C model includes a model quality evaluation step during calibration and validation, which allows for the assessment. We value the reviewer's feedback and have taken it into account to ensure the accuracy and reliability of our findings. Our objective was to develop high-resolution, meaningful, and practical results that can effectively support decision-making processes for producers operating in regions with specific climate, soil, and water conditions. We fully agree that ground-truthing the model is crucial for verifying the accuracy of soil and water quality simulations, and we have actively sought multiyear measurements to achieve this. We have collaborated with the USDA Agricultural Research Services, the U.S. Geological Survey, the EPA, as well as regional and local soil and water conservation groups in the watershed to gather field-monitoring data over time. Further, we share your view on the significant benefits of cover crops. Our watershed modeling work for the Raccoon River Watershed, South Fork of the Iowa River, and the Iowa River basin during the past decade has consistently demonstrated the excellent performance of cover crops in reducing soil loss as well as nitrogen and phosphorus runoff at the watershed scale. We agree that further understanding the impacts of cover crops on water and carbon interactions will provide valuable insights for farmers when making practical decisions. Thank you for highlighting these important aspects, and we remain committed to incorporating field-monitoring data and evaluating the benefits of the best management practices in our project to ensure its relevance and applicability in bioenergy production.

We would like to clarify that while this particular review emphasizes our efforts during the past three years, our team has been actively involved in water analysis for cellulosic feedstocks since 2007 with the support of BETO. We have conducted extensive research on the water footprint and water availability of various cellulosic feedstocks, including corn stover, wheat straw, perennial grasses such as switchgrass and miscanthus, forest wood residues (both hardwood and softwood), woody crops, and algae. Further, we have assessed water sustainability for the second *Billion-Ton Report* scenario in 2011 (BT2) and the third *Billion-Ton Report* scenario in 2017 (BT16). The results of these county-level analyses are accessible on the WATER model website (http://water.es.anl.gov). We fully agree that considering water resource limitations is crucial when evaluating the potential feedstock availability for biofuel production. Looking ahead, we are actively considering the development of water assessments for the 2023 *Billion-Ton Report* update scenario in our upcoming project cycle. Your feedback aligns with our goals, and we appreciate your acknowledgment of the importance of water resource analysis in biofuel development. We remain committed to advancing our understanding of water sustainability and its implications for bioenergy feedstocks.

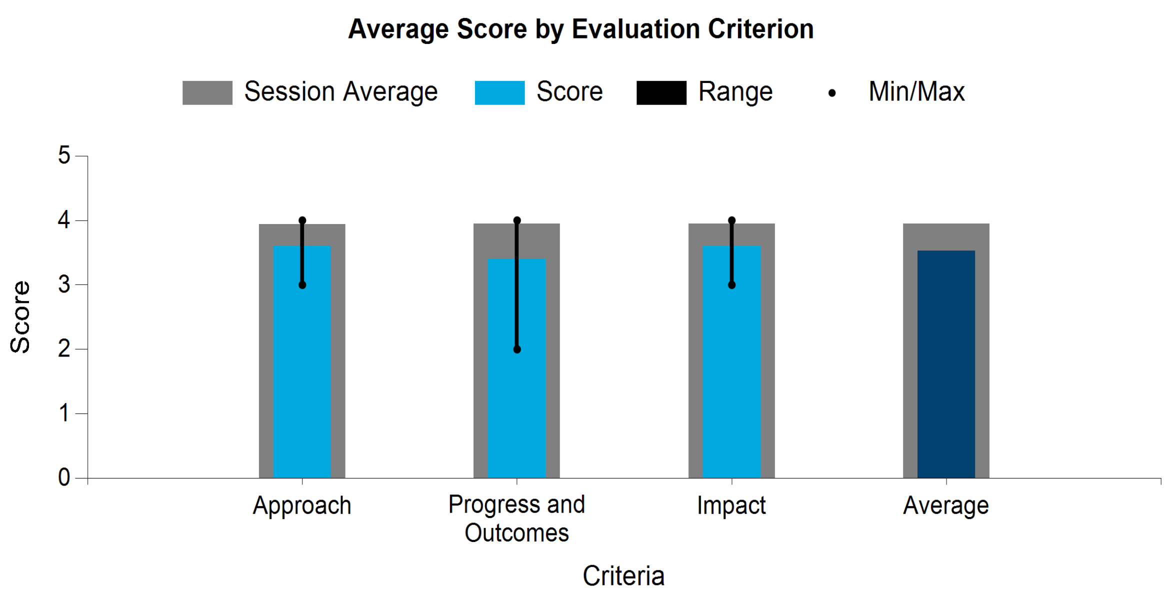
INTEGRATED LANDSCAPE MANAGEMENT

Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	4.2.1.20
Presenter(s):	Damon Hartley
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$900,000

The primary focus of the Integrated Landscape Management project is to develop modeled pathways to augment bioenergy feedstock supply practices with established supply chains such as traditional agricultural production systems. It is intended that potential pathways yield economic and environmental improvements while supporting an emerging bioeconomy. The Integrated Landscape Management project was initially focused on the utilization of modeling to show that a viable strategy may be to integrate lignocellulosic biomass production practices into agricultural production fields via sustainable crop residue harvest, collection, and dedicated energy crop cultivation in suitable field areas. For the last two years, the Integrated Landscape Management project has focused on extending beyond the production of herbaceous feedstocks to include woody resources. The extension began with integrating short-rotation woody crops into agricultural production systems that are near areas of high concentrations of forest and forest operations. Short-rotation woody crop materials would likely more easily integrate into systems developed to use the forest resources, extending further beyond the farm and into the forest. The project examined using a landscape management approach to evaluate management strategies that can be used to maintain forest health and productivity. The Integrated Landscape Management project was last merit-reviewed in 2020 and is entering its last year of the current three-year cycle and will be merit-reviewed again in FY 2023.



COMMENTS

- The expansion of this project into woody feedstocks has led to some good research. Developing tools suited to evaluating site suitability for short-rotation crops fills a significant research need. The work to estimate ideal depot locations also seems to have strong potential impact. In particular, though, the work to estimate the impact of biomass removal for fire mitigation seems both timely and of great interest to stakeholders and decision makers. If the project staff can succeed in getting these tools into the hands of stakeholders (as their presentation suggests they are trying to do), this project could prove highly influential in the development of biomass production systems that are coupled with fire mitigation efforts. I also applaud the planned steps to next assess the carbon impacts of woody and herbaceous systems.

- This project has a very clear purpose in its current iteration—to expand on an existing modeling framework for herbaceous feedstocks and apply it to woody biomass and wastes. The project looks like it is making important progress incorporating many woody biomass-specific dynamics into its framework, particularly wildfire mitigation, illustrating the potential to develop a valuable method of determining where it would be most effective to collect woody biomass and implement forest management practices that would simultaneously reduce fire risk.

  There is already good progress on the project, with promising results on shifts in fire risk based on implementing practices. As with other projects of this type, I would recommend additional efforts to ground truth and validate the modeling outcomes. This project also appears to have had some impact already, with two industry partners interested in using the model.

- This project seeks to maximize feedstock production in diverse landscapes, municipal solid waste, woody material, and agriculture. The project team first focused on cultivated perennial energy crops, such as switchgrass and miscanthus. In FY 2021, they shifted to expand beyond agriculture and herbaceous feedstocks to include additional feedstocks, such as woody material, which is what is being reviewed here. The project developed a modeling framework that can simulate forest and biomass supply impacts from the application of management activities. I am curious to know more about how these modeling efforts account for different silvicultural applications. Also, what scale of analysis was used?

  To what extent, if at all, might the use of forest residues compete with other forest product industries, such as pulp and paper markets, pellet markets, or emerging markets for biomaterials, cross-laminated timber/mass timber?

  The project partners state that DEI was not a formal goal of this project, but success in this project will help rural businesses and increase the wealth in rural communities. This seems intuitively true, but what metrics support this?

  Site suitability focuses on biophysical constraints—what about social availability? Who owns the land, and how willing are they to grow cultivated perennial energy crops or supply forest residuals?

  Making these models accessible and useable for stakeholders seems particularly relevant and important given the project's objectives.

- The approach in this project is thorough and thoughtful. The idea that biorefineries would be somewhat biomass agnostic and would need tools to identify what is available, environmentally useful, and economically viable is an interesting future posit. Detailing the connection and collaboration with industry to confirm that they find this tool robust and useful would be a great next step.

  The patent and potential licensing of CropAIQ is tangible indication of the usefulness of the model.

  The inclusion of the proximity to transportation nodes and clusters of suitable fields makes the output of this program more likely to reflect on-farm realities and will likely help to overcome logistical complications a plant may experience in implementation.

- Despite the project name (Integrated Landscape Management), this project seems to focus only on woody biomass without considering other feedstocks (e.g., grasses), and the discussion was mostly about fire management. The PI did mention a larger project that will look at a portfolio of feedstocks to maximize the energy yield from a unit of land and other related projects that will work with stakeholders such as farmers, but those projects could not justify the significance and impacts of this project, and the current progress and outcomes are not impressive. Additionally, it seems that the main route for this project's impacts is through publications and software repositories, which is very focused on academia despite the potential of this project's impacts on a larger scale; therefore, the team is encouraged to design future activities that can be applied to broader areas and to get more stakeholders involved.

PI RESPONSE TO REVIEWER COMMENTS

- The Integrated Landscape Management project has been actively working on the concept of incorporating the production of biomass into traditional management practices for nine years, with the first eight years of the project working in the area of developing strategies to incorporate dedicated energy crops into agricultural landscapes, and seven of those years focused on establishing perennial grasses in agricultural settings in addition to collecting crop residue. Because of the heavy focus on perennial grasses and crop residues in the early stages of this project, to become a truly integrated landscape management project, we needed to expand beyond agriculture, perennial grasses, and crop residues into other landscapes and feedstocks. As we begin to expand into the forestry area, we must develop a new set of tools to be used for analysis and design, and for this reason, the project does not currently have outputs that are at the same level as the outputs we previously had in the agricultural space, such as CropAIQ, which was awarded a patent in 2020; however, we aim to match the significance of the work that we have done in the agricultural domain with our forestry work. The planned focus of this work is to understand how management activities within the forest can be used not only to manage fire risk but also to contribute to carbon sequestration. Within this work will be the evaluation of different silvicultural systems based on current and future stand conditions, which will include the impact of markets on the products produced and an accounting of carbon that is sequestered in long-lived forest products. Our interest is to have tools that we can use to examine large regions and potentially national-level potentials of biomass production and carbon sequestration, but the tools that we are developing are modeling forests at the stand level and will ultimately be useful to forest landowners and managers to design management strategies for their landholdings.

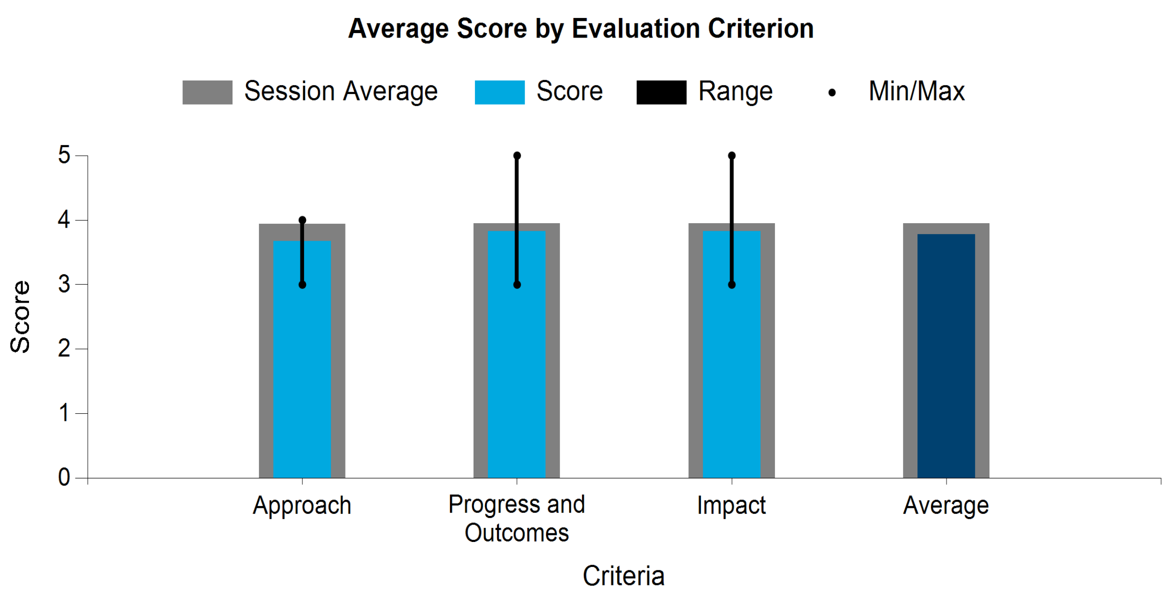
BIOFUELS AIR EMISSIONS ANALYSIS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	4.2.1.30
Presenter(s):	Vikram Ravi
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$600,000

The United States has goals to produce 3 billion gallons of SAF annually by 2030, increasing to 35 billion gallons by 2050 to decarbonize the aviation sector. Meeting these production targets will require setting up large numbers of biorefineries; however, the ability to comply with federal air quality standards is a prerequisite to being issued a construction permit. Negotiating the permitting process for a new biorefinery can be quite onerous and cost the investors significant time and money. Although there can be numerous reasons for delayed biorefinery construction, air permitting is fraught with pitfalls because the permitting process relies on precedence, which the future SAF biorefineries lack. NREL's Biofuel Air Emissions Analysis project is unique and innovative in terms of the tools, approaches, and analyses provided. NREL is the only national laboratory that is actively working at the intersection of federal air quality regulations and emissions and air quality analysis across the supply chain, including process design cases. This project is focused on providing much-needed data and analyses that address biorefinery air permitting. This project develops models and quantitative analyses, and it measures progress toward meeting air quality regulatory requirements. These models and methods have been applied to analyze the air permitting process related to wastewater sludge-to-biofuel conversion pathways using hydrothermal liquefaction (HTL) and study the impacts of the HTL pathway on local and regional air quality, including an assessment of health and equity impacts. In addition to filling research gaps, this project disseminates the findings to the relevant stakeholders at BETO, other national labs, and regulatory agencies.



COMMENTS

- The motivation for this research—helping biorefineries demonstrate compliance with federal air quality regulations—is laudable. I agree with the project team that such analysis would be highly useful for future biorefineries. The potential for impact is significant. Overall, I think the approach and progress to date are also good. One area where I would like to see more thought is regarding how biorefineries might be able to use these tools in conversations with federal air quality regulators. As the presenter said during the question-and-answer period, it is still unclear how results from this modeling workflow could be used in regulatory applications. I strongly encourage the researchers to continue engagement with the EPA's air quality and health effects modeling efforts to think through this important question.

- Thank you for the opportunity to review the Biofuels Air Emissions Analysis project. The project is reasonably aligned with BETO achieving its goals by providing data and information for the biorefinery air permitting process and helping the industry design processes that minimize impacts on the environment and communities. The project also includes important DEI considerations, and the advisory board is well connected with industry and regulators, including both Exon and the California Air Resources Board. The project's opportunity for improvement lies in updating FPEAM data inputs to make them more current (or allow for other sources of these model inputs). This would enable the assessment of the air impacts of other model results. Also, the PIs could consider more discussions with staff from the regulatory agencies to ensure that what is recommended to stakeholders would fulfil requirements. Thanks, and all the best going forward with this important project.

- This project nicely complements BETO's increased focus on equity by evaluating the potential risks of the bioeconomy to local air quality in finer detail and evaluating mitigation strategies. The modeling framework presented here was well designed and showed flexibility to evaluate different processing technologies. This has natural potential to integrate with any of BETO's work focused on new refinery siting.

  This project points to a potentially significant equity issue—that existing, centralized upgrading points would not be subject to air quality permitting. It would be helpful if, beyond siting new facilities, this work could be coordinated to identify mitigation strategies and opportunities for existing biomass processing.

- The goal of this project was to create industry design processes that minimize impacts to the environment and communities in the development of future biorefineries with an emphasis on air quality permitting. The project partners mentioned informing the stakeholders—are there ways in which feedback from the stakeholders has been incorporated into modeling and analysis?

  One reviewer mentioned that the project could include a more robust approach to stakeholder engagement and connections across other DOE modeling efforts. The project team has continued to communicate with teams at other national labs, but what about other affected stakeholder groups outside of research teams? This still seems like an important direction for the project.

  The breakdown of health impacts by race in different regions is helpful in showing disparate impacts. The project team should continue to work on developing these kinds of equity metrics related to air quality as it relates to distributive justice. It would also be interesting to look into procedural justice issues (decision-making process issues) and recognition justice issues (how past conditions inform the future).

- This project is important to the BETO portfolio because it works on the permitting pathway for the construction of biofuel facilities. This work is scaffolding that enables the faster implementation and production of low-carbon fuels.

  This work can be made more accurate and inclusive by allowing for variable feedstock scoring dependent on actual recorded farm practices, not regional or county averages. This is important for two reasons: First, farm practices can widely vary between farms, and by allowing for actuals, it can incentivize the adoption of better-than-average practices. Second, this can allow for farmers to be participatory in the evaluation and understanding of the models that are assigning them environmental impact metrics. This type of ground-truthing can end up improving and extending the models to be more representative.

- This project considers the impacts of on-site air pollutant emissions from biorefineries. The outcomes from this project include the open-source FPEAM (already publicly available) and contributions to other federal agencies or industries on the health impacts of biorefineries. It is meaningful work to provide inputs on the overlooked health impacts of the bioeconomy, especially for disadvantaged communities. But better approaches can be used for more accurate and impactful results (e.g., measuring the actual air emissions from pilot facilities rather than modeling using literature data, engaging with permitting agencies on the types and methods of pollutant tracking).

PI RESPONSE TO REVIEWER COMMENTS

- While not all tools and analyses developed as part of this project are designed for a regulatory application, we can explore ways to more effectively communicate how findings from the project can be used in a more suitable manner by the industry to lessen the permitting burden. We will continue to engage with the EPA's air quality and health modeling efforts.

  The logistics modeling component of FPEAM was recently updated to the most recent version of the EPA's Motor Vehicle Emission Simulator (MOVES) model, and we plan to update some underlying FPEAM data based on scenarios for the next *Billion-Ton Report*. We will continue to engage with various stakeholders on how our data, tools, and analysis can be made more robust.

  Regarding the concerns about "potentially significant equity issues" at centralized upgrading points, there will be permitting requirements for these sources per the prevailing regulatory environment as prescribed by the permitting agency. Analysis only suggests that no major source permitting is required unless the facility is located in a serious, severe, or extreme area of nonattainment for ozone.

  Thank you for the valuable comments and feedback. We will explore ways to further improve stakeholder engagement. Thank you for highlighting the value of distributional justice analysis, which aligns with the prospective analysis done as part of this project. Other projects have engaged in procedural and recognition issues, and we can explore how our work aligns with their analysis.

  We use the best available data within the project's constraints, and we will continue to improve our data as suggested by the reviewer. We agree with the reviewer that a local scale analysis (not the focus of the project's presentation during the Project Peer Review) can be improved by accounting for local farming practices that can influence analysis outcomes, although it can be a very resource and time-intensive exercise.

  The HTL analysis presented for the Project Peer Review does not have any measured emissions data available as of now, and most specific pathways we analyze have no real-world examples available that will be applicable at the same size and scale of the facilities for which we perform analysis. For these reasons, we use the best available estimates based on modeling and literature estimates, and we perform an evaluation of our emissions estimates where possible (and will continue to do so, as suggested by the reviewer).

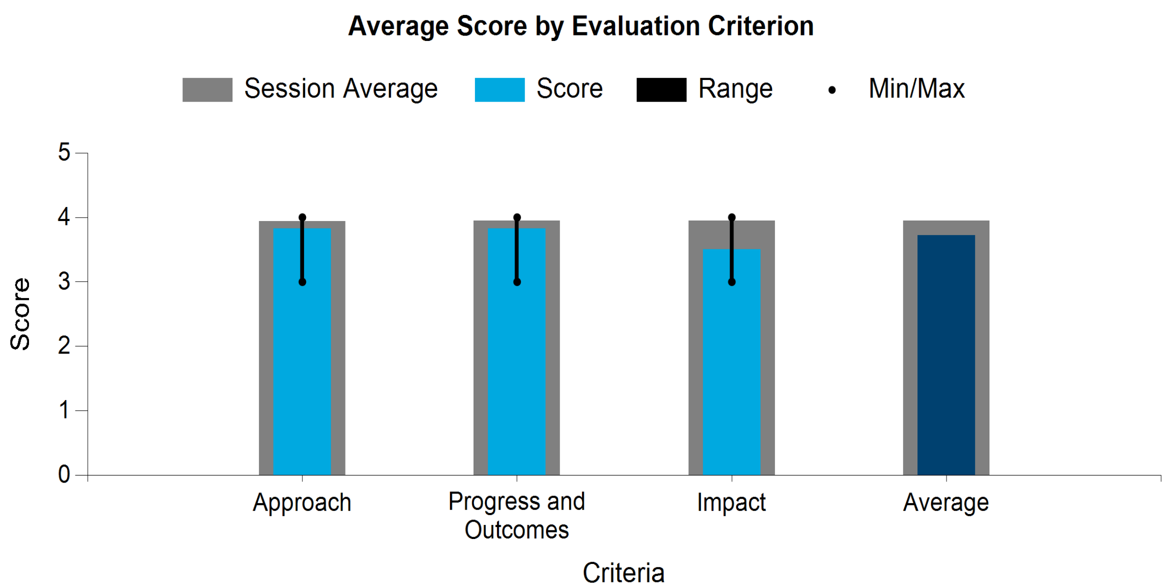
ENVIRONMENTALLY EXTENDED MULTI-REGIONAL PROJECTION OF LIFECYCLE AND OCCUPATIONAL ENERGY FUTURES (EMPLOY)

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	4.2.1.31
Presenter(s):	Andre Fernandes Tomon Avelino
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,200,000

This project provides BETO with strategic decision support for the evaluation of its R&D portfolio and future decarbonization scenarios by developing, validating, and applying a coherent methodology and consistent economy-wide model framework to quantify the net effects of an expanding U.S. bioeconomy. The framework fills an analysis gap previously identified by the Project Peer Review and supports a related milestone in BETO's Multi-Year Program Plan. The model complements pathway-specific TEA and LCA using a top-down framework to compute environmental, resource use, socioeconomic, and occupation metrics, and it provides retrospective (2002–2017) and prospective (2020–2050) economy-wide assessments for individual technologies or technology portfolios with regional-level detail to determine the trade-offs between deployment strategies for bioeconomy commodities. Presently, EMPLOY covers several commercial and near-commercial biofuel routes, including SAF, and an emerging pathway for plastics upcycling. EMPLOY has provided analyses for the *Third Triennial Report to Congress* on the environmental effects of the RFS, its results have been cited by the EPA's regulatory impact analysis for a proposed rule change in the RFS 2023–2025, and its capabilities have been presented to members of the aviation industry.



COMMENTS

- Economy-wide modeling perspectives on U.S. bioenergy are few and far between. It is a gap that needs to be filled, and I applaud DOE for funding research in this area. I think the model is choosing appropriate areas for development, expanding biofuel pathway representation and improving geographic resolution. Including a rest-of-world aggregate will also be an improvement. There are clearly areas where this model could be used for DEI-relevant work through the analysis of socioeconomic impacts, as shown in slide 9 of the presentation. The project does appear to have a very broad scope. Attempting to cover economic and workforce impacts at the same time the researchers are building out a biophysical representation of environmental impacts is a lot; however, I am encouraged that the researchers are linking to bottom-up models rather than trying to endogenously incorporate so much scope. I would encourage them to think about where their value add lies and not try to take on more than that.

- Thank you for the opportunity to review the EMPLOY project. This modeling project is reasonably aligned with BETO achieving its goals, particularly with expanding U.S. bioenergy and investigating the impacts on the economy. The plans for the incorporation of state-level energy policies and dynamic consumption structure/relationship to socioeconomic forecast assumptions are positive aspects of the project. The model's consistency across input sources is a critical issue that the project has addressed well with consistent assumptions in the baseline. Although the project plans to achieve DOE goals, the scale may have issues for incorporating different EJ analyses. Also, the mix of GAMS and R programming language makes it difficult to disseminate and could have accessibility issues; however, the project is an ambitious and useful tool that takes advantage of BETO's available models and data sources.

- This project is well timed and well suited to the priorities of BETO because it connects the bioeconomy to the recent focus on the socioeconomic risks and opportunities of the bioeconomy. The authors have focused on providing critical information to guide policymakers and has already been used in high-profile applications, such as the EPA's RFS *Triennial Report to Congress*. The key outputs that are particularly compelling include employment impacts and spatial trade-offs for pollution.

  One area of concern is the sheer complexity of the model and the risk of overreaching, particularly as the model tries to balance a complex set of economic and physiochemical processes. It would be helpful to more clearly demonstrate where the model is filling in new gaps and where the model outputs may be redundant with separate models, particularly on pollution estimates. Ideally, the model could be aligned with or integrate the results of those outside models and can focus on its key strengths and added value to the program on social and economic indicators.

- This is an ambitious project that covers multiple sectors to assess environmental and economic impacts. I agree with the 2021 reviewer that if the goal is to capture socioeconomic effects, a more diverse range of indicators could be incorporated. Adding labor and workforce metrics was a good initial step to understanding the potential economic benefits; I wonder if there are other metrics to address equity impacts in terms of workforce issues.

  Expanding the spatial dimension from the national to the state level to highlight regional trade-offs of specific pathways and decarbonization strategies is good, but it would be interesting to break that down into even finer-grain analysis to look at local impacts. Census track data are readily available, or county-level analysis could be useful. This seems especially important given the initial findings that discuss rural versus urban differences, and it is consistent with BETO's goal to increase regional studies and regional data. This would also allow for a better understanding of disparate impacts.

  It would be good to get the EMPLOY model in an accessible form that could be useful for decision makers and also to account for climate change and potential policy changes.

- Overall, this project is ambitious in scope and impactful in use. It has a strong connection to supporting policy decisioning and impact with the EPA and SAF Grand Challenge connections.

  The difficulty of modeling the Inflation Reduction Act policy was acknowledged in the presentation because of the way it impacts supply shock as opposed to demand shock. If possible, the model's accuracy should be tested against historical data on supply shocks to determine its ability to predict the effects of supply shocks on the economy.

The use of future models that incorporate climate change should be explored as this will provide policymakers with a more accurate picture of the future economic landscape. It is recommended that the model be updated when new climate change models become available and that its performance be tested against real-world data.

- The project has clearly defined goals, intermediate targets, and expected outcomes. It leverages process-based models and includes retrospective (with validation through back-casting and comparison with historic data) and prospective analyses. It considers multiple environmental impact categories (i.e., not only limited to GHG emissions); however, the use of the Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) also leads to potential inconsistency/incomparability with other models, such as GREET (e.g., GREET updates the N_2O- and CH_4-to-CO_2 with Intergovernmental Panel on Climate Change reports, whereas TRACI has not been updated for a long time). The project team also considers multiple scenarios based on the *Annual Energy Outlook* report. One strength of this project is the consideration of workforce development, which enables the model to consider how the expansion of the bioeconomy would affect urban and rural communities and contribute to EJ and DEI. One major caveat of this project is that the model is not publicly available (and the model uses GAMS, a commercial tool that requires a commercial license to use), which greatly limits the user basis, makes it very hard to assess the underlying assumptions and approaches, and creates difficulties in gathering constructive comments and feedback.

PI RESPONSE TO REVIEWER COMMENTS

- The EMPLOY team thanks the reviewers for their time, constructive comments, and suggestions provided during and after the presentation. EMPLOY aims to provide an economy-wide perspective to the introduction of new energy technologies in the United States, thus revealing indirect impacts and their trade-offs across sectors and regions in terms of economic, environmental, and resource use and workforce metrics. These results can then be used to study strategies to mitigate negative effects and increase positive ones. EMPLOY models the interactions between all sectors of the economy, and therefore its complexity and data requirements significantly increase at finer spatial scales. Primarily due to public data availability, the model is being developed at the state level. The team understands that to better highlight EJ implications, a finer spatial scale (such as at the census tract level) is essential. EMPLOY's EJ goal is to provide initial insights in terms of direct and especially indirect EJ effects across sectors throughout the United States, whereas most EJ models focus on localized direct effects. Due to the spatial scale of the model, equity metrics besides workforce ones might be difficult to evaluate. Nonetheless, we will explore the possibility of adding additional EJ metrics or linking EMPLOY's output to finer-scale NREL models, such as InMap. As part of the calibration process for EMPLOY, we perform a back-casting estimation against historic economic data to check for model fitness. Future shocks are based on external models, such as the BSM, which is also validated against real-world data; hence, this process is used to measure the degree of confidence in our estimates. Nonetheless, forecasted results from EMPLOY in FY 2024 will also include a sensitivity analysis across inputs to create ranges around our estimates. In FY 2025, the model will be expanded to account for international trade, thus revealing the importance of global supply chains to the growth of a domestic bioeconomy. At that stage, we will explore the possibility of connecting to a climate change model to create external supply shocks. Additionally, although the model currently uses TRACI characterization factors, those can be updated by incorporating other data sets, depending on DOE's preference. Due to the complexity of EMPLOY as well as data requirements and connections to other NREL models, currently, the model is not designed to be publicly available but to be used internally by DOE and NREL. Nonetheless, the team is always improving the model's codes, and we will explore the possibility of having our optimization routines in the same coding language as the rest of the model (R language) for efficiency and better workflow. Additionally, the team is currently drafting a manuscript with EMPLOY's modeling framework for submission in a peer-reviewed journal, and we will publish additional peer-reviewed papers with future model developments and results.

VISUALIZING ECOSYSTEM SERVICE PORTFOLIOS OF AGRICULTURAL AND FORESTRY BIOMASS PRODUCTION

Oak Ridge National Laboratory

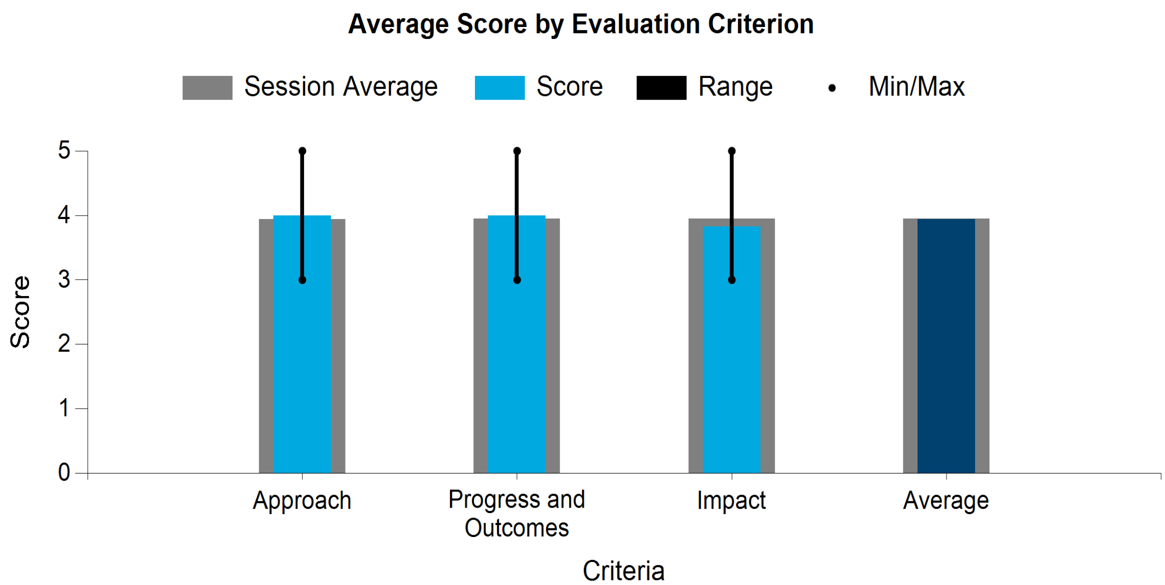
PROJECT DESCRIPTION

WBS:	4.2.1.40
Presenter(s):	Yetta Jager
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,250,000

Our project seeks to quantify pathways to producing biomass feedstocks with high potential value for producing ecosystem services. We met our go/no-go milestone by determining that the value of ecosystem services in riparian buffers of the Mid-Atlantic region converted from growing annual crops to switchgrass and coppice willow exceeded 25% of fixed production costs. We modeled ecosystem services, including increased SOC, reduced N_2O emissions, and reduced runoff of total nitrogen and phosphorus. The Biofuel Infrastructure, Logistics, and Transportation (BILT) model optimized ethanol refinery locations for these feedstocks, supplemented by forest residues. Our analysis suggests that 90% of carbon (19.4 Mt CO_2) could be avoided by using high-ecosystem services-value feedstocks while avoiding sensitive areas where air pollution concerns are high. ANL used these inputs to conduct an LCA using GREET in which ethanol achieved >82% GHG reductions compared to gasoline.

Beyond the results associated with key project milestones, we have produced the following results:

1. In the Arkansas-White-Red basin, we estimated that water quality improvements exceeded production costs for nearly half the cellulosic biomass supply, offsetting more than 20% of the 3-billion-gallon target for SAF.
2. A preliminary assessment of animal wastes showed that on average 18% of total nitrogen (20,859 Mg) and 21% of total phosphorus (2,276 Mg) could be removed if all manure were collected to produce RNG.
3. We completed climate flood risk modeling and used it to assess avoided insurance costs when planting perennial feedstocks. Preliminary estimates suggest an increase in average avoided costs from approximately $48,000 (current) to $54,000/county/year due to increased flooding under future climate conditions.



COMMENTS

- Tools to assess and monetize the potential ecosystem service benefits of biomass production and tools to help site future biorefineries in light of the potential positive and negative impacts seem like worthy scopes. Quantifying the potential revenue and impacts of riparian buffers and flood management could both provide strong value to stakeholders.

  The planned next steps for this project seem logical and potentially highly impactful. I especially applaud the efforts to make these tools publicly available. Because the researchers are seeking feedback on potential continuations, I will offer two. Further analysis of the potential impacts of producing RNG from manure digesters on water quality is extremely timely given public debates in this area, and it could have a strong impact. The ability to provide inputs to EJ decision tools for evaluating biorefinery siting may also be impactful. Providing stakeholders with tools and insights in both areas would be excellent for further work.

- Thank you for the opportunity to review the Visualizing Ecosystem Service Portfolios of Agricultural and Forestry Biomass Production project. Based on the information provided, the project is well aligned with BETO's goals. I was impressed with the progress made thus far, particularly on the development of BioVEST and the creation of geospatial maps. The web tool for stakeholders, BioVEST, hosted on the Posit platform, is an excellent impact outcome. It was easy to use and was very accessible. One area for potential improvement is to consider focusing outreach efforts on bioenergy companies in addition to landowners to increase impact. Overall, the project appears to be on schedule and has made significant progress toward achieving its objectives.

- This project provides a very valuable theoretical component to drive the use of cellulosic energy crops, assessing their suitability for ecosystem services and assessing the value of those benefits. This complements the objectives of BETO well because it could help to improve the cost-benefit calculus for one of the most abundant sources of biomass necessary for broader DOE objectives, such as the SAF Grand Challenge. The approach used here was both regionally and technically well differentiated from other projects to reduce redundancy with other projects within the technology area, and it provided a comprehensive basis to inform potential producers of the value of energy crops and the siting of potential biorefineries.

As with other projects of this type, the theoretical results are very exciting. I would say that the main way to improve the impact and relevance of this project would be to build upon this valuable conceptual work to better understand farmers' perspectives and openness to these techniques. This could better inform the types of policies necessary to capture these cobenefits.

- This project focuses on demand for biomass feedstocks and argues that nutrient credits and ecosystem service credits/payments can offset 25% of biomass production, and 10% of fuel cost. The visualizations the team have created have the potential to contribute to the profitability of perennial and waste feedstocks, which are, as they note, barriers to development.

  The project used six indicators related to air pollution from the EPA's EJ screening tool to also consider equity issues in locating potential biorefinery sites. It was great to see this understudied dimension of bioenergy sustainability addressed, and I wonder if the project team can consider other factors outside of air pollution that might play into rural equity issues related to bioenergy.

  How are animal wastes used currently? Are these concentrated animal feeding operations where wastes are a nuisance byproduct? Do they serve as fertilizer? If the material is coming from concentrated animal feeding operations, how might incentives for bioenergy indirectly incentivize unsustainable farm practices?

  Analysis of ecosystem services tends to focus on SOC and nitrogen runoff. Are there other relevant ecosystem services that should be considered?

  The project team does a good job working with related models, tools, and projects to build understanding of the economic dimensions of bioenergy production (GREET).

- This project's inclusion of flood insurance analysis as a potential benefit to incentivize communities was innovative. A useful next step here would be to engage with the insurance industry as well as state-level governments to elicit feedback. Additionally, it would be good to include crop insurance implications because improved resilience and reduced crop failures would be very valuable.

  The EJ screening seemed strong for Task 4. This could be better by considering economic impacts, if they are not already included.

  I highly recommend developing a data source for keeping ecosystem payment data current. Several groups—including AFT, *Farm Journal*, and The Context Network—all produce regularly updated carbon market pricing for growers. NRCS programming could also be an important pricing indication. Because ecosystem services are a rapidly changing market, this model will need to be responsive to be useful. The model could also allow for user inputs for key pricing data as a flexible way to run economic scenarios.

- Despite some delays due to external factors, this project largely stays on track. It is encouraging to see that BioVEST is interacting with other BETO models, but the interactions seem superficial, and there are a lot of opportunities for improved accuracy/more considerations of uncertainties. For example, the manure-to-natural gas project seems to rely on a previous NREL analysis of natural gas production potential; SOCs used in the LCA analysis are fixed values, etc. The project team is recommended to focus more on the accuracy of the analysis. Additionally, with the new stakeholder-related capabilities added to BioVEST, it would be instrumental to have it tested by partners and the public for comments.

PI RESPONSE TO REVIEWER COMMENTS

- Generally, the reviewers found the project to be well aligned with BETO's goals. The development and deployment of BioVEST on the Posit platform was appreciated as a way to increase project impact. Progress toward the objectives of quantifying potential income from ecosystem services, including flood insurance, was appreciated, as was the use of multiple models and the focus on the full life cycle. The reviewers suggested several future directions. (1) Allow users to provide input to EJ decision tools, and quantify the economic impacts of including them. (2) Focus on outreach efforts, including bioenergy companies in addition to landowners and farmers, and have partners test the tool. (3) Provide real-time data on ecosystem payments, incentives, and carbon prices. (4) Increase attention to accuracy and uncertainty analysis. (5) Perform further analysis on producing RNG from manure digesters, and address concerns that the use of these wastes for energy may incentivize unsustainable practices. Our proposed renewal of the project will seek to address the first four of these, with a significant focus on outreach, dissemination of results, user elicitation, scenario analysis to evaluate incentives, and the use of real-time price sources. Although we are interested in continuing our RNG research, the expansion of other parts of the project would make it difficult to address at the current funding level. We will also prioritize moving from Tier 1 to Tier 2 methods of modeling carbon sequestration, and we have recently conducted a sensitivity and uncertainty analysis of BioVEST.

SCALING UP DECARBONIZATION AND SUSTAINABILITY (SUDS)

Argonne National Laboratory

PROJECT DESCRIPTION

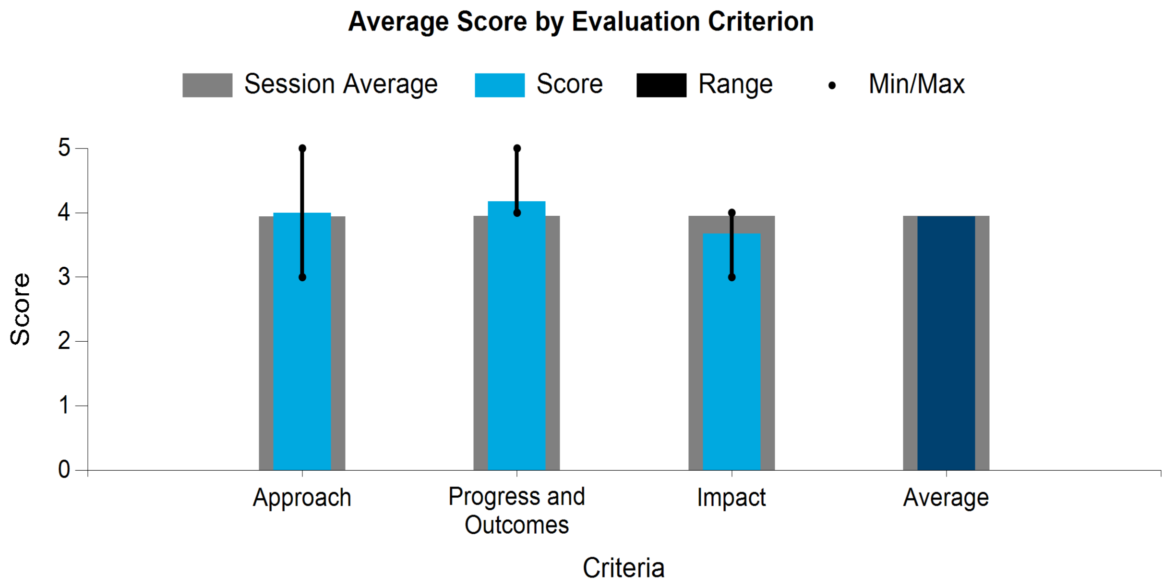
The sustainable generation of biomass can be achieved using perennial bioenergy crops to support the bioeconomy while providing a range of ecosystem services. Our group continues to explore the potential for farmer adoption of perennials through a combined effort of tool development, modeling, technology research, economic analysis, and field and lab work.

WBS:	4.2.2.12
Presenter(s):	Cristina Negri; John Quinn
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,605,000

Our new project builds on accomplishments in the prior project cycle and adds new directions. A key component of both projects is the creation and development of an online geospatial tool, SUPERBEEST. This tool is designed for a full range of users, with interests at scales ranging from the field level to one or more counties or watersheds. Its purpose is to assist with decision making regarding the conversion of row crops to perennials. It identifies economically and/or environmentally marginal farmland that is optimal for the change, providing users with the ability to explore different scenarios. It also identifies candidate locations for saturated bioenergy buffers to increase biomass production while reducing the loss of nutrients to surface water. Under development is the ability to determine the possible improved ecosystem services in a study area with integrated perennials relative to the business-as-usual scenario. The net economic impact of such a change will be estimated by relying on ever-changing valuations for ecosystem services, in particular, carbon sequestration, reduced GHG emissions, and nutrient trading schemes. Government and corporate programs will be evaluated for their relevance.

In addition, we will continue the development of a soil core scanner for the rapid estimation of SOC content, a project initiated with internal research funding (laboratory directed R&D) and important for verification of the carbon sequestration effects of deep-rooting perennials. We will assess root mass and SOC at our mature shrub willow research site in Illinois, perform baseline and future assessments of carbon sequestration and GHG emissions at a set of new switchgrass fields in marginal land in Iowa, and assess a saturated bioenergy buffer for its biomass generation and reduced nutrient loss.

Altogether, our current and future activities have the goal of reducing the cost for biofuel production while providing quantifiable environmental benefits, such as carbon sequestration both locally and globally.



COMMENTS

- This is a good project with a solid approach and a great deal of progress to show for it. Geospatial tools to help farmers understand the value proposition of perennial bioenergy crops, both from a traditional revenue standpoint and from an ecosystem services payment standpoint, have a lot of potential for impact. The capability to assess land marginality is great. The coupling of these modeling capabilities with real-world data from the willow test plots would be a powerful combination. The work to understand the potential for bioenergy crops to aid nutrient runoff reduction is also great. Keep doing that work.

  One area I would encourage the project team to consider doing more is considering transition costs and barriers. It is encouraging that the project is thinking about which equipment options exist and do not exist. But the target audience here are potential growers of perennial bioenergy crops. These tools need to consider things such as access to infrastructure for processing feedstock and whether plots being analyzed are compatible with existing machinery. These considerations are important to the core question: Can I grow it?

  Another thing I would strongly recommend is the public release of SUPERBEEST. While I understand that is not always a fast thing to do, I think it should be an explicit milestone for this project.

- Thank you for the opportunity to review the Scaling Up Decarbonization and Sustainability project. I find that the project is well aligned with BETO's goals, and after evaluating it with the corresponding outreach project, this includes goals related to DEI. SUPERBEEST's identification of marginal land that is ideal for a change, watershed-specific SWAT modeling, and the benefit transfer methodology can all provide potential support tools for bioenergy stakeholders. Further, the project's focus on the increased adoption of perennials, reduced feedstock production costs, improved carbon sequestration, biodiversity, and water quality, and decreased GHG emissions and topsoil loss contribute to farmers' needs for optimal cropping systems, determining low-input cost strategies, and a resilient and stable rural economy as a result of bioenergy adoption. The project is progressing on schedule, and the identification of a cheap method of measuring soil carbon is a notable achievement; however, there are no data on the use or dissemination of the project's free online tool, SUPERBEEST, and a clearer plan to include policy or farmer learning would be beneficial. Nonetheless, the project shows promise in tying together various work streams, and its ongoing refinement through outreach efforts is commendable.

- This project has a very ambitious approach and could be very impactful. The modeling tool developed for this project has the potential to help deliver on BETO's goals of delivering large quantities of sustainable biomass and simultaneously creating additional farm income and ecosystem services. The initial results from the model are extremely impressive, drawing together a variety of data sources to evaluate the optimal locations for energy crops on a very granular basis.

  Given the impressive theoretical findings in this project, this project would benefit from efforts to ground truth and validate the findings, particularly on farmer willingness to implement the recommendations on planting and to incorporate feedback from farmers and industry into the approach. It is very promising that the PI is already coordinating with Antares and pursuing comments from stakeholders through a separate project.

- This project aims to foster bioenergy supply by identifying marginal land that can be converted to perennial bioenergy crops. SUPERBEEST (one of the best acronyms that I've come across in terms of data modeling systems) employs a county-level approach that allows for nuances and complexities of biophysical landscapes. The SUPERBEEST approach allows for multiple scales of analysis—from farm-level to watershed-level scales—which could potentially be useful to different users, including farmer or landowner groups, researchers, agencies, and biorefinery developers. Has SUPERBEEST been tested with farmers? Outreach seems particularly important for this project.

  I wonder if social factors could be considered alongside biophysical dimensions. For example, the authors note that values of ecosystem services are greater than the loss of corn/soybean revenue on marginal lands, but will landowners/farmers change practices? What are the actual (or perceived) impacts on agricultural producers? Who decides what is marginal agricultural land?

  In terms of EJ implications, has a relationship between marginal land and low-income farmers been established? How might this part of the analysis be developed?

  Exploring the relationship between marginal land and income will be interesting and could make significant contributions to the understanding of equity issues in rural communities.

  What are the implications of SUPERBEEST in terms of the incentives necessary to achieve wider-scale bioenergy crop adoption? The authors note that if on-farm reduction costs are more cost-effective than what treatment plants pay to reduce nitrogen, it may be advantageous for treatment plants to pay farmers a credit to grow bioenergy crops. This can provide an additional market incentive to transition to bioenergy crops. Are there examples of this? How would this work exactly?

  How will moving targets such as potential carbon policies and incentives for ecosystem services that could influence conversion to bioenergy crops be incorporated in the model?

- This project's inclusion of a nitrogen water trading scheme is an effective and useful exercise. Often water and climate goals are separated, which misses the economic opportunities of aligning carbon markets with watershed district priorities. It also fits much better with how growers think about their fields and farming practices.

  Siting biorefineries in specific communities that meet EJ requirements is a strong approach to DEI.

  SUPERBEEST excelled in both partnering with local farmer-focused groups as well as prioritizing the gathering of first-party data. The partnership with AFT will help ensure that the farmer voice is well represented, and the commitment to gathering soil samples will help ground truth nitrogen and carbon outcomes.

There are several areas this project could improve. While the idea of identifying marginalized land for conversion to perennial crops is strong, it is important to include the cost of management change, the availability of markets, and the minimum viable acreage a processing facility would require. Growers will also likely be interested in the crop insurance implications of switching crops.

- This project aims to develop an online geospatial tool for decision making on the conversion of row crops to perennials (SUPERBEEST). The tool considers multiple aspects (productivity, soil, nutrient leaching) for marginality, and it can be used at different scales. It is promising as described, though currently it is not yet available to the public (I recommend making it publicly available even during this initial stage).

  The project also includes other activities to support the development of SUPERBEEST or demonstrate the potential usage of the tool (e.g., fieldwork for soil carbon data collection, nutrient credit trading analysis). It would be very exciting if the project team can have more involve partners throughout the project (e.g., as described for the saturated bioenergy buffer siting task, collecting comments from both farmers and wastewater treatment plant managers on the nutrient trading schemes).

PI RESPONSE TO REVIEWER COMMENTS

- We thank the panelists for their contributions of many positive comments and useful suggestions related to this project. As summarized in the comments, this continuation project aims to drive a thriving bioeconomy while decarbonizing agriculture through the adoption of perennial bioenergy crops by exploring the combination of biomass revenue, ecosystem services payments (including water quality trading schemes), and support for underserved rural regions. Many comments focus on the geospatial tool SUPERBEEST, which continues to be developed. Its planned scope addresses many suggested ideas or concerns. As described in the presentation, SUPERBEEST is adding biorefinery locations to provide users with information on distance to buyers and adding spatial EEEJ information to examine differences in farm income related to farmland marginality. Outreach is important for the future impact of this tool, and, as mentioned in the presentation, we are working closely with the ideal partner, AFT, in a related project (WBS 4.1.2.11 Ecosystem Services Entrepreneurship Technical Assistance). Through that project, we are gathering important input from farmers and industry to inform the technical path for SUPERBEEST development as well as pathways for bioenergy crop adoption by developing educational material and partnerships to identify and overcome some technical challenges of adoption. SUPERBEEST has had a partial public release and will be fully public soon, with announcements made at many relevant conferences and workshops. As mentioned in the presentation, we anticipate that changes in how SUPERBEEST provides economic estimates of changes in cropping at the farm, watershed(s), or county(ies) scale will require continuous modifications to be current and relevant to federal, state, and local government policies and corporate sponsorships. These updates will be necessary because of constant changes in governmental or corporate support for key ecosystem services, such as the water quality trading schemes highlighted in our demand analysis and TEA and the evolving support for carbon sequestration and reduction in GHG emissions. Our efforts with shrub willow, new switchgrass study sites, saturated bioenergy buffers, and scanning technology for SOC will all contribute to the scientific literature to support ground-truthing and model validation, and they represent important partner collaborations. Through the related project WBS 4.1.2.11, we are examining the important topic of crop management change and the associated costs. Crop insurance is a helpful new suggestion that may improve the economic proposition for farmers. Altogether, our intention is to contribute to an economically viable, environmentally friendly, socially equitable future scenario of sustainable perennial bioenergy crops supplying biomass to a growing market and offering low-income farming regions a robust cropping alternative.

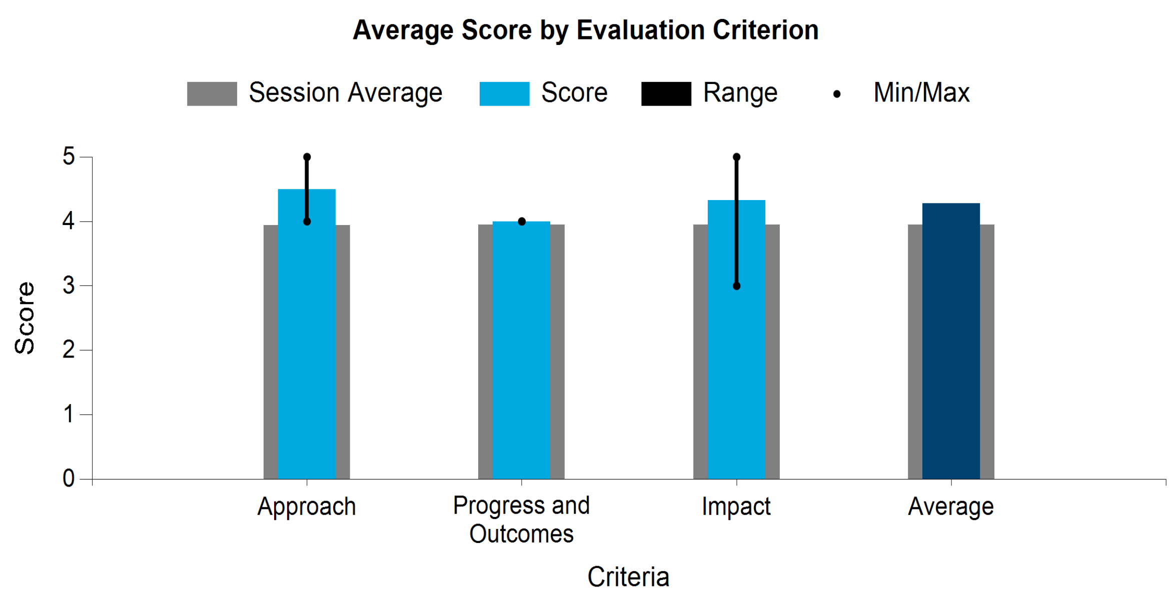
EXCHANGE: EXPANDING THE CONVERSION OF HABITAT IN THE NORTHERN GREAT PLAINS ECOSYSTEM

University of Nebraska – Lincoln

PROJECT DESCRIPTION

WBS:	4.6.1.10
Presenter(s):	Daren Redfearn
Project Start Date:	10/01/2021
Planned Project End Date:	03/31/2027
Total Funding:	$4,000,000

EXCHANGE quantifies and monetizes ecosystem services from the targeted deployment of perennial bioenergy grasses in semiarid, irrigated croplands. The selective return of native perennial grasses to irrigated landscapes fosters the diversification of row crops, livestock, and bioenergy production systems in water-scarce landscapes. This spatially directed innovation for integrating perennial and annual crops enhances climate resilience, sustainability, and security of domestic food and energy production. Expected impacts include improved (1) groundwater sustainability, water quantity, and quality; (2) nutrient retention; (3) pollinator/wildlife habitat to support increased biodiversity; (4) climate change mitigation through increased soil carbon storage and decreased agricultural GHG emissions; and (5) economic risk management by diversification of farm revenue streams. Soil sampling and water sensor installations were deferred due to the COVID-19 pandemic and project funding delays. EXCHANGE successfully established two small-plot trials and measured avian/arthropod populations at 10 paired grassland/cropland on-farm sites. Preliminary results show greater avian/arthropod populations in grasslands than croplands. The first perennial biomass harvests occurred in 2022. Soil GHG emissions summarization and biomass cell-wall parameter analyses are ongoing.



COMMENTS

- This project seems highly valuable, and I find little to criticize. Although the project seems to have gotten off to a slow start, the progress to date seems very promising. The scope of this project seems well suited to provide real-world data to address multiple important analytical needs for BETO. The data on energy grass cultivation seem likely to benefit efforts to develop those feedstocks and move them closer to commercialization. The quantification of ecosystem benefits from these cropping systems provides a separate set of potentially impactful data. While it remains to be seen how much of this project's potential will be realized, I find little to criticize so far.

- Thank you for the opportunity to review the EXCHANGE project. Based on the information presented, the project appears reasonably aligned with BETO's goals. I appreciate the approach of assessing bioenergy grass production to increase biomass for the bioeconomy while also reducing unsustainable stress on the Ogallala Aquifer and providing ecosystem services. It is also great to see the progress made in tasks 1–4 and the use of SOC measurements at different depths to assess GHG emissions. One opportunity for improvement could be to provide more information on the preliminary data that will be presented to give a better understanding of the project's progress. Additionally, it may be useful to provide more information on the site that was unsuccessful to gain better knowledge of suitable switchgrass acreage and the plant's resilience. Overall, it seems like the project is on schedule and making good progress toward achieving its goals.
- This project uses FOA funding to pursue a more focused analysis of energy crop cobenefits in the Northern Great Plains. This project is very useful to the portfolio because it connects theoretical benefits to real-world practice and data collection. While it is still in its very early stages, this project appears to be making progress toward its intended goals, with the early data collection showing results on wildlife ecosystem services, soil carbon change, and reduced N_2O emissions. In addition to a comparison of impacts of biodiverse farming systems to business-as-usual farming, it could also be helpful to evaluate the trade-offs associated with the planting and harvesting phases to get a more holistic comparison and better understand barriers and challenges.
- This project seeks to improve decision making by quantifying ecosystem services and incentives to bioenergy crops. The project yielded promising preliminary results finding that avian biodiversity was greater in grassland than cropland, and more insect pollinators were observed in grassland than cropland. The project also included a water modeling tool (MODFLOW) to capture changes to the aquifer from bioenergy production. The team brought together a wide range of approaches and tools, from range ecology to remote sensing data, and it has great potential to inform other models and projects.

  In addition to measurements at the field stations that showed promising results, it would be interesting to explore why the High Plains Agricultural Lab fizzled? It would be useful to explore this to understand what factors contribute to resilient systems.

  The two test sites, Scottsbluff and North Platte, compared aboveground biomass for switchgrass planting versus a low-diversity mix of big bluestem and other grasses. It would be interesting to see how different kinds of ecosystem services might compare between different types of perennial bioenergy plantings.

  The project states that it has potential to support rural socioeconomics in the Northern Great Plains region, which seems intuitively true, but having metrics to support that could make this claim even stronger.

  Creating best management practices for perennial bioenergy crops would have high impact value to farmers, and the project team is well qualified to disseminate results to farmers through Extension work.

  This project is an important inclusion in DOE's portfolio. The ground-truthing data collected here will help to aid growers' understanding of how to be successful and build confidence in the ultimate planting of switchgrass. This project also had the foresight to highlight biodiversity improvements, which are likely to be a driver of future environmental credits alongside carbon payments.

  The project could be made stronger by including industry biofuel representatives. Documentation of test site visits plus testimonials from local ethanol producers would help to build confidence in Nebraska.

The inclusion of the impact on the Ogallala Reservoir through switchgrass will also aid in the generation of additional economic incentives.

- This is a rare and much-needed project that aims to collect ground truth data to quantify the ecosystem service values. A variety of techniques were used to collect data related to SOC, GHG emissions, biodiversity, evapotranspiration, etc. Multiple plots were established and monitored to compare various scenarios (switchgrass versus low-diversity mix versus no-till corn, rain-fed versus irrigated, different sites). Field data were also leveraged in multiple models to understand the larger implications through TEA (economic), LCA (environmental), and ecosystem services valuation. The project has clear goals, coherent tasks, and is expected to provide critical information related to the application of perennial grass toward improving ecosystem quality while contributing to the bioeconomy.

PI RESPONSE TO REVIEWER COMMENTS

- The EXCHANGE team expresses our appreciation for the reviewers' efforts and input. We realize the time commitment involved to conduct a thorough Project Peer Review process. The review team's compliments on the achievements and suggestions for improvements are greatly appreciated. These suggestions will be extremely valuable in guiding the project moving forward. Generally, our plan is to include metrics on ecosystem services, trade-offs, and industry needs once additional data are available. The EXCHANGE project will provide supplementary data that can be coupled with some of our existing data sets to confront some important challenges identified by the reviewers. Several reviewers requested additional insight on the site information that resulted in unsuccessful bioenergy grass stand development. Part of the general premise for the project was to determine if these bioenergy cultivars could be used outside the recommended region. We generally do not recommend planting switchgrass, big bluestem, and Indiangrass for bioenergy production west of the 100th meridian. Of the three sites selected for small-plot bioenergy grass evaluations, two were successfully established (Scottsbluff, Nebraska, and North Platte, Nebraska), and one was an establishment failure (Sidney, Nebraska, is more than 150 miles west of the 100th meridian). Both the Sidney and Scottsbluff locations are classified as having a semiarid climate. Supplemental irrigation was available at both Scottsbluff and North Platte, whereas the Sidney site was dryland and nonirrigated. We purposely included a dryland (nonirrigated) site to test the risks associated with establishing bioenergy grasses under extreme conditions in a dryland, semiarid environment. All three sites were planted in spring 2021. The two sites with supplemental irrigation were successfully established in spring 2022, with the first biomass production data from those two sites collected in 2023. For the Sidney location, grass emergence and establishment were hampered by significant drought in 2021, resulting in thin stands. We chose to replant for the second time in spring 2022, and we planted corn for the business-as-usual comparison. Severe drought conditions persisted throughout the 2022 growing season, and grassy weeds continued to be problematic due to poor grass stands. The corn grew to about 4 feet but never produced grain. The Sidney site experienced two consecutive years of drought, resulting in poor seedling emergence and failed stand establishment. In spring 2023, we chose to abandon the dryland site (Sidney) and focus resources on Scottsbluff and North Platte. Again, the EXCHANGE team greatly appreciates the positive comments and feedback for this project. We look forward to continuing the process of data collection to support the understanding of the larger economic, environmental, and ecosystem services implications of bioenergy perennial grass production systems affecting the Northern Great Plains Ogallala Aquifer.

EVALUATION OF ENERGYCANE FOR BIOENERGY AND SUSTAINABLE AGRICULTURAL SYSTEMS (EC-BIOSALTS)

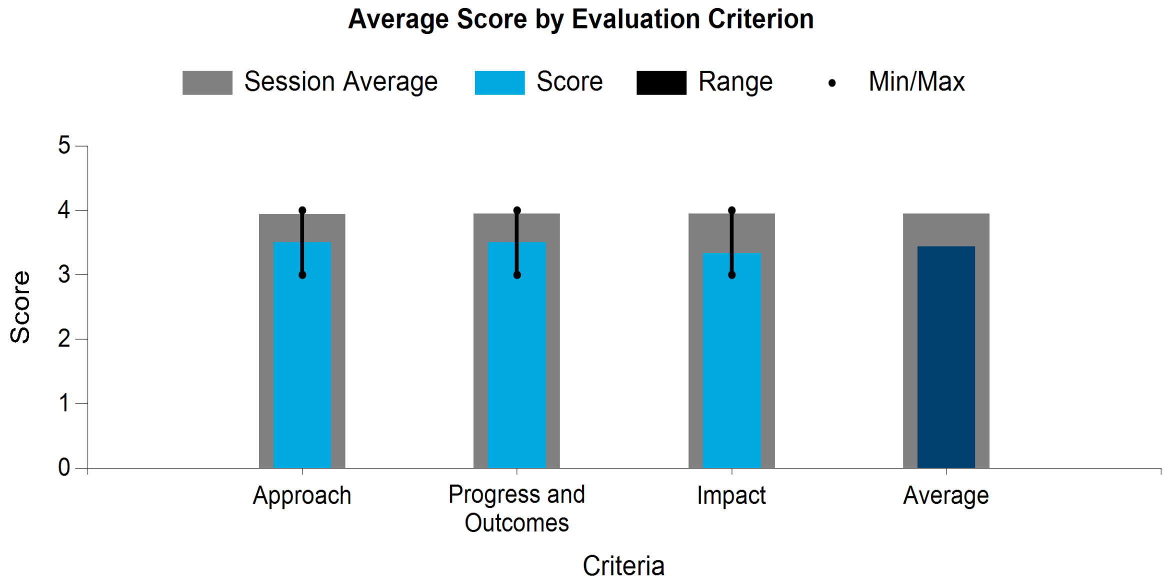
University of Florida

PROJECT DESCRIPTION

WBS:	4.6.1.20
Presenter(s):	Hardev Sandhu
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2025
Total Funding:	$4,991,921

Blue-green algal blooms and red tides are major environmental challenges in the U.S southeastern coastal plains, particularly in Florida, where they are a threat to public health and are affecting aquatic life, wetlands, and agriculture. Nitrogen (N) and phosphorus (P) runoff from agricultural fields are considered some of the major causes of blue-green algal blooms in rivers and lakes and red tides in the coastal waters. In this project, we are evaluating energy cane for ecosystem services, including reduced N and P losses and GHG emissions and improved soil carbon (C) storage and biodiversity in marginal agricultural lands of the U.S southeastern coastal plains. The overall goal of this project is to develop a bioenergy feedstock production system using an advanced energy cane cultivar (UFCP 84-1047) in marginal and fallow croplands of the U.S southeastern coastal plains. Specific objectives are to: (1) evaluate the yield and quality of currently available UFCP 84-1047 and advanced energy cane cultivar for bioenergy at the field scale in marginal and fallow croplands to predict biomass yield potential and determine suitable agronomic practices, (2) quantify the ecosystem services of UFCP 84-1047 compared to sugarcane and sweet corn cropping systems on marginal and fallow croplands, (3) test sensors for estimating environmental parameters and energy cane's agronomic attributes and ground truth information management platforms, (4) develop a machine learning-based model that can predict energy cane's agronomic attributes (yield and feedstock chemical composition) given a collection of environmental and crop management parameters, (5) use field-scale data to generate baseline and enhanced (with projected market values of ecosystem services) TEA to quantify opportunities to meet BETO's cost goal of <$3/gasoline gallon equivalent (GGE) with >4 ton per acre yield and a refinery delivery cost of <$84/ton, (6) develop an LCA, and (7) develop a market transformation plan. This project will enable the creation of a field-scale demonstration on how to sustainably embed bioenergy crops in marginally productive croplands of the U.S southeastern coastal plains, a region in the United States that could potentially supply large amounts of biomass for the bioeconomy. Field-scale production and demonstration will allow us to generate data of quality and quantity not achieved before for the proposed unique production system using one of the most productive bioenergy crops suitable for subtropical growing conditions. The expected multiple project outputs directly support the growing U.S. bioeconomy. These include remote sensing and modeling tools, high-resolution information on production, feedstock compositional characteristics, economic potential, LCA, a market transformation plan that specifies the path to the integration of biofuel and bioproduct production into the local and regional economic systems, and sustainability of energy cane in the U.S southeastern coastal plains. We anticipate being able to achieve BETO's biofuel price point goal of <$3/GGE. The development of remote sensing technology for the cost-effective and rapid data collection as well as machine learning model with agronomic predictive capabilities directly supports efforts toward using precision agriculture in bioenergy cropping systems. Additional impacts of this project are in the forms of field visits, training workshops, data dissemination through the KDF, peer-reviewed publications, and presentations at various national and international conferences.

Currently, we are in the 18th month of this project. Baseline data collection and energy cane seed cane propagation for field trials are successfully completed, which was required for our first go/no-go decision. The actual field trials are successfully planted at two locations: Everglades Research and Education Center in Belle Glade, Florida, and Indian River Research and Education Center in Fort Pierce, Florida. We are currently collecting data on energy cane biomass and ecosystem services in plant cane. Data on two ratoon crops will be collected in the third and fourth budget periods.



COMMENTS

- The goals and approach for this project seem valuable. Though energy cane may have a smaller overall range than some other potential cellulosic feedstocks, feedstock diversity is valuable. And there do seem to be some significant opportunities and potential environmental cobenefits. That said, it is difficult to provide much assessment of the progress, outcome, and ultimate impact of this project given that its start has been significantly delayed. For now, I will just say that the potential for an excellent project seems to be there, and I look forward to seeing how it progresses.

- Thank you for the opportunity to review the EC-BioSALTS project. The project is reasonably aligned with BETO's goals, particularly in their consideration of SAF. I was impressed with the team's detailed and comprehensive approach, including the development of a machine learning model for yield and feedstock chemical composition. The progress and outcomes of the project are on schedule, with data collection ongoing and several milestones completed. I appreciate the focus on environmental and economic measurements as well as the potential impact of the project on reducing GHG emissions through the use of energy cane-derived SAF. One area of improvement could be to discuss the machine learning data sets in more detail and to ensure the results can be replicable.

- This project is very focused and builds out understanding of the potential for energy cane in the southeast. Beyond energy potential, this project also illustrates several cobenefits, such as improved water quality and soil quality improvements that are unique to the Florida region. Particularly compelling was the potential for energy cane to benefit from existing supply chains and practices applied to conventional sugar cane.

  The project is still in the relatively early stages due to a delay associated with the negotiation period, so its progress is difficult to evaluate. Early results suggest success in matching measured data with previous reports on GHG fluxes and soil quality improvements. It also appears that in an LCA sense, the project is well on its way of demonstrating the GHG benefits of energy cane systems; however, as noted as a trend with these projects, it would be helpful to integrate more farmer and industry perspectives on the techniques implied by integrated land management and their feasibility. I think this would help to increase understanding beyond data collection, LCA, and TEA.

- This project seeks to quantify sustainability benefits such as GHG emissions reductions through LCA by evaluating supply chains in the production of energy cane. The project acknowledges that risks associated with energy cane production include prolonged drought, flooding, insect pests, and diseases. These seem like very real risks given current climate scenarios. The project aims to mitigate these risks through different genetic varieties of energy cane, but given the intensity and frequency of climate events in Florida, it seems worth exploring these risks a bit more.

  The project includes an advisory committee. What stakeholder groups are represented on this advisory committee, and how were different stakeholder perspectives integrated into the project development?

  The project claims to contribute to BETO's goals of DEI and workforce development by involving students from diverse backgrounds in research project activities. What did this look like? How many students were involved? What did they do on the project?

  How are the social dimensions of sustainability addressed? For example, how does the project address things outside of traditional LCA, such as access to land, land ownership and use, decision making about land, land ownership, workforce? How does the supply chain analysis account for labor issues, particularly given that citrus growers rely on migrant labor? What kinds of human capital (i.e., labor) are required for the production of energy cane? Perhaps this is something the project could consider in future iterations of this work.

- Overall, the opportunity for energy cane as a feedstock was not clear. The presentation identified major changes in orange production, but it was not clear if and why energy cane would be a suitable substitute. An evaluation of total addressable acres likely to adopt based on agronomic or land quality factors is required to better evaluate the importance of this potential feedstock. It would also be useful to evaluate how available land suitability and availability may change due to climate volatility.

- The partnership with LanzaTech is a nice connection with industry, and it would be helpful to include the parameters by which they evaluate the viability and competitiveness of a feedstock. Extension of stakeholder connections to environmental groups and growers would strengthen this project.

- This project focuses on the development of energy cane as a new bioenergy feedstock for the southeastern United States. It is meaningful in diversifying the portfolio of bioenergy feedstocks with options that might be more appropriate for a certain region, and a series of field and modeling activities have been performed/are planned.

  However, the research team did not fully justify the motivations/contributions of this project, especially given that the application of energy cane (although it is more cold-tolerate than sugarcane) is likely to be limited to a few states in the United States, and it is unclear if energy cane will be more beneficial for the ecosystem than perennial grass. Additionally, the team proposed to incorporate energy cane in conventional sugarcane and sweet corn cropping systems, but this will add non-negligible risk for farmers as they shift from established crops with a mature market to new feedstocks without potential buyers; therefore, the project team is encouraged to answer these questions through research activities in the future.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the panelists for their helpful feedback and suggestions. As reiterated in the comments, the overall aim of the project is to drive the adoption of a thriving and sustainable bioeconomy through the adoption of high-yielding energy cane cultivars in the fallow and marginal croplands of the U.S. southeastern coastal plains to produce SAF and coproducts. We intend to better demonstrate regional yield potentials and identify how to best transform the market in the region to support a thriving market for SAF and coproducts while providing improved ecosystem services and multiple income streams (e.g., biomass revenue and ecosystem service payments) for farmers/producers.

An important comment touched on the clarity and replicability of our machine learning model development process. In response, this process will be further laid out in progress reports and in our findings. The data sets needed for training and testing machine learning algorithms include energy cane biomass yield and quality, weather parameters, topographic features, and soil properties, which will be generated from field data and online databases. Weather parameters (air temperature, precipitation, etc.) will be generated from databases associated with nearby weather stations maintained by the USDA NRCS, National Oceanic and Atmospheric Administration, etc. Topographic features (elevation, slope, etc.) will be derived from the 3-m digital elevation model of the U.S. Geological Survey National Elevation Dataset. The rest of the data sets will be generated from data collected from the field site. Energy cane biomass yield and quality data will be generated from the outputs of the remote sensing task (using drones). Expected outputs from the remote sensing task are heat maps of the end-of-season biomass yield and quality at 1- to 3-m spatial resolution, which will be validated by actual biomass collected from each plot using 3 x 3-m quadrats throughout the growing season. Heat maps of 8–10 soil parameters will be generated from point sample measurements conducted as part of the study site characterization. The key is to create a gridded data set of the response variables (biomass yield and quality) and all the predictors or explanatory variables (climate, soil, topography, etc.) at a common horizontal spatial resolution for each experimental plot. The final choice of horizontal spatial resolution will be dictated by the spatial resolution of the biomass yield and quality maps produced from the remote sensing task, which is expected to be 3 m. We will follow a similar modeling framework from our work in the U.S. Midwest on the application of machine learning in predicting biomass yield, which has been published (https://doi.org/10.3390/en16104168).

Other comments touched on the LCA process. There is an emphasis on analyzing an LCA focused on life cycle GHG emissions, which aligns with DOE’s priorities. The results of the TEA and LCA will provide valuable insights into the major factors that contribute to both cost and GHG emissions of the project. These factors primarily stem from energy consumption and chemical usage (e.g., fertilizers) during farming as well as fuel production. The TEA and LCA team will conduct a thorough assessment to identify potential opportunities for achieving further cost and emissions reductions through various activities across farming and fuel production stages. Further, the team will explore innovative farming techniques, such as a reduction in nitrogen application within marginal lands and crop diversification strategies for soil and water management, that could contribute to these objectives. Additionally, the team will address the feasibility of implementing these techniques and consider their practicality in our operations. By integrating these findings and discussions, we aim to optimize our practices, reduce costs, and minimize our environmental impact. The social LCA, which examines the social dimensions of the pathway, is currently not within the scope of this project; however, we recognize that the inputs and outcomes from the current study can be used for future social LCA efforts. By using harmonized conditions, these analyses can effectively identify trade-offs between environmental and social impacts. Although it is outside the immediate scope, the findings of the present study can serve as a foundation for conducting comprehensive assessments that encompass both environmental and social aspects in the future.

As to the suitability and applicability of energy cane within the region, we will ensure that the following information is clear throughout our upcoming reports. High-yielding (advanced) energy cane cultivar production is a desirable substitute for fallow citrus lands for several reasons, primarily because our initial assessment showed that most lands that are ideal for advanced energy cane feedstock production for SAF and coproducts in Florida are fallow lands that used to be under citrus production. Except for a very small portion enrolled in the water farming program administered by the South Florida Water Management district, these fallow lands are mostly left unused, leaving landowners and farmers incomeless. Previous evaluation of energy cane in Central and South Florida showed high biomass yields (30–34 Mg/ha) on marginal sandy soils, which were under most of the citrus production in Florida. In addition, a more extensive deep-rooting system of energy cane than sugarcane and some other perennial grasses makes it more efficient in soil carbon sequestration and the use of water and nutrients, which can reduce nutrient runoff to water bodies. Energy cane cultivation is very similar to sugarcane, which is mostly mechanized and needs minimum human labor. Converting these fallow and/or marginal lands into sustainable energy cane feedstock production systems will boost the rural economy. Sales from energy cane biomass will provide income to landowners and farmers. Additionally, payment for ecosystem services (especially subsoil carbon sequestration because citrus fallow lands in this region primarily comprise sandy soils) will provide more income to landowners and farmers, providing further economic incentive for this diversification of crops. We are, in fact, conducting a formal analysis to assess the total addressable acreage of land in Florida that is likely going to adopt a sustainable energy cane feedstock production for SAF. The results of this analysis will be available by the end of this fiscal year, which are critical for our analyses to better understand the energy cane feedstock supply chain and impacts on ecosystem services.

We acknowledge the merits of the reviewer's suggestion to include climate change impacts on the land availability analysis. In this project, we are focused on the assessment and valuation of short-term carbon sequestration and other ecosystem service impacts at scale in Florida. Long-term impacts are beyond the scope of this project; however, inputs, process, and outcomes generated in this project when coupled with a downscaled climate data set at high horizontal spatial resolution can be used to determine long-term climate impacts. A downscaled climate data set at a high horizontal spatial resolution of 1 km could become available and accessible in a few years, particularly for North America, based on the work of climate scientists, including that of our colleagues at ANL. Future projects can leverage a downscaled climate data set of Florida at 1-km horizontal spatial resolution along with the foundational data sets and outcomes from this current project to better understand the long-term impacts of climate on the proposed energy cane feedstock production system in the U.S southeastern coastal plains region.

This project's focus on diversity and equity is primarily within diversifying the workforce development training for science, technology, engineering, and mathematics students. At national laboratories, DOE has a couple programs designed to provide a 10-week paid internship for talented students from academic institutions, including land grant universities, historically Black colleges and universities, and community colleges. Talented student research interns from diverse backgrounds and multiple academic institutions have been part of the ANL team since 2012 through the DOE's Science Undergraduate Laboratory Internship program. As part of the team, they are exposed to a wide range of activities geared toward building their professional and research skills during brainstorming and project planning meetings, teamwork activities (e.g., working in pairs during field data collection and laboratory experimental activities), literature reviews, technical report and journal paper writing, and data processing and analysis. Most importantly, each intern is required to work on a specific research problem (typically a subset of our BETO project deliverable) that could be done within the 10-week period. They will then present the results of their research as poster presentations in a laboratory-wide culmination activity for all student research interns. This summer, two student research interns (a male and a female) will join the ANL team for 10 weeks to work on not only the EC-BioSALTS project but also the other BETO-funded projects, such as the Affordable and Sustainable Energy Crops (ASEC) – Switchgrass and EXCHANGE.

Currently, the advisory panel includes members from the Florida Department of Agriculture and Consumer Services, South Florida Water Management District, Florida Department of Environment Protection, Florida Energy Systems Consortium, USDA Agricultural Research Service, University of South Florida, and LanzaTech. At present, there is no specific plan to target diverse stakeholders and other communities in the study area. Following the geospatial analysis of suitable agricultural lands for energy crop adoption, we can better understand the potential demographics of farmers and landowners.

Outreach is not built into this project, but the geospatial data derived from the project can provide context for future projects that will focus on outreach and education regarding these crops. We thank the reviewers for their feedback, and we look forward to working closely with BETO to maximize this project's potential during the next few years.

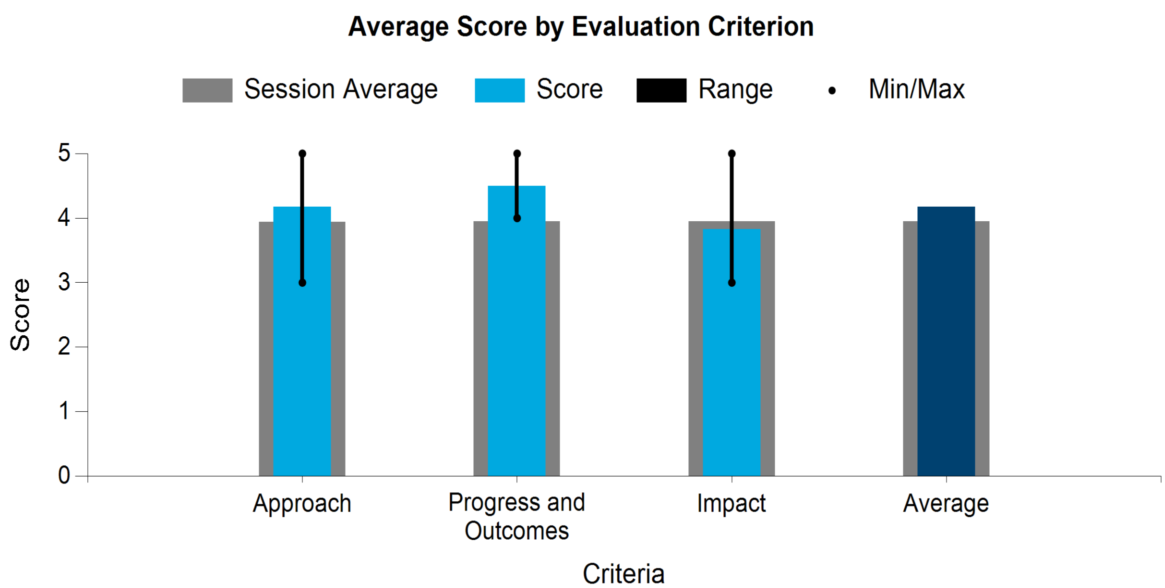
POSIES: POPULUS IN THE SOUTHEAST FOR INTEGRATED ECOSYSTEM SERVICES

Mississippi State University

PROJECT DESCRIPTION

WBS:	4.6.1.30
Presenter(s):	Heidi Renninger
Project Start Date:	10/01/2020
Planned Project End Date:	08/31/2023
Total Funding:	$2,544,896

The southeastern United States has great potential for growing poplar (*Populus spp.*) biomass, although costs are still higher than traditional fossil fuels. The incorporation and efficient quantification of ecosystem services may diversify income streams to reduce final costs, reduce market volatility risks, and provide additional benefits to society; therefore, our goal is to reduce the final cost of Populus feedstock production in the southeast by (1) enhancing productivity (through cultural planting practices and inoculation with endophytic bacteria), (2) quantifying ecosystem service provision (nitrogen mitigation and belowground carbon (C) storage), (3) developing remote sensing strategies to enable faster quantification of ecosystem services and productivity, and (4) integrating all findings into an updated TEA for short-rotation Populus plantations in the southeast. So far, we have identified Populus genotypes that exhibit biomass of more than 20 Mg/ha/yr on high-quality sites, increases of more than 91% with endophyte inoculation on poor sites, and increases of more than 30% based on cultural planting practices. Soil C in plantations increased by 13% and nitrate decreased by 20% compared with row crop agriculture. Near-infrared reflectance and LiDAR-predicted soil C and aboveground biomass with r2 of 0.73 and 0.97, respectively. In total, incorporating ecosystem services from Populus may be essential for meeting targets of $3/GGE for biofuels.



COMMENTS

- This project is doing highly valuable empirical work. Scaling up bioenergy crops cannot happen without work like this to test systems and growing strategies and gather data on the potential ecosystem benefits (and associated revenues). This approach will generate valuable data for other researchers and potential bioenergy crop growers. My only suggestion is that it seems like this project is an excellent context in which to develop harvesting machinery and logistics for poplar cropping systems. I encourage the project team to not neglect this opportunity as they pursue the valuable work of assessing genotypes and environmental impacts.

- Thank you for the opportunity to review the PoSIES project. From my analysis, the project is reasonably aligned with BETO's goals. I appreciate the use of short-rotation woody crops like poplar to assess ecosystem services, productivity, and variability while considering cost-competitive measures. The incorporation of technology such as lidar/drones to quantify soil carbon and biodiversity is commendable. The preliminary financial estimates and the quantification of impacts for farmers are also innovative. Additionally, the 22% decrease in nitrate relative to the agricultural field shows significant progress toward sustainable agriculture. As an opportunity for improvement, the project should further develop ecosystem services and quantifying disservices with dynamic considerations because these are likely to be sensitive to time. Additionally, and as other researchers noted, it may be useful to include harvest time as an endogenous variable in the optimization considerations. From what I understand, the project is on schedule, and I look forward to further updates.

- This project is a good opportunity to use FOA funding to do more targeted work on a specific feedstock in a region of interest to generate real-world data. The outcome of this work has broader relevance to unlocking a large potential pool of sustainably available biomass with some ecosystem cobenefits, which aligns well with BETO's and DOE's goals. The project has a very clear focus, and the emphasis on assessing and improving productivity from poplar stands, particularly on more challenging sites, fills an important niche. It is not clear from the approach, however, to what degree this project is focused on using marginal lands unsuitable for conventional production or whether it is intended to be implemented at larger scales on more conventional land types.

  While it is still relatively early in the life of the project, the initial outcomes and progress appear promising—in particular, the use of bacteria to improve productivity at more challenging sites as well as demonstrating cropping with reduced inputs.

- This project takes an innovative approach to examining ecosystem services and potential ecosystem disservices from poplar plantations grown in the southeast, potentially feeding markets for SAF. The project has great potential for impact to farmers, researchers, and bioenergy investors. The project team talks about working with stakeholder groups from industry, nonprofits, government agencies, landowners, and farmer organizations in yearly meetings and semiannual email reports. I am curious to know how feedback from those groups has been incorporated into the project? What function does the stakeholder advisory panel play in project development?

  Another question I had but that was thoughtfully addressed at the review: Is there potential for competition with other markets for these feedstocks? The project team mentions that if there are insufficient bioenergy markets, the material could supply traditional hardwood markets. Is there any concern about competition with pulp and paper industries, pellet markets, or emerging biomaterials (cross-laminated/mass timber, etc.?)

  The project team notes that hybrid poplar genotypes outperformed older eastern cottonwood genotypes. How do potential ecosystem services and disservices compare across the different genotypes? Impacts on wildlife? GHG? Water? How do different types of ecosystem services compare to one another in terms of assigning value to water quality versus biodiversity for example? That may be beyond the scope of this project but is possibly something to consider for future work.

  Poplar clones were developed by the USFS for the pulp and paper industry back in the mid- to late 20th century. What can we learn about the long-term sustainability of poplar from past studies on USFS efforts to pulp and paper production? Are there any long-term poplar study sites that have looked at some factors covered in this project?

Although it might be beyond the scope of this project, the team might want to check out the following to situate this project in the broader socioeconomic context: https://rowman.com/ISBN/9781793632357/Forests-as-Fuel-Energy-Landscape-Climate-and-Race-in-the-U-S-South.

Overall, this project had clear objectives and has made good progress on those goals. They have communicated and collaborated with other groups and partners from industry and NGOs. The project makes important contributions to understanding bioenergy production at a very practical, field-based level.

- This project adds important data to DOE’s understanding of the cost, productivity, and agronomic viability of poplar. The improvements in predicting carbon sequestration and tree mass gain are exciting outcomes of the work to date. This project also excelled in stakeholder engagement. Pricing carbon payments with a carbon project developer, wood demand with a pellet facility, technical assistance with a conservation group, and direct feedback from growers all lead to better outcomes of the research and make it more likely that recommendations will be adopted.

  There are several risks with planting a harvested crop on marginal land that this program can address. First, having clear delineations between the characteristics of marginal land that can impact grower outcomes can help better inform expectations and decisions. Second, an economic analysis of minimum viable acres would be useful to understand how much land should be dedicated to the effort in a single operation to be financially viable. Finally, it would be good to understand whether it would negatively impact the productivity of the poplars if fertilization of the main cash crop were to change and nutrient runoff were be reduced through improved farming practices or a shift in synthetic fertilizer application.

- This project evaluates the use of poplar (new genotypes, use of endophytes, etc.) for biofuels while providing ecosystem services. Highlights of this project include the establishment of multiple research sites (with measurements on SOC, water, biodiversity), improvement on data collection approaches, and involvement of multiple stakeholders (advisory panel with regular meetings); however, a key caveat is that the industry advisors do not seem to be interested in the genotypes developed in this project, and it is highly recommended that the project team works with the advisors to pilot-test the genotypes or to understand what metrics the new genotypes should reach before industries are willing to test them.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for all the helpful suggestions and the time and effort you took to review our project. We agree that harvesting machinery and logistics will be important as more broad-scale production occurs, although our study plots are not large enough to adequately answer this question. While not the scope of our study, other researchers have evaluated harvesting systems and timing (see https://doi.org/10.1016/j.biombioe.2017.09.003 and https://doi.org/10.1016/j.biombioe.2021.106075). The most useful new research would probably be TEA and LCA comparisons between 2- to 3-year coppice cycles with single-pass cut-and-chip harvesting compared to 10- to 15-year single-stem rotations harvested and chipped with traditional logging equipment in the southeastern United States. This is beyond the scope of our study in space (our plots are all too small for operational comparisons) and time (we do not have 10- to 15-year-old trees to harvest), but it would be valuable information for landowners. Minimum viable acres would also be interesting to determine, but that is also beyond the scope of our study. Landowners potentially also have the potential to work with neighbors to coordinate the harvesting of individually smaller plots if they are on the same planting schedule.

While not presented at this year's Project Peer Review, we are quantifying potential ecosystem disservices of water use, wildlife biodiversity, and trace gas and carbon dioxide emissions through time at various field sites. These will be compared across genotypes and planting designs and their scale compared with one another. We will definitely check out Sarah Hitchner's book because it sounds like it will be useful in putting our research into a broader context.

In terms of marginal land, we have a range of sites based on availability of more or less "free" land that is likely all considered marginal, or it would be in agricultural production. Implications for different degrees of "marginal" versus conventional agricultural land are probably better addressed through modeling, which our field data can contribute to, and some of which has been done already for our target system (see https://doi.org/10.1016/j.biombioe.2015.05.004, https://www.fs.usda.gov/research/treesearch/54326, and https://doi.org/10.1016/j.biombioe.2010.01.012). But we agree that more data connecting land characteristics (i.e., how marginal is the land) with growth and productivity predictions will be useful to landowners.

This study is also collecting a large amount of physiological data that can be used to drive process-based models of poplar growth at the genotype level. Our study is able to look a bit at the effect of the nearby fertilization of agricultural fields on growth because most sites are near agricultural land on a rotation between corn and soybeans (with corn being fertilized with synthetic fertilizer and soybeans not receiving extra fertilizer). Although soybeans fix nitrogen and may contribute more nitrogen to our poplar trees, it is likely much less than during corn production. We also have other sites that are not in direct contact with agricultural fertilization, but they are growing very well (suggesting that an external fertilizer source is not essential for good growth but may help).

Our stakeholder advisory board provides feedback on our data and will likely provide valuable input as we begin the TEA. It would have been good to have stakeholder input for project development; however, due to the short-term nature of the study, we needed to get trees planted as soon as possible, which was before stakeholders could provide suggestions for experimental design, etc. We have stakeholders who were a part of the original USFS trials and others with decades of experience in Populus research, and their expertise has been useful. Most trials in the past have focused on growth, disease resistance, and survival, with few looking at ecosystem services and impacts and tree-level physiology. We have a few of the older USFS genotypes in our study as well to provide continuity with older studies. To our knowledge, the older trials have not been maintained and monitored beyond the initial studies that planted them. In terms of competition with other markets, the hardwood pulp market is generally oversupplied, with exceptions in some geographies close to specific mills, so there is likely not competition there. Poplar is not currently considered suitable for cross-laminated timber products that are more suited to softwood species (southern pine, Douglas fir, etc.). On longer rotations, poplar has potential for plywood applications and even dimensional lumber. Grown on short coppice rotations, poplar is most suited for bioenergy, pellet markets, and emerging biomaterials, including lignin-based bioproducts; however, these markets are either in their infancy (bioenergy, SAF, and bioproducts) or have other sources of material (wood from thinned pine stands that are overly abundant in the south) in terms of pellet markets. But it is likely that as bioenergy and bioproducts markets emerge, industry will become more interested in the new genotypes being tested in this study. From past experience and our stakeholder panel, we know in general what industry values for genotypes (productivity, survival, disease resistance, wood quality parameters), but the production of stool beds to provide material to establish large-scale plantations of these new genotypes also will needs to be developed before they can be implemented in large-scale production.

BIOFUELS INFORMATION CENTER (BIC)

National Renewable Energy Laboratory

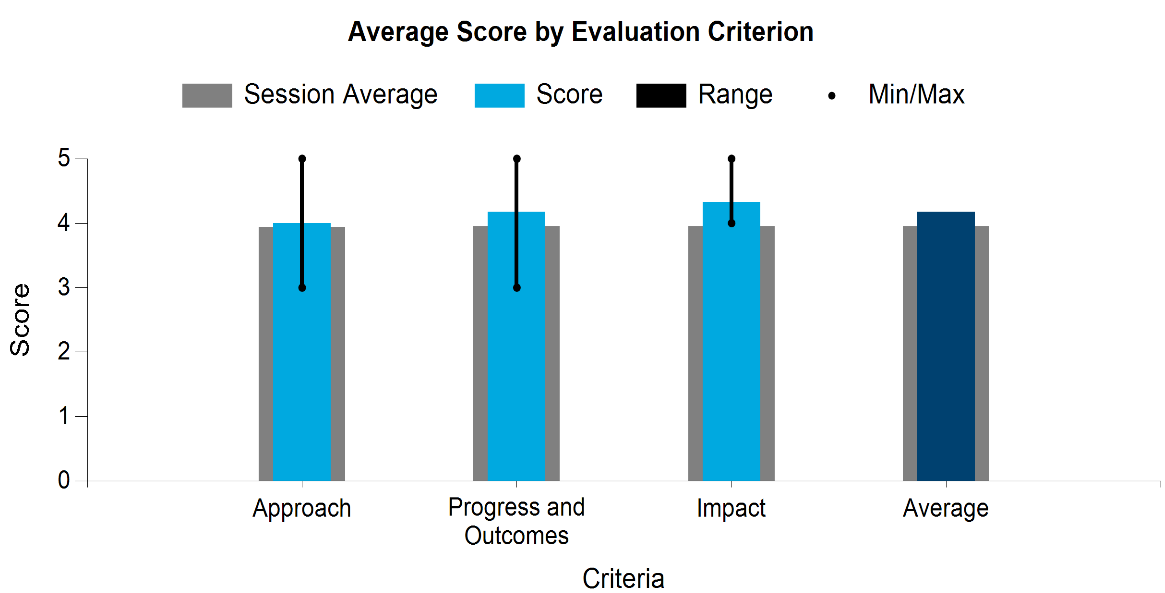
PROJECT DESCRIPTION

WBS:	6.3.0.1
Presenter(s):	Kristi Moriarty
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2025
Total Funding:	$1,060,000

The purpose of the BIC task is to provide relevant data, information, reports, and web-based tools to all bioenergy stakeholders. The BIC task began in FY 2008 to meet the requirement under Title II, Sec. 229 of the Energy Independence and Security Act of 2007, which requires DOE to develop a "Biofuels and Biorefinery Information Center."

The BIC task supports biofuels pages content on EERE's most visited website, the Alternative Fuels Data Center (http://www.afdc.energy.gov), and the BioEnergy Atlas tools (currently archived; previous address https://maps.nrel.gov). This task results in more than 1.7 million webpage views per year. In FY 2022, the task completed the final year of the five-year USDA Biofuels Infrastructure Partnership (BIP). The BIP expanded infrastructure for E15 and/or E85 to approximately 850 stations, and NREL received and reviewed data for quality and analyzed all infrastructure and sales data collected by USDA. Stations are privately held, and previously it was difficult to ascertain infrastructure and sales data. This unique data set allows insight into infrastructure data (number of pumps and tanks, cost to install new equipment) and sales data (price and volume for E10, E15, E85, and diesel by month). The 2021 BIP national summary report is with DOE for review prior to publication. Future work will include the biannual *Bioenergy Industry Status Report* (four previous versions have been published).

The task also supports the PI's time to engage stakeholders on infrastructure and the deployment of biofuels. This includes leading, membership, and participation in the following roles: member of the board of advisors at the Fuels Institute, voting member for multiple UL standards committees, co-chair of the Infrastructure Team at Agriculture/Auto/Ethanol, and member of the Coordination Research Council's ULSD Corrosion Committee. The PI routinely responds to industry inquires to assist in the regular deployment of biofuels.



COMMENTS

- The data products and visualizations generated by this project are important for a wide array of stakeholders. Overall, the BIC is a valuable public resource. I have no criticisms with regard to the approach and impact. My main suggestion is that the project team should consider how they might begin to provide information on biochemicals. It would be very valuable to visualize for the public where bio-based chemicals are being produced.

- Thank you for the opportunity to review the BIC, a project that is well aligned with BETO's goals. The BIC website provides comprehensive and valuable information on biofuels, and its progress and outcomes demonstrate that it is on schedule. The addition of bioenergy-based chemicals to the repository is a positive development, and efforts to improve data quality will be beneficial to all stakeholders. One opportunity for improvement is to better capture the impact of the project beyond page views, such as through user feedback or case studies. Additionally, it may be worth exploring the use of BIC as a tool for BETO modeling groups to better exchange and track various model output data streams. As many of the projects have shown, there is immense inter-dependability across frameworks, and it is difficult to keep data consistently updated, track which model output came from which run, and substitute models that become discontinued in such an interconnected framework. Overall, BIC is a valuable resource for stakeholders in the biofuels industry.

- This project has a very clear objective and role, and the relevance and importance of the project is underscored by its wide adoption, as measured in page views. This project fills an important niche because the data are extremely challenging to collect and yet they are compiled in one convenient place with excellent organization and data visualization. Beyond page views, it appears that this project has also attracted significant attention from industry and policymakers.

- This project is very helpful in maintaining an open and transparent information economy around bioenergy. The project team has clearly collaborated with related projects, advisory boards, and different agencies to provide data, information, reports, and web-based tools to a wide range of users. The project team has made progress toward addressing their goals. BIC will have immediate beneficial impacts to many people and organizations and is worthy of funding. I encourage the project team to consider how BIC can be used to further the understanding of diversity and equity issues related to bioenergy development. There are many ways in which these web tools are helpful in that regard, but emphasizing those more could help align this work with broader DOE goals.

- This project is crucial to bringing data from USDA's BIP to the public. Time spent cleaning and confirming the validity of data is valuable and will enhance the accuracy of all future modeling.

  The partnership between USDA and DOE for this program is an important one and is a strong component of this program. Stakeholder engagement with other agencies, industry, and academic institutions is comprehensive.

  The annual cadence of updating the model is appropriate and useful without being too frequent.

  Because public engagement and the usability of data are goals of this project, it is important to measure and report on the use in the form of page views, time spent on the website, downloads, etc. It would also be useful to measure user satisfaction and gather recommendations for improvements.

- Despite the limited budget, this project has curated a great number of easily accessible resources that have benefited a wide group of stakeholders (nearly 1.8 million page visits in FY 2022). The team is also adjusting/updating the information based on user inputs and trends (e.g., adding an SAF page). With the high level of interest in SAF, this project will likely have more users in the next few years, and some platforms and data collection methods can be modernized to enable easier usage and improve efficiency. Other web portals (e.g., the Bioenergy KDF) could also include links to BIC to increase accessibility.

PI RESPONSE TO REVIEWER COMMENTS

- The PI thanks the reviewers for their comments. Biochemicals: The project will include biochemical data and information in the *Bioenergy Industry Status Report* (FY 2023) and the revived BioEnergy Atlas tools where possible (FY 2024). Diversity and equity: The project will include appropriate data layers in the revived BioEnergy Atlas tools. Stakeholder engagement: The project will seek input and recommendations from Alternative Fuels Data Center users. BETO modeling groups and outputs is appropriate for ORNL's KDF project rather than BIC.

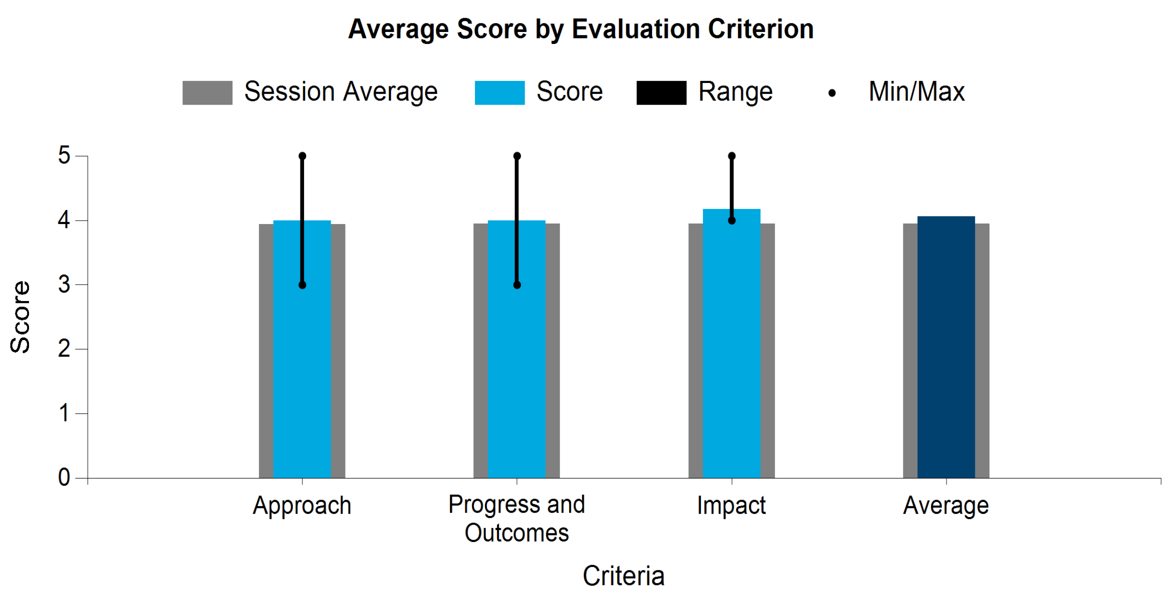
BIOENERGY KNOWLEDGE DISCOVERY FRAMEWORK

Oak Ridge National Laboratory

PROJECT DESCRIPTION

WBS:	6.3.0.2
Presenter(s):	Esther Parish
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,250,000

The purpose of this project is to develop and maintain a go-to web-based repository of BETO-funded data sets, reports, and publications for researchers proposing new projects needed to accelerate decarbonization and development of the U.S. bioeconomy. The Bioenergy KDF (https://bioenergykdf.net/) has been fundamental in the previous distribution of the *Billion-Ton Report* data sets and visualization tools, and the project is currently working to develop a new database and data download interface for the next *Billion-Ton Report* (expected to be released by the end of 2023). Last year, the project worked with BETO to gather SOT, LCA, and TEA reports and data sets from across the DOE labs and make them available to researchers through one central location. The project has also been working with the Biomass Feedstock Library at INL to align the information that recent BETO FOAs stipulate each awardee must provide to the Biomass Feedstock Library at INL and the KDF at ORNL. The project has also been working to incorporate findable, accessible, interoperable, and reusable (FAIR) data principles through showcasing previously unpublished biorefinery data sets gathered through the Data Valorization project and by developing a new workflow module to automatically generate DOE Office of Scientific and Technical Information digital object identifiers for user-contributed data sets and reports with a standard KDF prefix and a human-readable inset value (e.g., 10.23720/BT23/XXXXXX).



COMMENTS

- The recent progress toward developing new capabilities of the Bioenergy KDF has been highly encouraging. This is an excellent project with a good approach and strong potential for impact. The unknown factor has always been whether the project leads will be able to develop tools and resources that are sufficiently accessible and understandable to potential users. In many ways, the project is finding success here: The goal to make data and data sets FAIR is being realized. For example, the TEA spreadsheet on the landing page synthesizes critical research that is useful to a wide array of stakeholders in an easily accessible way. Creating a tool to mint new digital object identifier numbers, and using a dedicated prefix, will also make research more easily discoverable. My main feedback is to keep seeking new ways to make more of these data FAIR.

- I appreciate the opportunity to review the Bioenergy KDF project. The project is well aligned with BETO achieving its goals, as an excellent repository of BETO-funded data sets, reports, and publications. The team has made significant progress in adding numerous features and tools, and they focused on researchers as the primary target user. The project could focus more or investigate the feasibility and usefulness of facilitating data exchange between BETO researchers. The project has excellent potential for impact, considering outreach to users; however, the team should consider including usability experience to improve user-friendliness and creating more opportunities for data sharing across tools and frameworks.

- This project has a very clear role in the portfolio and excels at it. It provides a comprehensive repository of BETO resources and makes them accessible for users. Recent updates to the website have improved the user interface and even consolidated complex TEA data to make it easier to cross-reference. The user data suggest that in terms of page views, the popularity of the portal is growing. It could be helpful to develop other metrics to track uptake.

- The goal of this project is to develop and maintain a go-to web-based repository of BETO-funded data sets, reports, and publications. One primary audience is researchers proposing new projects needed to accelerate the decarbonization and development of the U.S. bioeconomy.

  To date, the webpage reflects BETO's emphasis on the economic and environmental dimensions of sustainability. As DOE tries to engage more with questions about equity, socioeconomic impact, and access to decision making, BETO should also move in this direction, and the webpage should reflect these important aspects of sustainable technological development.

  I would love to see more of the platform's emphasis on EEEJ—either weaving it throughout by highlighting how the different databases and models speak to these issues or having a designated landing page. If the terms *energy equity* or *environmental justice* are too esoteric, maybe talk about impacted communities on a section of the outreach page? Maybe this could go under the sustainability tab on the webpage? Is this something the ASEC projects cover? What was the focus of those three projects?

- This project provides excellent access to data and improves the usability of research. The new Office of Scientific and Technical Information and DOI system appears to be useful categorical hygiene.

  While government and lab teams are likely to be aware that this resource exists, it would be good to have an outlined outreach plan to industry to use this system with documented results.

  Previous commenters have asked for site usage, and KDF is currently getting registered with appropriate security measures to allow for that reporting. These metrics are important but may not tell the whole story because value may come not only from the volume of use and number of users but also the quality of use as well. Please also include metrics on quality, such as demographics of users, data accessed, and user satisfaction.

- KDF is a good example of the FAIR principles and has the potential to be the centralized repository for BETO's DMA work. Visualization of the *Billion-Ton Report* has been of great help to researchers. Future work should consider consolidating BETO's models and databases (e.g., with INL's Bioenergy Feedstock Library) so that regular users can just use KDF to find and navigate the resources they want. Additionally, when presenting the *Billion-Ton Report*, it would be great if factors in addition to cost (e.g., GHG emissions, water availability) can be presented together with cost.

PI RESPONSE TO REVIEWER COMMENTS

- ORNL's Bioenergy KDF team would like to thank all the reviewers for their constructive feedback. We will continue to work on making the Bioenergy KDF data sets more FAIR. Google Analytics was deemed a security risk, but we have now installed a Siteimprove tool that will help us gather and track metrics associated with user demographics and interaction with the various pages and tools housed on the Bioenergy KDF. We have also arranged for a usability experience expert to help us design the new 2023 *Billion-Ton Report* data visualization and download tool that will be rolled out near the end of 2023. We will seek to facilitate ways to help BETO researchers exchange data sets with one another through this shared platform, and we will work with BETO to possibly design a landing page to reflect the new and ongoing efforts related to EEEJ. The focus of the three ASEC projects has been on gathering field measurements and environmental metrics associated with dedicated energy crop production: The ASEC project led by the University of Illinois is focused on advanced switchgrass cultivars, the ASEC project led by Texas A&M is working with three new genotypes of energy cane and three new genotypes of biomass sorghum, and the ASEC project led by North Carolina State University was focused on the production of miscanthus.

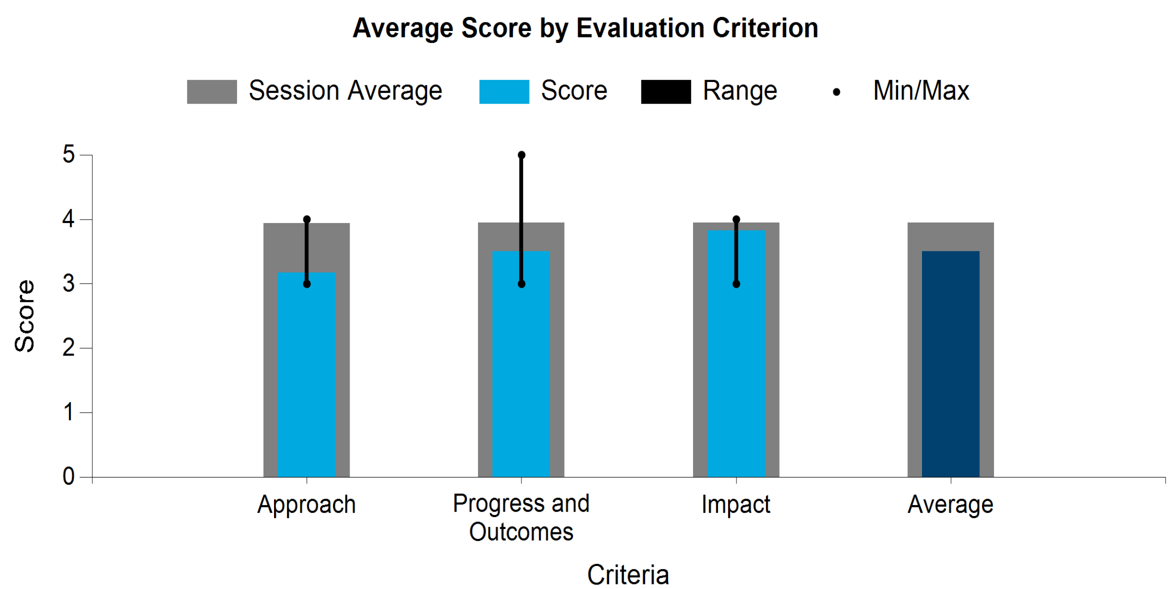
NET-ZERO CARBON TECH TEAM

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	NetZero
Presenter(s):	Aye Meyer; Hannah Goldstein; Ling Tao; Michael Wang; Uisung Li
Project Start Date:	01/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,050,000

The NZTT is tasked with investigating the potential to generate carbon-based fuels with much lower carbon intensities compared to those of conventional fuels, approaching or exceeding net-zero GHG emissions. In this project, researchers from four national laboratories (ANL, Lawrence Livermore National Laboratory, NREL, and PNNL) have teamed up to evaluate carbon conversion pathways for their potential to produce net-zero carbon fuels. This project directly supports BETO's missions on carbon reduction and SAF conversion strategies by collaborating with the U.S. DRIVE NZTT formed by industry experts. In FY 2020–2021, four fuel pathways were selected for scrutiny to discern their costs and benefits and their ability to provide net-zero-carbon fuels. In FY 2021–2022, six more fuel pathways were selected for scrutiny to discern their costs and benefits and their ability to provide net-zero-carbon fuels. These pathways represent a diverse set of options for producing net-zero-carbon fuels, covering a range of feedstocks, process inputs, products, coproducts, environmental impacts, and technical maturities. The project team concludes that multiple pathways exist to produce commercial net-zero-carbon fuels. Most pathways require both technical maturation of core conversion processes and one or more process inputs (e.g., feedstock, electricity, process heat) to be substantially decarbonized to deliver a net-zero product. The uniqueness and key contribution of this study is that both sustainability constraints and cost perspectives are simultaneously investigated, so, consequently, this integrated study can quantify the impacts of a variety of economic and environmental metrics. Applying this simultaneous analysis approach to several highly varying technologies allows for the identification of overarching trends, such as those highlighted in previous sections. This current analysis, together with future studies, can inform strategic decisions for the development of future net-zero-carbon fuel production technologies.



COMMENTS

- Overall, this project makes a lot of sense. The identification of liquid fuel pathways that could approach net-zero carbon is a worthy goal with potentially substantial impacts. This project could make substantial contributions in that area. But I see two weaknesses in the approach that I am hoping the researchers can amend going forward.

  First, while the TEA modeling appears to consider financial uncertainty case by case, as shown in the error bars on slide 11 of the presentation, the LCA results for each case do not appear to consider uncertainty in emissions. When considering which liquid fuel pathways have the greatest chance of reaching carbon neutrality, one very significant consideration is which pathways start with greater or larger downside risk of emissions. The greater the risk of high emissions, the less attractive the pathway should be from a strategic perspective if the goal is carbon neutrality. Looking at the appendix slides, it appears that the various cases consider different sources of process energy, which is one source of uncertainty worth considering. But it does not appear that the upstream risk associated with feedstock cultivation/collection is considered. This risk exists to some extent for corn stover because too much removal may lead to a loss in soil C. But the risk is substantially greater for corn to ETOH. It also appears that the risk of carbon leakage is not being quantified in the scenarios. For CCUS pathways, these risks need to be quantified with appropriate methods, and it is strange to see them missing from slide 11. The recent National Academy of Sciences study on biofuel LCA methods provides a good guide to the key considerations for this type of methodology (https://doi.org/10.17226/26402). Future work in this area needs to make uncertainty analysis a core part of the LCA scope.

  Second, there appears to be a mismatch between the goals of the project and the downselection of pathways for deeper analysis. A large amount of the analysis presented to the reviewers focuses on corn ethanol to jet fuel pathways. Looking at slide 13, however, it appears that corn ATJ has some of the highest potential emissions and least potential for negative emissions. Focusing on corn ATJ over the stover, biomass gasification to Fischer Tropsch and wet waste HTL pathways does not seem to make sense from a deep decarbonization perspective. Perhaps this was simply a case where an odd example was selected to illustrate the larger project. But I would hope that in the final year of the project the researchers would narrow more of their focus to those pathways with greater potential for deep decarbonization rather than spending further resources quantifying the emissions of corn ATJ.

- Thank you for the opportunity to review the NZTT project. From my evaluation, the project is reasonably aligned with BETO achieving their goals. The team has made progress in investigating different pathways and feedstocks, adding decarbonization strategies and fuel pathways across a significant number of combinations. The project's impact is substantial, with outreach to the fuel industry, electric partners, and automobile sectors; however, the team should consider investigating methods to better show results across large numbers of fuel production pathways and better reflecting on uncertainty to more effectively communicate with stakeholders.

- The increased focus on net-zero goals makes this a very timely and relevant project. It nicely combines the technology area's existing research and expertise with TEA and LCA and puts it into a new perspective, evaluating all the different technology levers to reduce the GHG intensity of existing or future fuel pathways, and then estimating the incremental cost impact of those interventions. There is a natural synergy with the use of GREET to evaluate the LCA impacts of technology changes along the supply chain and NREL's TEA expertise. In terms of the project design and progress, I think the project has a very clear path forward. There is high relevance to the SAF Grand Challenge and very meaningful partnerships to be developed with industry groups.

  In terms of fitting within BETO's overall strategy, I do have some minor concerns. In contrast to most other projects in this technology area, this work appears to be largely focused on incremental changes and benefits for existing, commercialized technologies (at least based on the initial progress). While this is laudable, I am wondering if the relatively low costs and high opportunities for incremental gains here may crowd out interest in some of the more challenging feedstocks. There also appears to be some optimism associated with CCS results versus real-world practices that may overstate the potential for CCS. It would be helpful to expand the analysis to more feedstocks emphasized in other DMA projects and to include error bars to show a wider, more realistic range of CCS outcomes for the selected fuel pathways.

- The NZTT seeks to investigate options for generating liquid carbon-based fuels with a reduced carbon intensity such that, from a life cycle carbon accounting standpoint, they have a net carbon emissions profile approaching zero. This goal requires more than 400 biorefineries, and 1 billion tons of biomass and/or gaseous carbon oxide feedstock will be needed to produce 35 billion gallons/year by 2050. Where will all of this take place? How will the siting of biorefineries occur? How can this team collaborate with other groups who are looking at the EJ implications of feedstock production and refining?

  Each different feedstock has its own set of supply chain challenges—how are these accounted for?

- This project has successfully demonstrated pathways to reach net-neutral liquid fuel biofuel production along with the costs and trade-offs of those options. While a national-only evaluation could result in overlooking regional drivers of decarbonization, the inclusion of regional complexities of CCS and CCU drivers help to mitigate that risk. Of particular note, this project has a comprehensive and clear engagement with many stakeholders across the academic, industry, and policy sectors that it touches.

  This project is missing an evaluation of EJ and could incorporate it to strengthen its outcomes.

- This is a multi-national lab effort that leverages various BETO models to examine the various technology pathways for sustainable bioenergy. It involves the federal government and various industry partners (electric utility, fuel, automobile) with regular meetings. Work on this scale is needed to leverage and synthesize BETO's DMA efforts and map out a blueprint for bioenergy decarbonization. The main recommendations are to rigorously consider uncertainties in the analyses (especially LCA) and to make the analyses (including underlying models, assumptions, etc.) and their results publicly available so that they can be used by other researchers and industries to tailor the analyses to their individual needs.

PI RESPONSE TO REVIEWER COMMENTS

- We sincerely appreciate the reviewers' recognition of the importance and contributions of this project's efforts for the last two years to the BETO program. The main objective of this project is to identify and evaluate the economic and environmental implications of various potential pathways for net-zero-carbon fuel production. The research scope and directions of this project have been actively discussed with the engaged industry stakeholders (U.S. DRIVE NZTT) and DOE to ensure the optimal utilization of available project resources and alignment with DOE's decarbonization strategies.

  Regarding the suggestion on performing more uncertainty analysis, our team has evaluated pathways for future fuel production instead of only analyzing existing fuel production pathways; thus, this analysis heavily relies on process modeling because industry data sets that illustrate the possible ranges of each parameter are currently unavailable. Consequently, conducting uncertainty analysis and generating error bars with limited information can potentially lead to misleading results. Even if there were available data sets, conducting uncertainty analysis (e.g., stochastic and/or sensitivity analysis) would require significant efforts to collect, process, and analyze the data. While we acknowledge the importance of analyzing uncertainties to provide valuable information about the risks associated with these pathways, it was not the primary focus of our analysis in this project. The project team has been focused on identification opportunities and challenges of various fuel production pathways under different low-carbon technology options. To evaluate uncertainty and risks associated with these pathways, a separate and more dedicated effort would be necessary.

Certain other outstanding issues, such as the impact of SOC change resulting from corn stover removal and emissions leakage from carbon capture and sequestration, are being evaluated by other DOE projects and expected to be further assessed. Analyzing these specific impacts is beyond the scope of this project. The uncertainties associated with CCS significantly vary based on factors such as capture technologies, capture efficiencies, the volume of gas captured, geological locations, and storage efficiencies. Similarly, assessing the ranges of these parameters falls outside the scope of this project. Moving forward, the project team will provide qualitative assessments of uncertainties, risks, and associated implications in the technical reports. The primary focus was to determine the availability of low-carbon liquid fuel production options in the near future and assess the associated resource utilization, so we did have extensive discussion and considerations on pathway or feedstock choices.

In response to the reviewers' comments on the pathway selections and consideration of biomass feedstocks, the selection process for feedstocks, conversion technologies, and decarbonization options not only heavily relied on the feedback and input from these stakeholders but also was a result of extensive discussions among NZTT team and subject matter experts. One distinguishing factor of this project compared to others is its strong communication with industry stakeholders. In addition, the presentation of the corn ethanol-derived jet fuel production pathway among other evaluated pathways was not a random choice; it was intentionally included to showcase the potential of emission reductions through various options. It is also because the main goal of this project is to identify opportunities and challenges associated with various net-zero-carbon fuel production pathways rather than conduct a screening solely based on carbon intensity scores. To meet the U.S. SAF Grand Challenge volume targets of 3 billion gallons/year by 2030 and 35 billion gallons/year by 2050, all possible available low-carbon SAF production pathways will need to be used. As a result, we incorporated a variety of feedstocks (cellulosic biomass, wet waste, and waste CO_2) and a wide spectrum of conversion pathways, although we only presented the corn ethanol ATJ case during the BETO Project Peer Review. We do believe creating a balanced and comprehensive portfolio is crucial, so we plan to provide defensible analysis results to assist DOE and stakeholders in building a decarbonization road map.

We would like to thank the reviewers for their insightful questions on the siting of the future biorefineries and EJ-related complications. The analyses presented in the project encompass the initial two-year efforts primarily focusing on integrating TEA and LCA for decarbonization strategies. The team and our industry collaborators did recognize the importance of regional implications for future biorefineries, so the project has shifted its focus toward evaluating regional aspects that encompass factors such as feedstock availability, renewable electricity, water, and infrastructure in the third year as ongoing efforts. Similarly, related to the comments on CCS, our evaluation primarily accounted for the reduction in GHG emissions and the incremental cost associated with implementing CCS. Starting from the third year, our team began evaluating regional factors in various pathways to incorporate more realistic conditions, such as the transportation of CO_2 from the source to storage, to provide additional perspectives. This comprehensive evaluation aims to identify both the challenges and opportunities associated with the selected pathways, ultimately assisting in the strategic siting of biorefineries. While evaluating EJ falls outside the specific scope of this project, we believe that the project's outcomes can serve as inputs for assessing the EJ implications at a regional level. By considering the broader regional context and incorporating the findings of this project, stakeholders and BETO can gain insights into the potential EJ implications related to the implementation of the selected pathways. We recognize this is an important subject, and we will consider incorporating EJ with our analysis in the future.

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Feedstock-Conversion Interface Consortium (FCIC) is one of 12 technology areas that were reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 11 presentations were reviewed in the FCIC session by six external experts from industry, academia, consulting, and other government agencies. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer the corresponding Program and Technology Area Overview presentation slide decks, which can be accessed at the Peer Review website: www.energy.gov/eere/bioenergy/2023-project-peer-review.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $33.2 million, which represents approximately 6% of the BETO portfolio reviewed during the 2023 Peer Review. During the Project Peer Review meeting, the presenter for each project was given 10–20 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Mark Elless as the FCIC review lead, with contractor support from Atilio de Frias of Allegheny Science and Technology. In this capacity, Mark Elless was responsible for all aspects of review planning and implementation.

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM REVIEW PANEL

Name	Affiliation
Mr. Philip Weathers*	Weathers Associates Consulting
Mr. Chris Burk	Lee Enterprises Consulting
Ms. Bryna Guriel	Genomatica
Ms. Vicky Putsche	VLP Consulting Company
Dr. Julie Tucker	U.S. Department of Agriculture Forest Service
Dr. Paul Weider	Retired (Shell Oil)

* Lead Reviewer

FCIC REVIEW PANEL SUMMARY REPORT

Prepared by the FCIC Review Panel

INTRODUCTION

The FCIC is a collaborative program among nine different national laboratories, comprised of nine project tasks and one management task. The strategic focus of the consortium is to develop first-principles-based knowledge and tools to understand and mitigate the effects of biomass feedstock and process variability on biorefineries.

The program starts with the feedstock variability incurred during growth, harvest, and storage through preprocessing and into the throat of both high-temperature and low-temperature conversion reactors. The intent of the project tasks is to develop and implement mitigation strategies and tools to overcome the feedstock- and process-induced variability in the integrated operations of biorefineries.

The program also has crosscutting tasks to analyze the impact of these mitigation approaches on system reliability and process economics, as well as the environmental impacts of the integrated process. Future work will continue to optimize feedstock cost by developing high-value coproducts as well as by reducing the variability. The program also calls for in-line sensors and control logic to reduce the process variability and improve system reliability.

This feedback from the Peer Review panel will discuss how well the strategy has been implemented across the project tasks, the level of involvement of industry and other stakeholders, and the success the program has had in communicating and applying the tools that have been developed. The Peer Review panel will also offer key recommendations on how the program should evolve.

STRATEGY

The FCIC has a clear mission, which is defined as developing first-principles-based knowledge and tools to understand and mitigate the effects of biomass feedstock and process variability on biorefineries. The review panel recognizes that each of the tasks has individual goals and milestones. However, the reviewers felt the overall program lacked measurable goals and desired outcomes. Each individual task demonstrated the impact it had on a specific aspect of performance, but there needs to be a more complete demonstration and integration of the impact on the entire process, from preprocessing to the throat of the reactor. The panel did not observe significant collaboration across the tasks where the learnings from one task were being applied in the downstream tasks. One specific example was the lack of use of the characterization techniques developed by Task 2 in other tasks of the program.

There is a clear need for initial techno-economic models in each of the tasks, as well as interim techno-economic analyses (TEAs), as progress is made in improving operational reliability and minimum fuel selling price (MFSP). The lack of initial and progressive techno-economic models/analysis was identified as one of the primary gaps in assessing and achieving the strategic outcomes desired by this program.

The processes of feedstock growth, harvest, and storage are not adequately addressed in terms of their contribution to feedstock variability. The use of air classification for anatomical fractionation was mentioned in multiple reviews, but it is not clear whether fractionation is an economical way of reducing downstream variability or improving operational reliability. A TEA looking at the economic impact of discarding a significant portion of the biomass or processing the fractions separately would help determine whether fractionation is worth pursuing further.

Storage has been considered in terms of the impact of feedstock degradation, especially in bales of biomass; however, the potential of bale fires in corn stover, as experienced in pioneer biorefineries, necessitates that other storage formats of biomass be considered. Pelletizing and silage-style storage are two possibilities. An initial TEA and looking at technology to lower the cost and improve the life cycle analysis (LCA) of these alternatives should be conducted.

Although the FCIC mission includes the introduction of biomass to the throat of the reactor, this has not been thoroughly addressed. Flow of biomass into the reactor against pressure is an area of concern for biorefineries. The biomass coming into the reactor could be dry or mixed with another medium such as high-pressure steam. This is a technology gap that should be confirmed with industry and potentially added to the portfolio of FCIC tasks.

The review panel noted that the research done by the labs was excellent quality but appeared more academic in context. The FCIC program should be complimented on holding an information session with stakeholders and doing at least one industry survey for high-temperature conversion. To maintain program relevance, engagement with industry and other stakeholders must be an ongoing process. Stakeholder engagement should increase in both depth and breadth. The FCIC Industry Advisory Board (IAB) needs wider participation from biorefineries, technology providers, and the equipment industry. FCIC should consider adding representation from other federal agencies, such as the U.S. Forest Service and U.S. Department of Agriculture (USDA).

The use of additional information-gathering sessions could also help revise the priorities of the program. The program should consider gathering representatives from active biorefinery projects as well as from projects that failed to move to demonstration or commercialization, which could be useful in refining the list of critical priorities. These sessions should incorporate input from the Sustainable Aviation Fuel (SAF) Challenge and Multi-Year Program Plan 2023 (MYPP23) documents. BETO could also consider a coordinator to act as an interface between the consortia (FCIC, Conversion, etc.) and industry to both gather the needs of industry and communicate the technology and tools available at the national labs.

The use of funding opportunity announcements (FOAs) and cooperative research and development agreements (CRADAs) should be strengthened to move FCIC and national lab researchers closer to industry and other stakeholders. Each FOA/CRADA should have a participant(s) from the national labs to transfer the technology and learnings of FCIC and other consortia to the project as well as to identify additional gaps or risks that the national labs should be mitigating. Annual operating plan (AOP) funding could also be used to support researchers visiting biorefinery pilot and demonstration facilities to better understand the issues of operation. Preprocessing and material handling should consider doing experimental verification at equipment vendors' locations.

Diversity, equity, and inclusion (DEI) continues to be a work in progress. The FCIC task teams have tried to put together activities to support the intent of DEI, but the effectiveness varies between the tasks and is clearly challenging when taking a bottom-up approach without upper-level support or drive. The DEI effort needs to be more focused on specific, measurable, achievable, relevant, and time-bound (SMART) goals: for instance, the number of minority interns or postdocs who are part of the team, the percent of funding for minority-serving institution (MSI) researchers as part of the team, the number of field days hosted for science, technology, engineering, and mathematics (STEM) classes at national labs, a community-specific website, and information day events. One suggestion would be to focus DEI activity coordination at the FCIC or BETO management levels. Coordination activity could include setting specific goals and identifying activities and milestones for each of the task areas. A specific presentation of the DEI progress and impact could be part of the Peer Review.

STRATEGY IMPLEMENTATION AND PROGRESS

The funding for FCIC has been supporting the area of feedstock variability, specifically in the area of material handling and flowability. The tasks focused on preprocessing and material handling are most closely aligned with the priority of flowability. In each case, however, the focus is somewhat narrow. Preprocessing has focused most of its work on knife milling, with minimal effort being reported on other methods of comminution. Material handling has focused much of its work on hopper flow, with no studies of material conveyance in pipes, which is a source of concern while moving biomass from one unit operation to another in biorefineries. The panel also noted that significant effort has been spent on anatomical fractionation using air classification. The value of anatomical fractionation in improving the economics or operational reliability is unclear and may not add much value to the strategic goals. As a side observation, anatomical fractionation was tried in the cellulosic ethanol industry in the late 1970s.

The High-Temperature Conversion task has developed first-principles models for particle behavior in the reactor. The work of this task is at the leading edge of the technology. However, the models do not appear to address the introduction of the feedstock into the reactor throat against a pressure boundary, which is a primary barrier to biorefinery performance.

The Low-Temperature Conversion task has developed statistical models to determine the impact of feedstock variability on process yield. Much of the effort to date has been in comparing drought-stressed to non-drought-stressed corn stover, which showed insignificant differences in product yield. The task should demonstrate that their approach can identify differences in feedstock variability that impact process variability and recommend process changes to mitigate these differences.

With the recent publication of the SAF Grand Challenge Roadmap and the MYPP23 documents, the technology managers may want to consider a restatement of the program goals to better align with these recent strategies. This program has the potential to advance the supply, lower the cost, and improve the quality of feedstocks, which can improve operational reliability of biorefineries and lower the cost of SAF. Its goals and funding should support these strategies.

In addition, BETO should encourage direct interaction between FCIC/national lab researchers and industry using FOA, CRADA, and AOP funding sources. The increased engagement with industry, through multiple channels, is perhaps the best way of ensuring beneficial outcomes for both BETO and its industry partners.

RECOMMENDATIONS

- Strategic Alignment
    - Ensure that the mission of FCIC is aligned with the goals of the SAF Roadmap and MYPP23.
        - Focus on increasing the supply, improving the quality/consistency, and lowering the cost of the feedstock going to the biorefinery.
        - Ensure that all tasks are considering the three identified program feedstocks (corn stover, forest residue/thinnings, and municipal solid waste [MSW]).
        - Solicit input/feedback on FCIC activities and strategy from other federal agencies, such as the USDA and U.S. Forest Service.
        - Consider adding purpose-grown energy crops to the portfolio for evaluation.
    - Evaluate the feasibility and economics of pelletizing feedstock.
        - Consider using blended feedstocks of stover, forest residue, and MSW.
        - Focus on lower-cost pelletizing with improved consistency and quality.
    - Integrate FCIC learnings across the FCIC tasks.
        - Utilize the critical quality attributes (CQAs) from Task 2 in the downstream tasks.
        - Expand the work from Task 2 to include the upstream supply chain (growth, harvest, and storage).
        - Establish feedback from the conversion tasks to the upstream tasks to guide the mitigation of challenges and risks identified in the biorefinery.
- Strategic Partnerships
    - Industry
        - Expand the membership of the IAB to include representatives from biorefineries, especially at the demonstration and pioneer scale.

        - Use AOP and CRADA funding to enable researchers or staff to spend time in biorefineries to observe the operating issues firsthand and provide feedback to FCIC and the labs.
        - Fund FCIC/national lab participation in FOAs and CRADAs for pilot, demonstration, and pioneer plants.
        - Fund FCIC staff to work in equipment manufacturer facilities to utilize the models developed by FCIC and run verification on production-scale equipment.
    - Federal Agencies
        - Solicit input/feedback from the USDA and the U.S. Forest Service on improving feedstock availability, cost, and quality/consistency.
- Economic and Environmental Impact
    - TEA/Techno-Economic Modeling
        - Require an initial TEA/techno-economic model (TEM) for each task.
            - Update the models as the tasks progress, and use the level of improvement as interim goals.
            - Include the impact on MFSP and internal rate of return (IRR).
        - Require an initial TEA/TEM for FOAs and CRADAs.
            - Update the models at specified milestones.
            - Include the impact on MFSP and IRR.
        - Continue the application of scenario TEAs (Task 8).
            - Work with industry applications/scenarios to demonstrate the economic benefit of process alternatives.
    - Require LCA goals and calculations for tasks and FOAs.
        - Update LCA models at specified milestones.
- Measurable Goals
    - The overall FCIC program should have measurable (SMART) goals.
        - Progress toward these goals should be part of the Peer Review presentation.
        - Each task should ensure that the goals cover the use of all three feedstocks and consider a broader range of process options (such as multiple methods for comminution in preprocessing).
        - Each Peer Review presentation should discuss the progress in meeting the milestone timeline for the project.
- DEI
    - Consider consolidating the DEI efforts at the FCIC or BETO level.
        - Assign a DEI coordinator to work with the task teams in developing meaningful activities.
        - Give a DEI program update presentation at the Peer Review.
    - The DEI effort should be focused on SMART goals, for instance:
        - The number of minority interns or postdocs who are part of the team
        - The percent funding of MSI researchers as part of the team
        - The number of field days hosted for STEM classes at national labs
        - A community-specific website and information days.

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM PROGRAMMATIC RESPONSE

INTRODUCTION

BETO would like to thank the reviewers for their detailed comments and review of the projects involved in the FCIC.

Based on the recommendations from the Fiscal Year (FY) 2021 Peer Review panelists, FCIC (a) implemented more SMART metrics, such as clear 1-year and 3-year outcomes, with an emphasis on examining new feedstocks for production of SAF; (b) continued to develop tools and knowledge for use by industry; and (c) released the FY 2023 CRADA call for more meaningful and diverse industry engagement. The office included many of these recommendations in its guidance and requirements as part of the FY 2022–2024 merit review process.

The recommendations listed above from the FY 2023 Peer Review panelists seek to extend these previous recommendations by aligning FCIC more strategically with the SAF Roadmap, developing more strategic partnerships with industry, further assessing the economic and environmental impacts of the tools developed, continuing to use SMART goals, and engaging in more meaningful DEI efforts, perhaps at the program rather than project level. Our response to these recommendations is given below.

Recommendation 1: Strategic Alignment

The reviewers noted that BETO should ensure that the mission of the FCIC is aligned to the SAF Roadmap and MYPP23. Specifically, FCIC should continue to (a) increase the supply, improve the quality, and lower the cost of producing conversion-ready feedstocks to the biorefinery; (b) ensure that all tasks consider the FCIC feedstocks (corn stover, pine residues/thinnings, and MSW); (c) solicit input from other federal agencies (e.g., USDA, Forest Service); and (d) consider adding a purpose-grown energy crop to the portfolio. The reviewers also noted that the flexibility and economics of pelletizing feedstocks should be evaluated, with blending of the three FCIC feedstocks considered and a focus on lower-cost pelletizing with improved consistency and quality. Finally, the reviewers recommend that BETO integrate the learnings of FCIC across all FCIC tasks by utilizing CQAs from Task 2 in all downstream tasks, expand Task 2 activities to include upstream activities, and establish feedback from the conversion tasks to the upstream tasks to guide future improvements.

BETO concurs with these recommendations. For several years, BETO has emphasized that increasing the supply, improving the quality, and reducing the cost are the three critical factors for producing conversion-ready feedstocks in the Renewable Carbon Resources (RCR) subprogram and will ensure that these critical factors are carried to the FCIC. While the emphasis has been on engaging industry for risk identification and tool development/effectiveness, we will solicit input from other federal agencies for their expertise in handling FCIC feedstocks and purpose-grown energy crops. Blending of feedstocks has not yet been conducted in FCIC, as a focus on individual feedstocks was deemed necessary to improve the conveyance of these feedstocks. Blending is seen as an opportunity to improve quality and/or decrease cost and remains a viable option in the future. In addition, high-moisture pelleting to reduce pelleting cost and improve conveyance has been completed in RCR; learnings from this study are available to FCIC. Finally, all of FCIC has adopted the quality-by-design (QbD) framework, with CQAs guiding the research and development (R&D) of all downstream tasks or hand offs. While upstream factors, such as growth, harvest, and storage, help inform the CQAs identified by Task 2, those upstream factors are considered outside the scope of FCIC and instead reside in RCR. Such factors are transferred to FCIC by core R&D conducted by RCR.

Lastly, the QbD framework has been adopted by other research projects outside of FCIC. For example, fast pyrolysis and sugar pretreatment projects funded in the conversion R&D space are now actively exploring the criticalities of various feedstock impurities to improve the robustness of the processes and catalysts being used.

Many FCIC researchers are involved in other research efforts within BETO and DOE-funded work, and this framework can be shared with those projects to enable their success.

Recommendation 2: Strategic Partnerships With Industry

The reviewers noted that FCIC should seek strategic partnerships with industry and federal agencies. For industry, the reviewers recommend that the IAB should include representatives from biorefineries, expand opportunities for FCIC researchers to visit biorefineries to see firsthand the problems they face, fund FCIC participation in FOAs/CRADAs for biorefineries at various scales, and fund FCIC researchers to work at equipment manufacturers to utilize the models developed by FCIC and run verification on production-scale equipment. For federal agencies, input should be solicited from the USDA and the Forest Service on improving feedstock supply, cost, and quality.

BETO strongly concurs with these recommendations. Each year, FCIC leadership examines the composition of the IAB to make sure that its members can provide insight on emerging areas of interest, and FCIC leadership will consider adding new members to this board with biorefinery experience. The partnerships to date on the previous CRADA calls have yielded high-quality collaborations and afforded opportunities for the consortium to apply the knowledge generated to date with industry. BETO awarded three projects its FY 2023 CRADA call, furthering its pursuit to transfer the tools and knowledge developed by FCIC researchers into the hands of industry. Industry response to this CRADA call was very strong and covered a variety of unit operations and fuel production pathways. The consortium will be encouraged to employ the strategies recommended by the review panel, particularly visiting biorefineries and equipment manufacturers to learn firsthand the issues that need to be solved and the modifications to existing equipment that are needed to better convey biomass. The ultimate objective of the consortium is to disseminate learnings to industry to aid in de-risking processes; success would include vendors and engineering firms using FCIC results to deliver performance-guaranteed processes and investors feeling sufficiently confident in these processes to invest. Finally, BETO has a strong collaboration with USDA, particularly through the Biomass R&D Board Interagency Working Groups on Feedstock Production and Management and Feedstock Logistics. Learnings from these working groups have and will continue to be transferred to FCIC.

Recommendation 3: Economic and Environmental Impact

The reviewers noted that initial TEAs should be included in all tasks and FCIC-related projects. BETO strongly concurs with this recommendation. BETO uses such measures to help direct the R&D of a project, providing economic considerations to inform a down-selection of possible future avenues of research. There are numerous TEAs and smaller case studies that have been developed by the experimental tasks and Task 8 that will be published in the very near future.

The environmental impact of the technology developed by FCIC is also of major importance to BETO. To help decarbonize the aviation sector, the carbon intensity of the processing needed to produce conversion-ready feedstocks that convey well in biorefineries must be kept to a minimum. Advances in unit operations that reduce those operations' energy input are needed to reduce the overall carbon footprint of the integrated system. We will ensure that all FCIC projects from FY 2024 onward will determine the carbon intensity of each unit operation examined for each feedstock. BETO acknowledges that LCA in the consortium up to this point has almost exclusively focused on carbon intensity, and other environmental sustainability considerations (water use, use of hazardous chemicals, emissions) have not been considered.

One such example is the work to evaluate milling energy consumption and associated emissions. The FCIC tasks extensively explored dry versus wet milling, and both economic and environmental trade-offs were quantified. Ultimately, it was determined that wet milling could result in economic and environmental improvements in the form of reduced electricity consumption, reduced particulate emissions, and overall improved carbon intensity.

Recommendation 4: Measurable Goals

The reviewers noted that FCIC should use SMART goals for clear assessment of goal completion. BETO concurs with this recommendation. We will continue the use of SMART goals to track progress more clearly as part of our active project management. We will ensure that future Peer Review presentations will include progress toward these goals and the expected timeline for completing these goals. In addition, BETO will ensure that all three feedstocks (i.e., corn stover, pine residues, and MSW) are represented with a range of preprocessing options for accomplishing each goal.

Recommendation 5: Diversity, Equity, and Inclusion

The panelists recommend that DEI activities should be implemented at an FCIC or BETO level, not at the project level, and that a DEI update at the program level should be provided at future Peer Reviews. BETO strongly concurs with this recommendation and with the proposed SMART metrics for tracking DEI progress. As part of the FY 2024 national laboratory funding cycle, BETO distributed updated suggestions and guidance on DEI activities. The guidance includes considerations and examples across multiple areas that researchers can consider: integrating into existing DEI program participation, opportunities for the research team, and considerations for the research process and outcomes.

In conclusion, FCIC appreciates the expert feedback from our 2023 independent peer reviewers and appreciates the overall sentiment expressed that FCIC is helping solve the conveyance issues caused by poor biomass quality that plagued the pioneer biorefineries. With the recommendations summarized above in hand, BETO will continue to improve the tool set that can be provided to future biorefineries to improve their biomass throughout. BETO looks forward to presenting the results of the FCIC to the public once again in 2025.

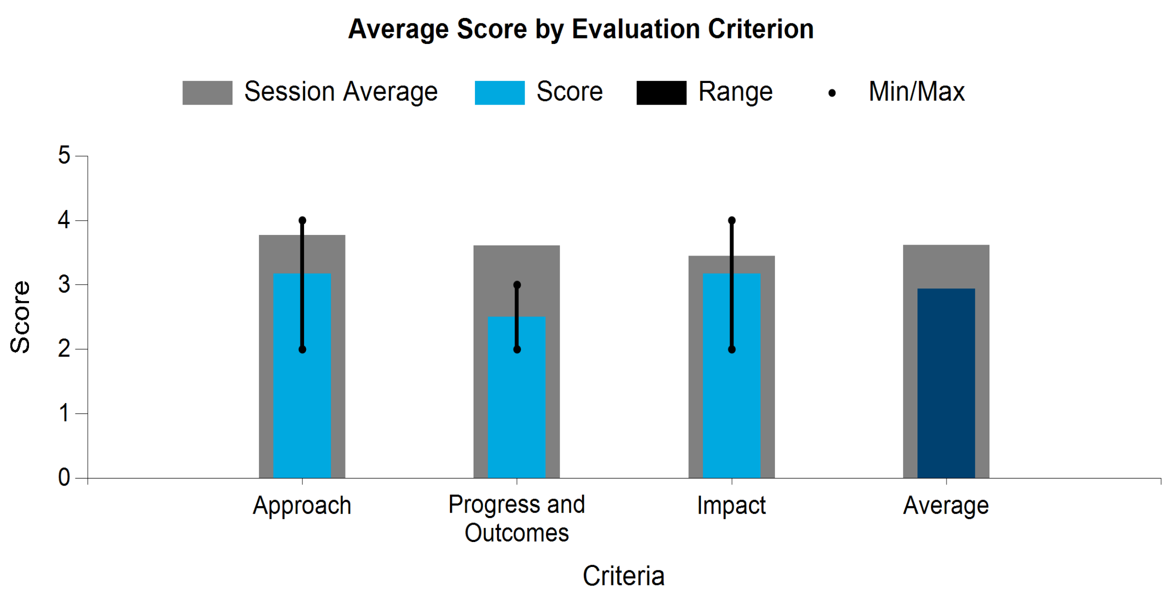
IDAHO NATIONAL LABORATORY DIRECTED FUNDING OPPORTUNITY: REAL TIME, INTEGRATED DYNAMIC CONTROL OPTIMIZATION TO IMPROVE THE OPERATIONAL RELIABILITY OF A BIOMASS DRYER

Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.2.7801
Presenter(s):	Damon Hartley
Project Start Date:	11/16/2020
Planned Project End Date:	9/30/2023
Total Funding:	$4,018,684

Variations in feedstock characteristics (e.g., particle size distribution, moisture, ash, and heat content) negatively affect the integration of biomass feeding systems and conversion processes and result in low or unreliable onstream time and long start-up times. The main objective of this project is to achieve 90% uptime of our industrial partner's low-temperature dryer and achieve the target reduction of steam exploded wood fiber moisture from about 25% to about 12% (wet basis) before densification through the development of a new, real-time, integrated dynamic control optimization solution. The goal is that the new control system will ensure the reliable, cost-effective, robust, and continuous operation of a low-temperature biomass dryer. The control system will require the development of control algorithms and the integration of various FCIC resources (e.g., sensors, in-line instrumentation, predictive modeling of mechanical behavior of biomass particles, process development unit). Upon the completion of this project, a new, real-time, integrated, dynamic, optimal adaptive control system will be demonstrated, at industrial scale, that minimizes cost while improving operating reliability and throughput and maintaining performance of a low-temperature fluidized bed biomass dryer.



COMMENTS

- The project has a real and clear industrial application; however, the actual scope and impact (cost) beyond the Idaho Forest Group is unclear. The overall TEA and LCA are needed to be able to holistically assess the impact. If successful, this appears to be a reasonable process contribution for a relatively low project cost. It is unclear whether this will be made widely available to industry or only to the Idaho Forest Group.

- The researchers are developing a sensor with the potential to improve the operation reliability of biomass drying. It is great that they are developing it in collaboration with an industry partner. They have clear performance goals for the technology (90% uptime and >90% of material having 12%–16% moisture content), but without knowing the baseline state of the technology, it is difficult to judge the potential for impact.

- The presenter took over the project 6 months ago. The project partnered with a lumber producer, which is a strength of this project. The technical challenges are well- understood and accounted for, especially in the context of operational safety issues with personnel and explosion potential. The project has been very delayed, but has worked to address the factors contributing to the delays. The project is currently not yet achieving the project objective of 90% operational reliability. The project could improve its sharing of lessons learned with industry prior to project end, especially considering that the research was done at an actual forest products facility. At the end of the presentation, the presenter said that a demonstration will occur in Idaho at a facility. This will be an important sharing of lessons learned. The potential for this project to be a significant benefit for industry is great, but the actual benefit currently appears to be low to negligible. DEI was not an objective at the outset of the project, but the presenter indicated that rural communities would benefit from project lessons learned.

- The concept of using process analytical technology to optimize a biomass drier is sound. One can use this as a feed-forward control or a produced product measurement. It appears to this reviewer that the project is significantly behind in its progress and objectives. The instrumentation selected for the measurement has not been proven to be capable of accomplishing the project objectives. The near-infrared technique is a surface technique, and the drying will take place initially on the surface, so measurement after drying is unlikely to be informative of the bulk moisture content—this is exacerbated if the particles are "chip sized." A bulk technique (time-domain nuclear magnetic resonance [TD-NMR] or even air-driven fractionation) would provide a better value than a surface technique. TD-NMR has been applied in the food industry in an online (process analytical technology) basis, but one must ask how much value is captured by making this measurement. Other methods to consider for after drying include midinfrared emissions from the hot particles.

- The project develops a dryer control algorithm to obtain the specific moisture content of the exiting pine particles. The primary control variables are feed rate and firing rate (temperature input). The project has been delayed while implementing additional safety requirements from the industrial partner. Although the project measures particle size distribution, the information is used to detect relative shifts in particle size distribution, which acts as a critical process parameter. The principal investigator (PI) should include risks/mitigations if the combination of feed rate and firing rate proves insufficient to meet the moisture content at an economically feasible output rate. The PI is requesting a 1-year, no-cost extension but has not included a new timeline or milestone dates.

- Approach: The team outlined a plan to develop online instrumentation to ensure the onstream time and moisture content of biomass through a dryer. While feedstock variability and its issues are well known and identified as an issue, the team did not characterize their importance in drying. Biomass drying is conducted in numerous industries and processes, and it is not clear whether the team is improving their drying process or the industrial standard. Although the Idaho Forest Group is engaged in the project, it would have been good to engage one of the many dryer vendors. The type of dryer used, as well as the specifics of the types of biomass for drying, were not included. Will these technologies work as well with other setups? The team addressed DEI, although it was not required, and they have one industry partner.

- Progress: The project has been delayed due to the need for additional safety considerations as well as COVID. The team has done a nice job of adjusting and doing work where and when they can until the safety issues are resolved. The results are still preliminary, so it is difficult to assess whether significant progress has been made. Impacts: Having the control algorithm and interface software for industry could have a significant impact, but assessing the magnitude of this impact is difficult because the team did not conduct any economic or LCA analyses, and, as noted earlier, they did not provide specifics on the failure rate of industry standard dryers. It is unclear whether the protocols would be transferrable to other dryer types, feedstock types, etc.

PI RESPONSE TO REVIEWER COMMENTS

- This project has been significantly delayed due to required safety upgrades and supply chain delays as a result of the pandemic; however, we have been able to develop preliminary modeling frameworks, in the absence of data, that are substantially increasing the speed of advancement that we have been able to attain since the system became fully operational. As for the significance of the project, this project was developed in collaboration with our industry partner, who was having a significant problem with meeting target specifications and maintaining operability of the system. Although the baseline conditions were not directly measured, 90% uptime and 90% of the material meeting outlet specifications will be a substantial improvement over previous operation. However, because detailed information on the initial operation of the drying system was not collected and is not available, any TEA or LCA comparisons would be inaccurate and not appropriate for comparison. Additionally, we recognize the limitations of the sensors that are currently being used, but because the material is blended and homogenized as it is being fed, we feel that the measurements are sufficiently accurate to guide the adjustments of the system. We will also evaluate the accuracy after drying to ensure that the technique used to measure moisture content is accurate, appropriate, and adjusted as necessary. It is possible that there is not enough adjustment in the parameters that we can access to attain the project objectives. If that is the case, then the system will need to be redesigned, and that will be outside the scope of this project. However, even in this case, although the specific model that is being developed will not be directly applicable to other systems, the developed framework will still have wide applicability across different equipment and feedstock types where multiple processing parameters can be adjusted to meet a desired condition.

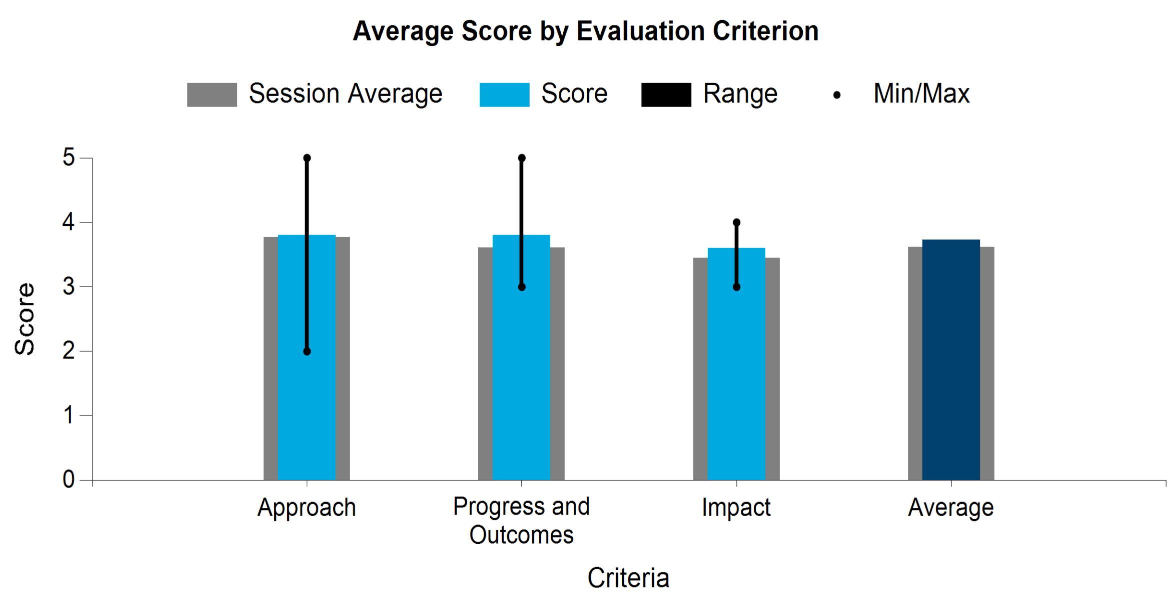
TASK 1 - MATERIALS OF CONSTRUCTION

Feedstock-Conversion Interface Consortium

WBS:	Task 1
Presenter(s):	Jun Qu
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,725,000

PROJECT DESCRIPTION

FCIC's Task 1, Materials of Construction, uses a systematic QbD approach with integrated efforts of characterization, modeling, and testing to gain fundamental understanding of the failure modes and wear mechanisms of biomass preprocessing tools. It develops analytical models to predict wear and establish material property specifications, selects and evaluates candidate mitigations based on modeling and lab-scale testing, identifies top-performing mitigation for process development unit validation, and shares the fundamentals and mitigations with the biomass industry. As of today, the team has gained fundamental understanding of the wear mechanisms of both hammer mills and knife mills, developed protocols for extraction and characterization of extrinsic and intrinsic inorganics, constructed analytical erosive and abrasive wear models, identified low-cost feedstock modifications for improving tool life, evaluated candidate tool coatings and surface treatments using bench-scale abrasion and erosion tests, and completed a set of small knife mill validation tests for candidate wear-resistant blade materials with TEA. We are currently developing bench-scale tests to study abrasiveness and fouling for both biomass and MSW and are planning for small shredder testing for validation of candidate wear-resistant blade materials.



COMMENTS

- Wear mechanisms that are based on feedstock variability (one of the main tenets of this overall project) were not well-presented within this task. Even though the wear solutions being proposed are interesting, little information was provided in terms of the overall process TEA or even LCA of these new/other materials and coatings, as IRR is not the best way to express the improvements.

- The researchers did excellent work on this task. In the approach, they clearly articulated the challenges and the metrics (both technical and economic) that they would use to measure progress. I have just one suggestion related to the general approach. It would be useful to see the economic metrics in the context of the larger system. How will these mechanism of corrosion improvements affect the minimum selling price? Also, it seems that the TEM could have been built prior to the research and used to direct efforts. Slide 19 presents a very nice TEA of the knife mill. This approach could be used as an example for other tasks. A few general comments/suggestions: (1) IRR loses its meaning at extreme values, so it's not the right choice to quantify these results. Simple payback period might be a better choice, in addition to percent reduction in minimum selling price. (2) It is unclear which factors are included in this analysis. For example, does it take into consideration production losses due to downtime? Or does it assume that multiple parallel machines alleviate this issue? (3) It would be great to see a tornado diagram showing the relative impact of the various process parameters on economic value metrics. It's great that the researchers made an open-source tool in Excel. I tried to download it, though, and could not get the form to work. Also, the download form requires too much personal information. Name, company, email, and state should be plenty. People shouldn't need to supply telephone numbers or mailing addresses.

- This task focus is much needed; however, it seems that most of the testing research is done in a lab rather than in the field. More of the latter than the former is needed. This task could benefit from working with industry so that most of the testing is done in actual industrial facilities. Testing of the same equipment at different facilities could have more illuminating results. Industry has a lot of operational challenges with equipment wear and tear as well as breakages that this task team could study with industry direction based on what the sector collectively identifies. It was very practical that the research showed higher throughput and lower energy consumption, and it was excellent that diverse costs associated with equipment materials performance were assessed. The material decision matrix will be very practical for industry. It's excellent that the team published an open-source prediction tool. There was no mention of DEI.

- This work is good; it combined solid engineering test data with sufficient modeling to guide the selection of construction materials for knife mills. Real data on the costs of operation of various materials was examined and presented. The results have an immediate impact on plant design and operability prediction for knife mill comminution. Knife mill comminution is one method of particle size reduction, and extension/comparison to other methods is important. I'm looking forward to the results on abrasion and gumming fouling. Extensions of wear and material selection to examining screw feeders (especially against back pressure) are urgently needed.

- The team has completed all the milestones defined in the original project plan. They have identified critical material attributes (CMAs) for feedstocks that impact tool wear rate as well as CMAs for knife mills' materials of construction. They defined three stages of knife wear and developed an Excel-based program for predicting edge recession rates in knife mill cutters. They demonstrated experimentally the improvement in knife wear by applying an iron-boride (Fe-B) coating or using tungsten-carbide (W-C) knives. They conducted a TEA based on a 350-day experimental study showing the advantage of Fe-B coating as well as tungsten-carbide (W-C) knives. However, Slide 19 does not explain why there is such a large difference between the IRR of Fe-B and W-C. It is not clear that the experimental study included feedstock other than "wet, dirty forest residue." Other tasks have focused on corn stover in addition to forest residues. The presentation did not address whether the CMAs change for forest residue versus corn stover or whether the wear model accounts for different feedstock characteristics. The next phase of this project should include additional materials, including corn stover and MSW (planned). The team should engage their industry partners to evaluate the correlation between their model and actual equipment performance as well as doing economic evaluations for their equipment (cost/benefit). This engagement could increase the acceptance of the model and material recommendations commercially. A DEI plan, to be completed by the end of the project, should be added to the milestones.

PI RESPONSE TO REVIEWER COMMENTS

- We truly appreciate the overall positive and encouraging feedback from the reviewers. Comments and questions are answered here.
- Reviewer 1, Q1: Wear mechanisms that are based on feedstock variability (one of the main tenets of this overall project) were not well-presented within this task. Response: The wear mechanisms for various types of feedstocks were investigated in FCIC 1.0 and determined to be strongly correlated to the extrinsic and intrinsic inorganic contents of the feedstock. Results were reported in the 2021 BETO Peer Review and published in a journal paper (https://dx.doi.org/10.1021/acssuschemeng.9b06429). The objectives of Task 1 in FCIC 2.0 are to develop and validate mitigation strategies for the wear issues of feedstock size reduction equipment.
- Q2: Even though the wear solutions being proposed are interesting, little information was provided in terms of the overall process TEA or even LCA of these new/other materials and coatings, as IRR is not the best way to express the improvements. Response: Limited to the 15 minutes of presentation time, we had to skip the details of the TEA process, which were reported in our recent journal paper (https://doi.org/10.1016/j.wear.2023.204714). We agree that IRR may not be the best for presenting the economic benefits of using new tool materials/coatings, because the tool cost typically is not considered a capital investment. This has been clarified in the publication and other measures, including the cost reduction in processing a unit weight of feedstock and MFSP.
- Reviewer 2, Q0: It would be useful to see the economic metrics in the context of the larger system. How will these mechanism of corrosion improvements affect the minimum selling price? Also, it seems that the TEM could have been built prior to the research and used to direct efforts. Response: The MFSP in dollars per gallon gasoline equivalent ($/GGE) was calculated to be $3.42, $3.37, and $3.35 for the baseline, iron-borided, and WC-Co (cobalt-doped tungsten carbide) blades, respectively. The MFSP values were actually presented in the table on Slide 19 of our Peer Review presentation.
- Q1: IRR loses its meaning at extreme values, so it's not the right choice to quantify these results. Simple payback period might be a better choice, in addition to percent reduction in minimum selling price. Response: We agree and appreciate the suggestion for using the payback period.
- Q2: It is unclear which factors are included in this analysis. For example, does it take into consideration production losses due to downtime? Or does it assume that multiple parallel machines alleviate this issue? Response: Yes. The production losses due to downtime were taken into consideration in the calculation. Limited to the 15 minutes presentation time, we had to skip the details of the TEA process, which were reported in our recent journal paper (https://doi.org/10.1016/j.wear.2023.204714).
- Q3: It would be great to see a tornado diagram showing the relative impact of the various process parameters on economic value metrics. Response: We appreciate the suggestion and will generate a tornado diagram in the future presentation of economic impact.
- Q4: It's great that the researchers made an open-source tool in Excel. I tried to download it, though, and could not get the form to work. Also, the download form requires too much personal information. Name, company, email, and state should be plenty. People shouldn't need to supply telephone numbers or mailing addresses. Response: We will try to simplify the download form and add introduction.
- Reviewer 3, Q1: This task focus is much needed; however, it seems that most of the testing research is done in a lab rather than in the field. More of the former than the latter is needed. This task could benefit from working with industry so that most of the testing is done in actual industrial facilities. Testing of the same equipment at different facilities could have more illuminating results. Industry has a lot of operational challenges with equipment wear and tear as well as breakages that this task team could study

with industry direction based on what the sector collectively identifies. Response: We certainly agree with the reviewer. A round-robin type of study with multiple industrial partners testing the same equipment would be very beneficial for understanding the impact of feedstock variability and operating conditions to provide insights for developing more effective and economical mitigations. That would require a collective effort between BETO and industry.

- Q2: There was no mention of DEI. Response: FCIC thrives on the premise that diversity is essential, equity is inherent, inclusion is innate, and accessibility is achievable. These principles guide Task 1's vision to create a welcoming environment that attracts, supports, and inspires a diverse and engaged workforce; fuels its scientific mission and impact; and fosters greater accessibility for diverse communities.
- Reviewer 4, Q1: I'm looking forward to the results on abrasion and gumming fouling. Response: We are currently working on MSW-caused abrasive wear and gumming/fouling and will report in the next Peer Review.
- Q2: Extensions of wear and material selection to examining screw feeders (especially against back pressure) are urgently needed. Response: We fully agree and plan to propose this to BETO in FY 2024 or FY 2025.
- Reviewer 5, Q1: Slide 19 does not explain why there is such a large difference between the IRR of Fe-B and W-C. It is not clear that the experimental study included feedstock other than "wet, dirty forest residue." Response: Limited to the 15 minutes of presentation time, we had to skip the details of the TEA process and feedstock processed, which were reported in our recent journal paper (https://doi.org/10.1016/j.wear.2023.204714).
- Q2: The presentation did not address whether the CMAs change for forest residue versus corn stover or whether the wear model accounts for different feedstock characteristics. Response: Our earlier investigation suggested that the tool wear is more strongly correlated to the feedstock ash content than the type of feedstock itself (https://dx.doi.org/10.1021/acssuschemeng.9b06429). Therefore, the current version of the wear model simply uses the amount of ash as the input. The impact of feedstock type could be added to the model in future development.
- Q3: The next phase of this project should include additional materials, including corn stover and MSW (planned). The team should engage their industry partners to evaluate the correlation between their model and actual equipment performance as well as doing economic evaluations for their equipment (cost/benefit). This engagement could increase the acceptance of the model and material recommendations commercially. A DEI plan, to be completed by the end of the project, should be added to the milestones. Response: We agree and will work on them.

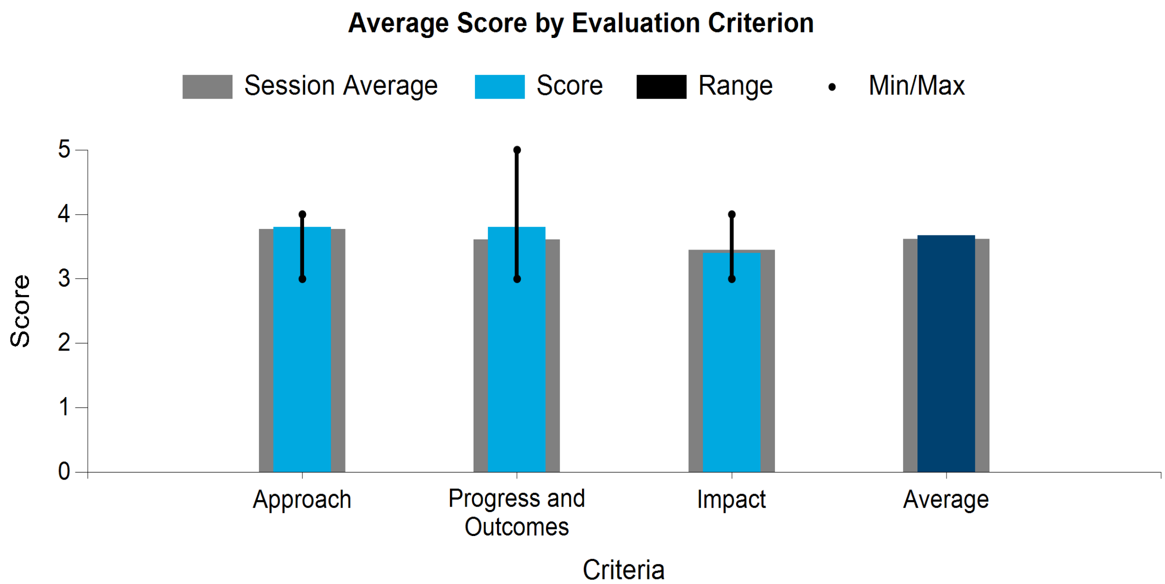
FCIC OVERVIEW AND TASK X - PROJECT MANAGEMENT

Feedstock-Conversion Interface Consortium

WBS:	Task X
Presenter(s):	Ed Wolfrum
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,150,000

PROJECT DESCRIPTION

FCIC is a collaborative project among nine different national laboratories, led by BETO, and is developing first-principles-based knowledge and tools to understand and mitigate the effects of biomass feedstock and process variability on biorefineries. The purpose of the FCIC Project Management task is to provide scientific direction and leadership to the consortium and to provide project management to ensure robust operational planning and execution. The key challenges are ensuring superior coordination and communication among researchers across nine tasks and nine national laboratories and ensuring industrially relevant outcomes. We are addressing these challenges by using robust, well-accepted project management tools to ensure good communication among all stakeholders, and by engaging industry in multiple ways to ensure the work we are doing is relevant.



COMMENTS

- The IAB should have more industry and less academia. Overall, the consortia appear to be thoughtfully designed, but the feedback loops between projects, data, CRADA calls, industry, etc., remain unclear. I understand that there are challenges with getting meaningful input from industry. Surveys appeared to be successful in the high-temperature conversion task. I suggest continuing to pursue all avenues for input. The Project Management task is clearly a challenge, with so many tasks and labs doing the work. It would have been helpful to understand how information and data are flowing between projects in order to inform the work being done.

- The plan is strategic and recognizes the need for industry engagement. FCIC should solicit priority needs from key sectors that need more research to catapult feedstock utilization, especially for SAF and biofuels, and support the sectors. FCIC is using diverse communication and outreach approaches via a website, fact sheets, webinars, and case studies to communicate about FCIC work. FCIC should count on this diversified approach but determine which audiences are still not being reached. I would like to hear more about another IAB and how it informs and directs prioritization of FCIC work. When a reviewer asked how the IAB engages with FCIC, there seemed to have been very little engagement recently, and communication primarily flows from DOE to the IAB rather than the reverse. This is a missed critical opportunity. Industry or sectors should be driving the direction of FCIC research. The presenter did not emphasize DEI.

- An overall comment: Presentations in this area tended to be a bit too "information rich"—too much data presented in a short time. The primary messages should be distilled and presented in a more concise manner. There were a tremendous number of acronyms used in these talks, often without definition of what they stood for. The use of QbD)—versus the old-school "product by process" championed by DuPont in the 1960s—can learn a lot by what the commodity chemicals industry handled back then. Anatomical fractionation of biomass has provided some very interesting science and engineering data, but I struggled with how this information will aid in processing or economics. The primary failure in feedstock handling of the pioneer biorefineries was the feed of biomass into "the throat" of pretreatment; this had to do with trying to push biomass into a high-pressure zone and not appreciating the complications that would result. Yet most of the properties presented here neglected the challenge of feedstock introduction into a high back pressure process. The communication of results and industrial outreach outlined in the presentation is critical and should be a two-way street—the programs can inform industry, and industry can refine focus. Related to the FY 2023 DEI plan, I suggest a contact between the National Renewable Energy Laboratory (NREL) and the newly opened Colorado State University Spur campus, where they have focused on water, food, and the environment. They are missing the critical energy component, and this would mesh well with the Colorado State University Spur mission and NREL's DEI mission.

- The FCIC Project Management task has successfully implemented the QbD terminology across the nine program tasks and has created the common theme of "feedstock variability" across the tasks. The management team has set up a routine communication process among the tasks and across the nine national labs. They are using project management approaches to track the successful and timely completion of all FCIC milestones. They are supporting DEI goals by tracking plans for the tasks as well as having set up a DEI plan for the management team. They have identified key feedback from the 2022 Merit Review and recognized the need to form stronger partnerships with industry as well as continuing strong interaction with the IAB. The management team should help drive industry partnerships across the nine task areas and set goals to create CRADAs with both equipment manufacturers and biorefineries in as many of the task areas as possible. These partnerships will have the strongest potential for commercializing the FCIC technologies. A useful tool for the tasks to use in developing partnerships could be creating a database of companies developing both process equipment and biorefineries, including the technologies being developed and the state of their development. The use of a survey, as was done by Task 6, could be a useful approach. Partnerships with USDA and feedstock suppliers to assist in the reduction in variability from growth, harvest, and storage should be considered, especially for Task 2. Another way to increase involvement with both industry and academia would be to find ways for the various FCIC tasks to be involved in FOAs, especially pilot, demonstration, and pioneer plant FOAs. The management team should continue to focus on improving and integrating the QbD process across the tasks, ensuring the learnings from one task area are applied in downstream tasks. Developing control limits for critical process parameters (CPPs) would be a valuable tool in the operating environment for both preprocessing and biorefineries. A common feedstock suite of corn stover, forest residue, and MSW should apply to all tasks, including both the pyrolysis and gasification pathways of Task 6. As more companies are beginning to commercialize SAF, the team should consider the composition and size of the IAB. In other words, the IAB should include representatives from equipment companies and biorefineries (both low- and high-temperature technologies). The IAB could also act as a gateway to industry partnerships. The management team should also ensure that each of the tasks has completed a DEI milestone as part of their project goal.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their helpful and instructive comments and suggestions. We group these comments into two main opportunities for improvement: (1) increasing interaction with industry, and (2) strengthening our work supporting DEI. To improve our industry interactions, we will add additional industry (rather than academic) members to the existing FCIC IAB in 2023 to get more input at the overall FCIC level, as well as feedback on individual FCIC tasks. We believe the current FCIC CRADA call will provide additional avenues for industry interaction (as of this writing, over 25 industry proposals have been received and are undergoing review). If this CRADA call is successful, we will recommend issuing future calls as other BETO consortia (e.g., Agile BioFoundry, Chemical Catalysis for Bioenergy) have done. We will also develop and implement a plan to reach out to industry stakeholders, including existing BETO FOA recipients, to understand their needs more thoroughly. We will consider using one or more surveys (as suggested by one reviewer) to collect information more effectively. We will also consider developing an industry stakeholder database to understand and categorize specific industry needs that FCIC could address. We agree that our work in DEI needs improvement. We will add explicit consortium- and task-level DEI goals to our FY 2024 work plan to support our end-of-project goals, and we will reach out to local universities later in 2023 to better understand DEI engagement opportunities (as suggested by one reviewer).

TASK 2 - FEEDSTOCK VARIABILITY

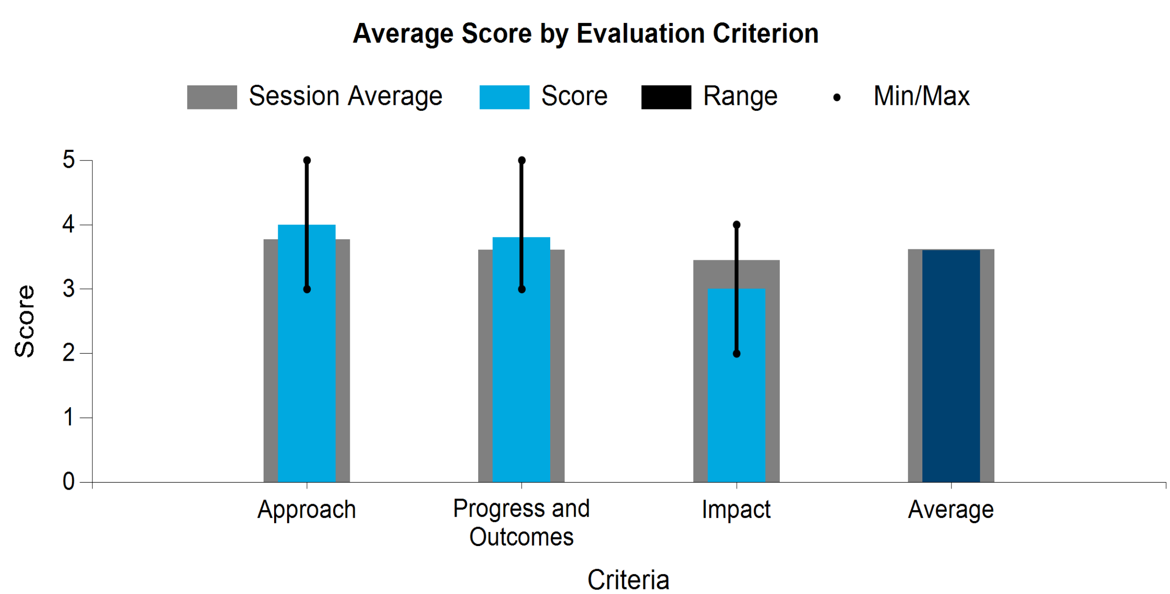
Feedstock-Conversion Interface Consortium

PROJECT DESCRIPTION

WBS:	Task 2
Presenter(s):	Bryon Donohoe
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$3,690,000

The feedstock variability project provides information and tools to detect and quantify initial feedstock material attributes and guide management methods for accommodating feedstock variability.

Lignocellulosic feedstocks are heterogeneous, making bioprocessing challenging. Advanced fractionation methods use chemical and physical qualities and how they vary across scales to optimize feedstock handling and customize pretreatment procedures to feedstock fractions with variable and multiscale recalcitrance factors. Quality and end-user application-specific routes can exploit feedstock variability to extract value from lignocellulosic biomass fractions. The key results from this project cover distribution, sources, and mitigation methods for inherent feedstock features that FCIC has shown to impact corn stover, pine residues, and MSW material handling, preprocessing, and conversion. This data is provided through peer-reviewed articles, trade journal submissions, and interactive feedstock variability models that let users decide whether a set of attribute combinations is useful. This fundamental understanding and characterization tools will help stakeholders establish attribute-driven, feedstock-independent strategies for assessing feedstock quality and choosing process designs that control or accommodate variability from the field to conversion. This information and resources will also enable feedstock valuation by critical attributes.



COMMENTS

- The metrics provided in this approach are very qualitative. The metrics for narrowing the attributes list are not well-defined; these metrics are critical and should be well-informed by industry. There is a good list of industry engagement for this type of work.

- The researchers seem to be doing an excellent job of quantifying and understanding the sources of biomass resource and feedstock variability. This may indeed be high-impact work. Surely some of these tools are more important than others. As a sorting tool, either TEA or interviews with industry partners might be used. Even if it is impossible to quantify impact with any precision, TEA could be used to identify problem areas that might benefit from one of the solutions that the feedstock variability team has developed or has considered pursuing. When narrowing down parameters, the team might consider two groups: (1) tools for routine measurements in design and operation feed systems, batches testing, etc., and (2) "big gun" techniques that might be used by researchers in special circumstances.
- There appears to be a heavy emphasis on corn with some work on MSW and wood, but no explanation for why. A strength of this task is engagement with diverse industries and companies. It would help to know how the team prioritizes which partners to work with. The team should prioritize research on the highest priorities identified by industries that are closest to commercialization or that have greatest potential for largest scale, are most environmentally beneficial, and have climate-friendly outcomes. Variability matters for some feedstock applications but not all. It would be helpful to understand how the team prioritizes which feedstocks need more variability research to advance greater utilization of that feedstock. The forestry sector has a unique need to produce homogeneous feedstock of a specific size and quality for all types of end uses. This task team should consider working with this sector to develop harvesting and in-field processing systems that can easily and economically create a more uniform desired feedstock. Task 2 should continue to publish work in trade journals. This is extremely important and will likely have greater impact than publishing in science journals. It is excellent that this team is developing best practices guides. The team should expand the number and diversity of best practices guidance documents.
- This is a task being pursued with a broad spectrum of analytical technologies that appears to use the best tool for the job rather than just being locked into near-infrared, which is refreshing. There is a tremendous amount of fundamental information presented here, but linking this to "real-world" attributes of biomass feedstock is not clearly delineated. This could just be because there is so much information presented in a short time. For instance, on Slide 21, in a small box on the side, it is noted that "10% increase in lignin => 25% increase in grinding energy" ... This is huge! This needs to be expanded upon, explaining how this is measured and what impact it has on overall processing. There are numerous other process variables other than drought stress to focus on, such as the effect of overfertilization on biomass properties, the impact of high chloride content of soils on biomass chlorine content (critical to both pyrolytic and enzyme processing), and grower-location-driven variation in biomass variability. I was impressed by the TD-NMR work presented and would like to see if this could be applied as an online technique.
- The team has made excellent progress in refining analytical methods for the six CMAs they have defined. They have effectively used these techniques to describe the impact of drought and storage conditions on corn stover. Subtask 2.9 calls for adding MSW as a feedstock for evaluation. Although they have meetings with the other task teams and have published various reports targeting these tasks, it is unclear whether Tasks 3, 5, 6, and 7 are using the six CMAs from this task in their evaluations. Task 7 utilized both drought-stressed and non-drought-stressed stover supplied by Task 2 for their evaluation, but it did not appear that they considered any of the six CMAs in that evaluation. Many of the other tasks are also using forest residue (pine) in addition to corn stover. Adding forest residue as a model feedstock will increase the linkages to the other tasks. Industrial engagement appears to be in the early stages of involvement. Two partners, Alder Fuels and VERDE Nanomaterials, are involved in producing biofuels or biomaterials and could provide valuable feedback on the impact of feedstock on their process. Adding preprocessing and material handling equipment manufacturers as partners would provide another source of input on the importance of these six CMAs. Slide 5 discusses CMA, CPP, and CQA for growth, harvest, and storage. Working with feedstock suppliers from growth through delivery on the importance of the CMAs to downstream processes could help these suppliers find ways to reduce feedstock

variability. Overall, the team should look for ways to increase the relevance of their work to the other FCIC tasks as well as industry and demonstrate the advantages of utilizing these methods beyond the traditional compositional analysis.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments and the time they took to understand our project and recommend changes. We appreciate the compliments on the breadth and depth of the analytical approaches we used to assess feedstock variability. We agree that rating the tools/techniques and reducing the list of attributes to the most important still requires work. We agree with the concept of characterization tools being divided into two groups ("routine" and "big gun"). The downstream study of conveyance efficiency, conversion yield, and TEA are our major criteria for narrowing the attributes list we are investigating. TEA is now being used; however, Task 2 should and will plan to employ industry interviews. We've done more work with pine residue than we've had time to present. Our first findings revealed decreased variability overall, which could be explained by shifting anatomical fraction ratios as the pine trees aged. These findings contributed to a greater emphasis on corn stover throughout the current evaluation period. However, we recognize the importance of broadening and balancing the feedstocks under consideration. We intend to get more involved with forestry and will look for appropriate relationships, particularly in the area of in-field processing technologies. Working with feedstock suppliers on issues ranging from growth to delivery would be another excellent opportunity to discover the significance of material attributes in downstream processes and help reduce feedstock unpredictability. We will begin with supplier interviews and work our way up from there. Determining and relating to "real-world" qualities will continue to be a core problem and fundamental focus of our work in the future. We also hear and understand that we must continue collaborating with the other FCIC activities to increase the relevance of our upstream variability analysis to the downstream conveyance and conversion operations. Finally, we welcome the new sources of variation proposals. This is another topic on which we can get more information from our feedstock supplier interviews.

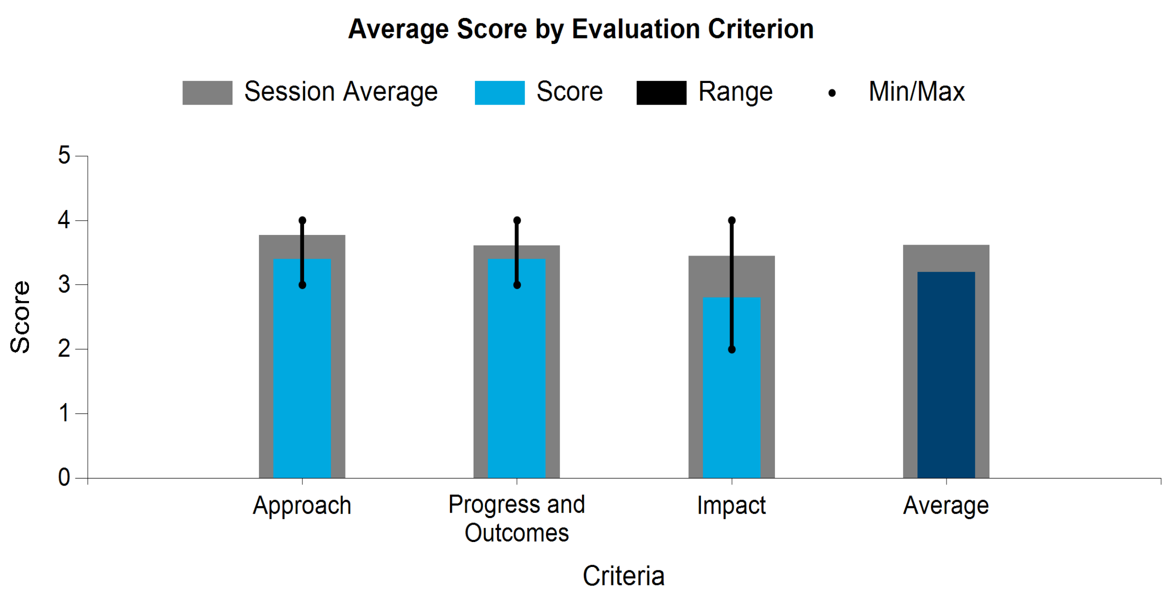
TASK 3 - MATERIAL HANDLING

Feedstock-Conversion Interface Consortium

PROJECT DESCRIPTION

WBS:	Task 3
Presenter(s):	Yidong Xia
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$5,130,000

The overarching objective of the project is to develop first-principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through the processing train to the reactor throat. The project takes a synergistic approach, including integrated multiscale characterization, experimental flow testing, and physics-based modeling, to understand, model, validate, and solve the biomass feeding and handling problems. The scope of work consists of establishing controlled particle and bulk flow tests using industry-relevant biomass feedstocks and for evaluating flow performance under various combinations of CMAs and CPPs; developing experiment-validated, physics-based discrete particle models for gaining a fundamental understanding of flow characteristics and upscaling of first-principles-based constitutive models as input to continuum flow simulations; and developing experiment-validated, physics-based continuum-mechanics models for predictive studies of engineering-scale flow performance under relevant combinations of CMAs and CPPs Computational tools implemented with the developed flow models will be released as open-source software and/or open-source add-on modules for proprietary software upon the completion of the project.



COMMENTS

- Materials handling is one of the most critical and underestimated aspects of a biorefinery. A widely available simulation tool could hold value to the industry; however, feedback should be requested from users of the models that have been released to assist with continuous improvement.

- The research team has used a first-principles approach to developing several design tools that will apparently be useful to industry. They should consider taking the concept of "impact" one step further, though. For example, one impact statement reads, "For handling operations with a high flow rate, the new model is essential to accurately predict the flow behavior and throughput." The question remains:

What will be the impact of being able to accurately predict flow behavior? In one slide, they present a graph of angle of repose and comminution energy versus nominal particle size. It would be useful and fairly straightforward to put some costs to these numbers. The importance of comminution energy can only be judged in the context of the total energy consumption for the larger process. Similarly, they might try to connect flowability to system downtime and put a cost on that. With the resulting model, they could tune the parameters toward a point or range of optimization.

- This task is more focused on developing tools to ameliorate material flow, but it would be equally impactful to study types of commercially available equipment that improve flow. These types of tests can be conducted at operating facilities, especially with forest biomass of varying size distributions. It is very helpful that this task defines the criteria and scope being used at the outset. It is unclear what is driving this team's focus on the wedge hopper and screw conveyor. Are those industry priorities? Wedge hopper design is an example of the type of work that would most benefit industry, because most material handling is done with commercially available equipment that is then modified when material handling problems are encountered. It is unclear how much testing the team conducts at industrial facilities. The team should prioritize this. The presenter mentioned DEI efforts. The team should continue to hire students from underrepresented universities.

- The approach of this project involves first-principles measurement, linking to real process behavior, and developing distributable computer models to test design. This results in a useful precommercial tool. The slide outlining the comminution energy of the Forest Concept Crumbler to flowability is a significant accomplishment—going from a 6-millimeter to 2-millimeter crumble takes six times the energy! This is critical to TEA and LCA as well as process economics. The stated objective, "develop tools that enable continuous, steady, trouble-free feed into reactors," hits on the critical failure points of the pioneering cellulosic biorefineries. However, the program's progress has taken this through to the "reactor throat" but does not deal with the reactor throat pushing feed biomass into the reactor (against pressure), which is the most critical step and where most failure in operability occurs. This is a disconnect that limits the commercialization impact.

- The team has made good progress on developing models and hopper design charts for granular flow in hoppers and identifying the appropriate CMAs and CPPs. Their implementation strategy is to provide these models as open source with a user manual. They have used lab-scale experiments to verify the flowability and hopper discharge models and created hopper design charts for use by industry. It appears that the experimental work has been completed using lab-scale or Idaho National Laboratory pilot equipment. The project should increase its interactions with industry partners. Creating CRADAs or other linkages with industry partners as they design and test new equipment would enhance the verification of the models and design charts. The quad chart discusses using milled corn stover and corn stover/paper blends as the model feedstock for this task. Adding nonrecyclable MSW and continuing the work with forest residue would provide better alignment with other FCIC tasks and be more relevant to potential industry partners. The modeling and experimental work should be expanded to screw conveyors because there was little information discussing the modeling or design charts of screw conveyors. The team should also survey industry to determine whether there are flowability issues in parts of the process beyond hoppers and screw feeders.

PI RESPONSE TO REVIEWER COMMENTS

- We sincerely thank the reviewers for their thoughtful and constructive comments on this project. Please find below our replies to the reviewers' comments. Interfacing with industry is vitally important to maintain relevant scope. Although interactions with industry have been limited up to this point, this project is developing a strategy to increase such interactions. BETO CRADA projects led by industry partners and supported by national labs, such as through the 2023 FCIC CRADA proposal call, provide a venue to allow national labs to directly engage with industry partners to resolve specific flowability issues at the industrial/commercial scale by leveraging the material handling expertise developed in this project. However, limited interaction does not mean no interaction. In conversations that we have had with those in industry, flowability issues have been identified as a significant problem at industrial/commercial scales. This has led the team to focus on feedstock flow studies based on wedge hoppers and screw conveyors because of the prevalence of these two types of units in industry. The wedge hopper used in this project is a custom design in which the exit opening size and side panel inclination angle can be easily adjusted. The design enables hopper discharge tests to create data for flow charts requiring only one hopper, instead of multiple hoppers with different configurations. The screw conveyor used in this project allows easy change of screw configurations to test for suitable screw designs depending on feedstock properties to avoid jamming or excess energy use. Beyond hoppers and screw feeders, flowability issues have also been pointed out by industry partners to occur in their specific handling units, but often in the units where feedstock flow is primarily driven by gravity. We also recognize that at the reactor throat, flow disruptions due to pressure-driven transport could and often do happen. In the past, this project focused on addressing some of the known challenges, e.g., transport in compressive screw feeders. Beyond specific equipment types, this project is also focusing on a variety of materials. In the third year of the current 3-year project, the team will experimentally and computationally study the flowability of nonrecyclable MSW following previously established research procedures based on granular biomass flow, and will synergistically collaborate with other FCIC tasks, such as Feedstock Variability and Preprocessing. The impact of an accurate flow model to predict flow behavior will de-risk the determination of design parameters of material handling units such as hoppers for industry users. For example, if a flow model overpredicts flow rate at the hopper exit, it could mislead equipment designers into using a smaller opening size than required. A smaller opening size would result in a lower flow rate (lower throughput) or clogging and arching. Since the initial release of these flow models, the project team has continued to improve the models by extending their applicability to material attributes and flow operation units, often upon application of these models to other BETO projects that involve industry partners and their modeling needs for predicting and assessing flow performance of specific feedstock materials.

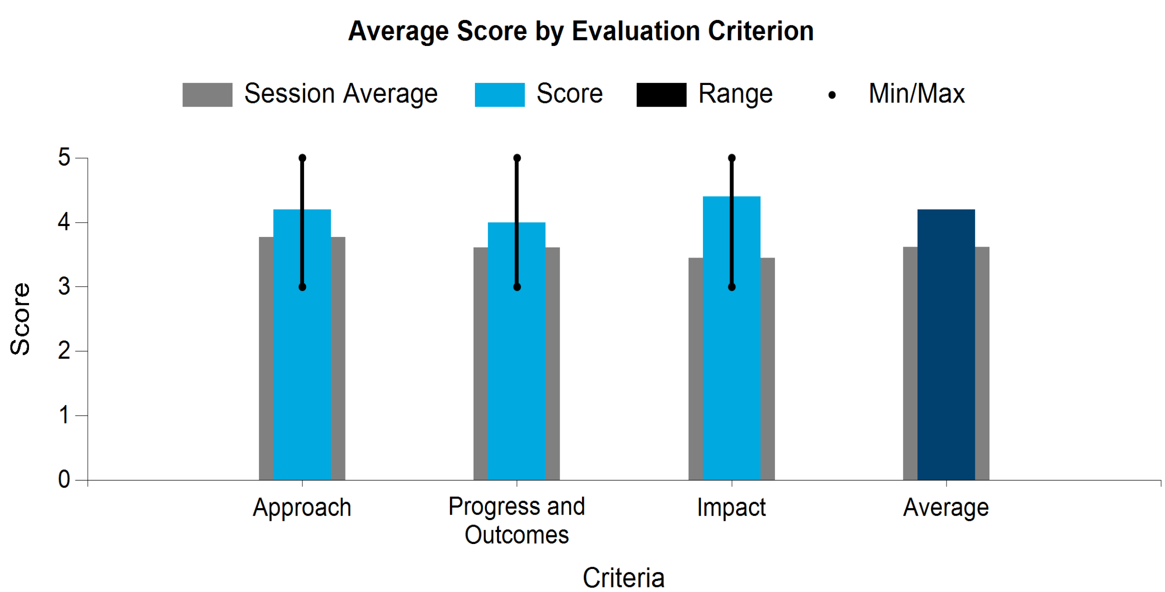
TASK 4 - DATA INTEGRATION AND WEB PORTAL

Feedstock-Conversion Interface Consortium

PROJECT DESCRIPTION

WBS:	Task 4
Presenter(s):	Rachel Emerson
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,650,000

The objectives of the Data Integration and Web Portal Task are (1) to provide a web-based collaboration platform and database (the FCIC Data Hub) for integration, preservation, and sharing of FCIC datasets, metadata, and analytical results within a uniform QbD framework; and (2) to provide a portal on the Data Hub for industry stakeholder and public access to FCIC results, data, and software. The Data Hub's QbD framework provides workflows and data tables for cataloging and tracking critical property attributes of feedstocks, intermediates, and products as well as CPPs of unit operations within the low- and high-temperature conversion pathways. The QbD data table interfaces provide easy, rapid, and transparent access to supporting data and evidence of criticality in biorefinery processes and materials. FCIC analysts, experimentalists, modelers, and managers benefit from having a shared, online workspace wherein data may be exchanged, tracked, transformed, analyzed, and preserved within a formal structure that supports efficient tracking of progress toward FCIC goals. Industry stakeholders seeking to build new bioeconomy infrastructure for production of renewable fuels and chemicals benefit from having ready access to findable, accessible, interoperable, and reusable FCIC data and knowledge via the Data Hub web portal.



COMMENTS

- Next to the TEA work, this is likely the next most impactful piece of this work, as it is the actual dissemination of the information being generated next to the available models, though it appears to be delayed until the Data Stakeholder Workshop, which is likely a valuable outreach activity within this work. Creating a user-friendly user interface as well as consistent data and nomenclature are/will be critical to overall success.

- This is a great resource in development. As discussed in the Q&A, it will be critical for BETO to secure long-term funding for it. While I think that this platform will be great for facilitating communication between national lab researchers and industry, I am not enthusiastic about the idea of including a forum or chat feature. There are other platforms that are designed for discussion, so I don't think that FCIC should spend their limited time duplicating that effort. Perhaps there could be a dedicated FCIC subreddit or something along those lines. I work with lots of start-ups to build TEMs for their technologies. NREL TEAs are very important to many of them as sources for base-case process designs, capital expenditure factors, equipment cost correlations, material prices, etc. The start-up community would really benefit if this web portal included that sort of information (e.g., case studies, databases of reference equipment/plant costs, raw material prices, etc.).
- Data integration across disciplines and diverse datasets in one portal will prove to be useful for multiple stakeholders, sectors, and researchers. It is excellent to have a repository of so much diverse research and products. It is very helpful that the database includes journal articles and case studies in the repository. A fair approach and harmonizing data are important priorities to continue. It's impressive that the team already assessed the impacts from and on ChatGPT. The team should consider whether and how to offer a peer-to-peer support communications platform as part of the database, where an online community might emerge for inter- and intrasector cross-pollination. The small team doesn't seem diverse, and there was no mention of DEI.
- I will start by saying that reviewing data portals is outside of my area of expertise. What has been done seems comprehensive and essential. A great invention means nothing if nobody knows about it, so communication should be as quick and broad as possible. The recording of data, methods, procedures, and conclusions is essential to accelerate and maintain a developing industry. Basing the Data Integration and Web Portal on commercial software is a wise decision; leave the software development to experts with a commercial incentive to improve. I would suggest having a messaging or (monitored) chatroom feature so that communication with and between PIs and industry is facilitated.
- The team has developed and deployed the FCIC Data Hub and populated it with QbD data, Task 8 case studies, publications, and presentations. They formed an advisory panel and received guidance on the functionality and content of the Data Hub. The have identified a Data Hub champion at each of the national labs to encourage the use of this tool, and they are working to create standard data terms. The Data Hub has been opened to non-DOE users on a limited basis. The team is currently evaluating the use of artificial intelligence in interpreting FCIC Data Hub knowledge. The team has made good progress on developing and populating the Data Hub. The task has an end-of-project milestone target of at least 100 active commercial users on the system. To achieve this goal, the team should set intermediate, quarterly goals for recruiting and involving active commercial users. The milestone to have 20 non-DOE users is due by March 31, 2023. It is not clear if this is on schedule. Similar goals should be set for researchers, academic partners, and staff. These intermediate goals should be visibly tracked using the User Activity Tracking module that has been developed. It appears that internal use of the Data Hub is behind schedule, as the inaugural Data Stakeholder Workshop scheduled for September 22 was delayed. The presentation mentions that the LabKey software is used in support of DEI in high schools. A more specific DEI activity could be identified for this task.

PI RESPONSE TO REVIEWER COMMENTS

- We are grateful for the insightful feedback from the Peer Review panel and for their service to BETO. Creating a user-friendly interface for the FCIC Bioenergy Data Hub that facilitates industry stakeholder access to harmonized and easily downloadable datasets has been a top priority for our team. We appreciate that bioenergy start-ups rely heavily on TEA models from the national laboratories to create base-case process designs; as such, we will continue to work with the Task 8 (Crosscutting Analysis) team to make FCIC case studies available via the Data Hub. Our use of commercial, built-for-purpose scientific data management and collaboration software for the Data Hub provides new channels of communication with our stakeholders, who now mainly access FCIC knowledge via published journal articles and technical reports. The software includes tools for issue tracking, discussions, and surveys that will help us build an interactive online community of Data Hub users working within the nascent bioeconomy. These innovations will also support greater DEI outreach, as will be emphasized by the Task X leadership team for the FCIC.

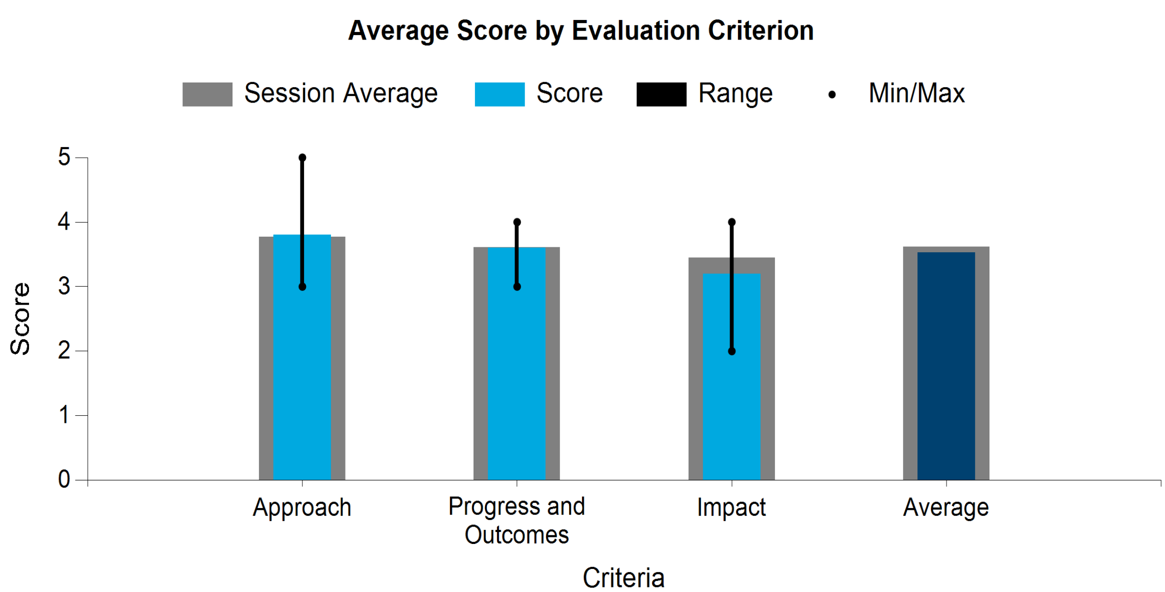
TASK 5 - PREPROCESSING

Feedstock-Conversion Interface Consortium

WBS:	Task 5
Presenter(s):	Jordan Klinger
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$6,225,000

PROJECT DESCRIPTION

The objectives of Task 5 are to develop first-principles-based comminution design manuals and machine-learning-trained process control algorithms to be used by mill manufacturers and biorefineries. Mill manufacturers will be able to develop new mill designs with the manuals to solve issues of fines generation and broad particle size distributions that negatively impact downstream flow and feeding (rat holing, bridging) and downstream conversion processes (over- and underconversion of biomass). Biorefineries will be able to utilize the process control algorithms and code, which analyze photographic images of the processed materials and determine whether they are out of specification in a feed-forward configuration, to adjust mill process parameters to correct the fault(s). Our multiscale approach considers feedstock attributes from molecular structure to bulk particle morphology, which enables identification of relationships between preprocessing and feedstock performance in downstream conversion processes. The external marketing plan for Task 5 involves several areas of focus in the research and engineering community. First is the continued R&D of open-source comminution simulation software and process control software, with ongoing releases (including updates, maintenance, and user-friendliness improvement) and peer-reviewed publications in industry-interested journals, e.g., *Powder Technology*, *Biomass and Bioenergy*, and *Biosystems Engineering*. Task 5's success in continued publications on comminution tools and models and process control software will allow the Task 5 team to disseminate proceedings in professional and trade conferences such as the American Society of Agricultural and Biological Engineers, International Powders and Bulk Solids conferences, and American Institute of Chemical Engineers annual meetings. Through these meetings, the Task 5 team will extend relationships with existing industrial partners (JRS, Forest Concepts) and new partners.



COMMENTS

- The impacts of this work could have cost implications, but this was not addressed in any TEA presented. This task appears to have more collaborators (some potential) than other tasks.

- The stated objective of this task was to "develop science-based design and operation principles informed by TEA/LCA that result in predictable, reliable, and scalable performance of preprocessing unit operations." TEA does not seem to show up anywhere in the work. The work done under this task may be very high value, but we cannot know without putting some dollar signs on it. That said, the researchers on this task seem to have collaborated well with industry partners, which speaks qualitatively to the relevance and value of what they are doing. Energy consumption and material loss are presented as "economic metrics" later in the presentation. These are perhaps "economic-adjacent metrics," but they are not really "economic metrics." An appropriate economic metric for this task (and others) might be something along the lines of "percentage reduction in predicted minimum selling price." This might then be further broken down into improvements due to reduced energy consumption and improvements due to reduced material loss. On Slide 13, the claim is made that the new tools will "allow biorefinery industries to quickly evaluate biomass quality, determine process parameters, and predict plant economics based on feedstock variabilities." It would be helpful for the reviewers (and probably the researchers also) to model a case study of how this would happen.

- This task seems well-organized and has a strategic approach to assessing and improving preprocessing issues. A weakness of this task is the fact that it is not working on several real-world preprocessing problems in the field. Some of the findings are insightful, but little is practical. The team should consider increasing engagement with industry at real facilities. The team should also consider scaling up pilot work to a larger-scale level before investing in even more associated analytical work. The focus is on comminution, which is OK as long as the preprocessing research need is greater for that compared to other preprocessing issues. The plans to incorporate this work into manuals and academic textbooks serve purposes beyond accelerating improvements in preprocessing. The presenter said that the goal is to incorporate the knowledge to diverse audiences, which is good. The presenter showed a slide illustrating the components of an MSW waste stream. Isn't this information already available? Not only that, but it seems little else was done, yet this task is focused on preprocessing. This MSW subtask work seems to have little value or practical application. DEI efforts include diverse initiatives, especially recruiting and job shadowing, which are very important.

- Comminution (size reduction) is one area of biomass preprocessing that has received too little attention. The industry has usually just resorted to hammer milling and "make it as small as we can afford." Thus, a step back to look at the fundamental mechanisms of fracture and size reduction to understand how to intelligently design equipment for a purpose has resulted in valuable modeling/design tools, at least for knife milling. The approach chosen and results presented seem comprehensive. I liked the linkage of micro-indentation studies to biomass bulk properties. There seem to have been a few discoveries *in silico* that have not been confirmed with experimental studies. What is missing here is that there are many different methods to accomplish comminution that rely on fundamentally different methods of fiber deconstruction. This work does not approach the optimization of particles size reduction by reduction methodology selection.

- The team continues to integrate experimental and modeling approaches to provide tools for preprocessing. The use of statistical models has enabled them to run smaller-scale experiments and still provide the verification of their physics-based models. The team has created a matrix of CMAs, CPPs, and CQAs across a variety of unit operations. They have identified mitigations for three primary risks. They are working to provide models for use by downstream tasks, such as Low-Temperature Conversion. The DEI plan of outreach to underrepresented high schools is a good approach for encouraging interest in bioenergy and STEM education. Specific milestones/goals for this outreach would strengthen the DEI plan. The team has made appropriate progress toward their end-of-project milestone to provide mill manufacturers with design manuals for corn stover and forest residue. Comparing the CQAs across comminution types of equipment (e.g., knife mill, hammer mill, crumbler) to provide biorefineries with the optimum choice of milling equipment for the feedstock they use would be a significant contribution to biorefinery design. More extensive work on MSW is required. Identifying the breadth of MSW composition is needed; for example, are some facilities including organic material such as food waste? The team should consider collecting information from operating plants such as Fulcrum. The use of real-time image analysis is showing the capability of characterizing incoming feedstock to a biorefinery. The team should continue working with D3MAX to apply the technology to their process. Expanding the use of imaging technologies to other downstream processes should be considered, including high-temperature conversion biorefineries. The team has identified numerous preprocessing equipment manufacturers as potential partners for commercialization. More detail on the deliverables of these partnerships would be helpful in understanding the commercialization potential of the tools. Active engagement of additional partners should be considered for the next phase of this project.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for their time and feedback on this project. Their thoughtful comments and expertise will guide the work scope development moving forward. Below are responses to select themes in the reviewers' feedback: the incorporation of TEA, seeking additional industrial guidance, and the value of MSW. TEA is a critical tool that should be used at every stage of a process to understand the cost-benefit trade-offs for a particular unit operation and/or process stage. It was an error in omission that the recent case study produced by Task 8 (presented shortly after this task) was not highlighted during this task review as well to show the complete story. During the development of experimental work in this task, for example, relevant pilot-scale process data were collected in the Biomass Feedstock National User Facility at Idaho National Laboratory for throughput and energy consumption of loblolly pine residues being size reduced in a hammer mill. In collaboration with Task 8, the research team collected these data in coordination with other ongoing studies to understand the fracture mechanics of particles as functions of impact velocity (and energy via the rotor speed) and moisture content (impacting the fundamental strength properties and behavior). As a result of this economic evaluation in the context of a high-temperature conversion pathway, we concluded that although pine particles are fundamentally more difficult to fracture and break at high-moisture conditions, milling the feedstock while it is wet resulted in significant cost savings. By staging the milling prior to drying, the overall comminution energy increased by more than a factor of two (from 26.2 kilowatt-hours/dry ton to 59.9 kilowatt-hours/dry ton); however, this increase in energy was dwarfed by the reduction in energy during drying (a decrease from 2,328 kilowatt-hours/dry ton to 1,238 kilowatt-hours/dry ton) through increased drying efficiency and lower entrance moisture. This energy savings represents a feedstock production cost reduction on the order of $17.10/dry ton. Considering the additional quality attributes that can be derived, such as increased overall operational effectiveness and reduction in fines, the base case MFSP dropped from $4.75/GGE to $3.51/GGE. The reviewers rightfully indicate that interfacing with industry to identify current barriers to commercial operations is essential to maintain relevance. Currently, the task maintains ongoing relationships with several comminution equipment manufacturers and feedstock suppliers, and is developing relationships, for example, within in-line vision and characterization companies. The task is continually seeking new partnerships, where possible, to apply the advanced learnings from our diverse preprocessing work to de-risk operation and improve reliability and understanding. For example, since the Peer Review (as publicly announced at the event), the 2023 FCIC CRADA call for proposals saw several new partnerships and connections form within this task. These funding opportunities led by industry provide targeted funding to apply FCIC knowledge and tools to overcome the current challenges and barriers industry is facing. These opportunities have been in the areas of comminution, material separations and variability, and chemical/mechanical deconstruction and fibrillation of biomass for access to carbohydrates and advanced conversion schemes. These real-world problems identified by industry range from very practical choices of selection of mill type to achieve particle size and morphology attributes, to what the impact of feedstock structure is on deconstruction performance and how these native structures, carbohydrate distributions, and fibrillation methods improve access to carbohydrates or formation of nanofibers. Although decisions regarding these engagements are still outstanding, it highlights the myriad industrial engagement opportunities the task can take advantage of in future work scope definition. Similarly, these recent engagements indicate a growing shift in the desire to potentially take advantage of municipal wastes and other waste feedstocks in industrial processes. Although this work scope and strategies are still being developed alongside other funded projects, the fundamental approach of the FCIC at large is needed to understand approaches to waste processing prior to adoption. Due to the availability and collection of MSW, the problem of waste accumulation is imperative across the country but can tend to disproportionately affect rural communities via landfill siting operations and land availability. Actively seeking waste solutions and development of businesses and innovation for these communities can provide strong leverage to address waste, as well as increase DEI and environmental justice. In addition to the current activity, these will be explored in future scope.

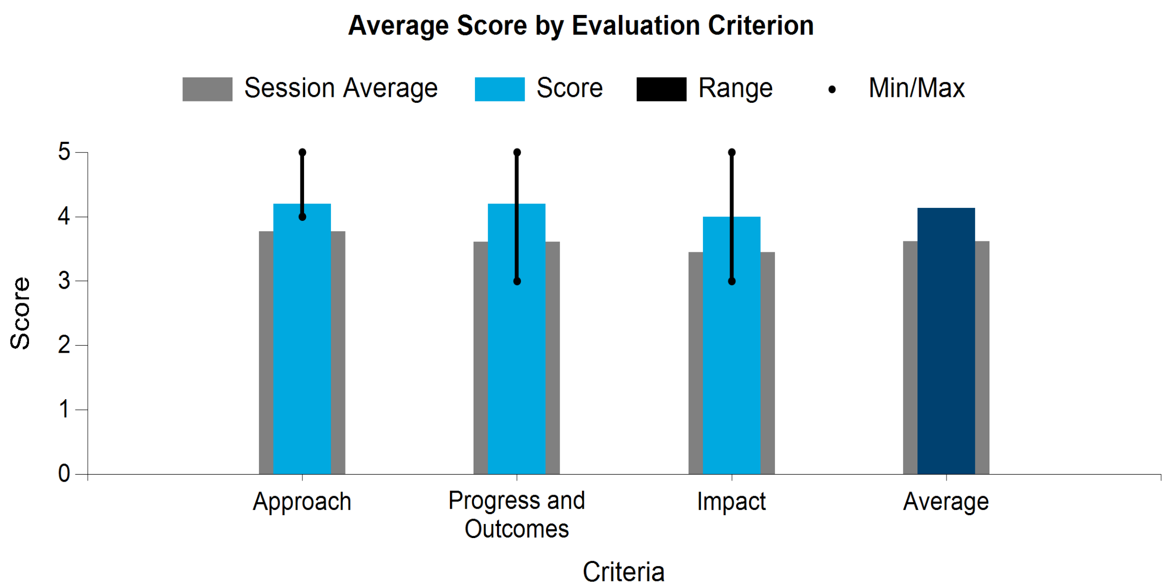
TASK 6 - HIGH-TEMPERATURE CONVERSION

Feedstock-Conversion Interface Consortium

PROJECT DESCRIPTION

WBS:	Task 6
Presenter(s):	Jim Parks
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$5,250,000

FCIC's High-Temperature Conversion Task (Task 6) addresses challenges with thermochemical conversion of diverse feedstocks. Conversion unit operations include fast pyrolysis and gasification. Feedstocks range from complex mixtures of woody biomass (forest residues) to MSW. The research identifies and quantifies the feedstock CMAs and product CQAs, consistent with FCIC's overarching approach embracing the QbD methodology. A primary outcome targeted by the research is experimentally validated computational modeling tool sets that can be used by the bioenergy industry to efficiently scale up and operate bioenergy technologies.



COMMENTS

- Valuable data and models were generated covering both pyrolysis and gasification. There was nice utilization of industry surveys and a summary of feedback on CMAs. It would be good to understand if additional feedback was solicited or received from industry, and if so, what that feedback was. There appears to be a current gap/inconsistency in the validation of the computational fluid dynamics (CFD) gasification model, which has been validated on feedstocks outside of the pine and corn stover that have been the express focus of the consortia.

- The researchers have done very nice and well-thought-out work. They did a great job of bridging the divide between science and industry, e.g., through industry surveys and by developing lower-order versions of their software to be used in Aspen TEA. At the beginning of the presentation, it would have been useful to know the breakdown of the costs typically associated with pyrolysis and gasification. This would have helped put the value and direction of their work into context. The researchers developed a lower-order version of their model for Aspen; they might also consider using their findings to develop an even-lower-order one for Microsoft Excel/Visual Basic for Applications. Reactants might be simplified to cellulose, hemicellulose, lignin, extractives, metaplastics, and water, and products might be simplified to char, oil, and light gases (or something like that). The Excel model could be used to perform sensitivity analyses on the feedstock compositions and yields to better understand the impact of these variables on process economics. An Excel model is also much more accessible than an Aspen model, and it might allow users besides the modelers to have a new window into the process.

- This task is extremely well-organized and presented. The application of the research outcomes for industry needs is significant. The team should continue to research gasification and pyrolysis for forestry feedstock because more research, modeling tools, and data are needed to better understand the conversion rates and economics of forestry feedstock of varying attributes to SAF and other high-value and even lower-value intermediates. It is very good that the team is doing validation at multiple scales. It's unclear why the team measured the breakdown of the forestry residue by weight but didn't measure the British thermal unit/energy value of each component, which is likely more valuable information for a final energy product. The TEA analysis is very insightful. Estimating translatable real-world costs is most helpful. It is fantastic to hear that the researchers reached out to and solicited input from industry leads. They should do more of this as often is practical. This appears to be a very diverse team in terms of gender, age, and ethnicity, which is fantastic. Communication and dissemination of research appears to be sound.

- This is a very difficult area with extremely complex interactions of heat and mass flow, reaction residence time, and many unknown factors. The objective of developing a "multiscale experimental and computational framework" is therefore a daunting task. In the presentation (Slide 18), a "generally good agreement" for model predictions is claimed, but objectively I must disagree with this assessment. If you look at the chart of model mass to experimental mass, there is a definitive skew in the experimental results from the predicted results. Good agreement would require the residuals of the experimental results to the prediction line to be randomly distributed about the line; instead, there is a definitive skew where the model mass fails to track the observed experimental mass (model mass holds at 60%–63%, whereas the experimental mass rises to almost 75%). This type of skew generally indicates something "missing" from the model. The new "micro- and macro-scale instruments" looked intriguing, but we ran out of time to discuss or highlight these.

- The team has made excellent progress in both modeling and experimental verification of the models. The progress is impressive on both pyrolysis and gasification (which was added after the 2021 Peer Review). The modeling efforts range from an extensive CFD model to TEA using Aspen. They have identified critical CMAs through experimentation as well as surveying 28 industry technology providers. They have created a partnership with the Sustainable Energy Research Centre in Italy to obtain gasification experimental results while the NREL gasifier is being recommissioned. The team has completed most of the end-of-project milestones listed in the quad chart and has used the industry technology provider survey to create the initial industry engagement toward commercialization. The opportunities during the second half of this project are:

    1. Develop a plan for addressing DEI in the project.

    2. Develop a strategy to lower the MFSP for both the pyrolysis and gasification pathways.

    3. Develop CPPs for both pyrolysis and gasification.

    4. Include MSW and corn stover along with woody biomass as feedstocks for both pyrolysis and gasification.

    5. Create additional industry engagement by developing partnerships for using the models and knowledge from this project in demonstration or commercialization efforts for both pyrolysis and gasification. Visits and presentations to pilot and demonstration facilities should be

considered. These partnerships could be funded by either CRADA agreements or funding opportunities.

PI RESPONSE TO REVIEWER COMMENTS

- The FCIC High-Temperature Conversion Task (Task 6) team appreciates the feedback provided by the review panel. Several positive comments were provided by the reviewers on the overall high-temperature conversion approach that covers both pyrolysis and gasification pathways. The reviewers complimented our focus on addressing the complex challenges associated with thermochemical feedstock conversion; the multiscale approach that combines both experiments and modeling; the overall approach bridging science and industry-relevant tools and knowledge; the overall outcomes of the project, including the data, models, and tool sets; the communication and dissemination of the research outcomes; the task's industry engagement; the inclusion of TEAs; and the diversity of the team toward DEI goals. We will continue the approaches leading to these positive outcomes. Several comments from the review panel offered valuable constructive feedback, including: (1) quantifying the outcomes of feedstock conversion in terms of energy content (e.g., British thermal unit) in addition to cost, yield, and life cycle carbon; (2) balancing the resource allocation between fast pyrolysis and gasification and providing further breakdown on the associated resource allocation between those pathways in future reviews; (3) pursuing further interactions with industry in the form of site visits and presentations; (4) developing more specific plans for DEI efforts; and (5) continuing the development of low-order models that can be used in techno-economic and life cycle analyses, and even providing more lower-order versions of the models in perhaps Microsoft Excel format that can be used by an even broader range of bioenergy industry stakeholders. This task considers all of these comments as relevant and useful and will incorporate these comments into our future plans. Another constructive comment related to including more feedstocks such as corn stover in the research and including MSW and woody forest residues in both gasification and fast pyrolysis pathways. While the task agrees that more research outcomes for more feedstocks would be highly beneficial, it will be extremely challenging to study all of these feedstocks for all pathways based on the current resources allocated to the FCIC. Nonetheless, this task will continue to develop tools that are generally effective for research of a wide range of feedstocks, and we will incorporate more feedstocks into our studies if additional resources can be made available. An additional constructive and guiding reviewer comment was to develop a strategy to lower the MFSP for both pyrolysis and gasification pathways. This comment is good feedback and challenges the team to go beyond the current status of calculating MFSP for a wide range of feedstocks and to, based on our tool sets, actually define strategies for lowering MFSP. The review panel had one negative comment on the characterization of the agreement between experimental and model results; a reviewer noted "a definitive skew in the experimental results from the predicted results." While we recognize that the agreement between experimental and model results was not exact, our comparison between experimental and model results was obtained by taking a fundamental science-based approach that incorporated extensive feedstock physical and chemical characterization, a chemical conversion kinetic scheme that included 25 reactant and intermediate species and 31 product species, and complete capture of any feedstock particle effects due to size, shape, and even biomass microstructure. By incorporating all these chemical and physical phenomena into our models, we were able to predict the outcomes of experiments very closely for an extremely wide range of forest residue feedstocks. The agreement was obtained without additional model calibration or fitting and demonstrates that our model is robust and capable as a valuable tool to industry despite the vast variability in bioenergy feedstocks. We consider our model as state of the art for fast pyrolysis, and to our knowledge, no other entity has demonstrated such an advanced fast pyrolysis model. Multiple reviewers noted and complimented the utility of the model outcomes, and we seek to improve upon our state of the art. The utilization of these modeling and knowledge outcomes will enable industry stakeholders reduce MSFP for sustainable fuel production in a cost-effective manner. Overall, we appreciate all the feedback from the review panel and look forward to incorporating the guidance as we move forward in the FCIC program.

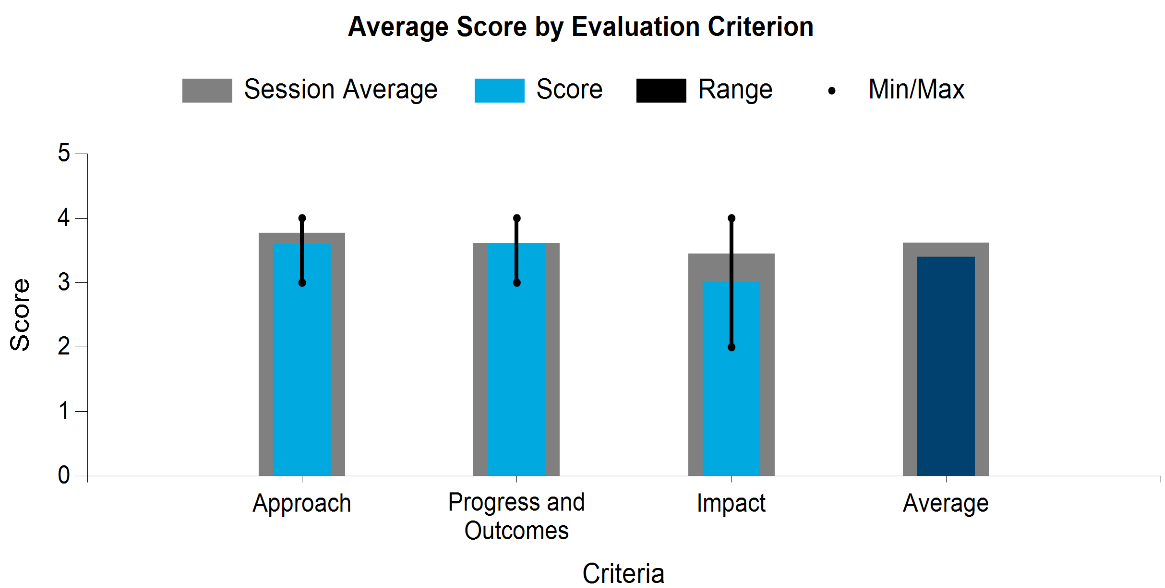
TASK 7 - LOW-TEMPERATURE CONVERSION

Feedstock-Conversion Interface Consortium

PROJECT DESCRIPTION

WBS:	Task 7
Presenter(s):	Phil Laible
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$3,210,000

The objective of this task is to determine the effects of feedstock variability on biocatalytic conversion (by both sugar and lignin pathways) and to develop tools to mitigate the risks posed. Long-term goals are to intelligently operate the sequential cascade of unit operations by understanding critical attributes of materials to adjust process parameters, limit impacts, and maximize feedstock utilization. Researchers are leveraging laboratory data and existing metabolic models to develop an integrated framework that predicts the effects of feedstock variability on microbial conversion performance, by identifying the genetic basis of the effects on conversion efficiency. This knowledge lets these approaches adapt to and/or engineer around attributes of feedstocks that negatively affect conversion. Impacts on productivity and substrate utilization have been observed for feedstock streams derived from both intrinsic and process-derived variability—in many cases differentially for the sugar- and lignin-converting organisms. Operational ranges of critical components in feedstock streams have been determined. These results are the first of their kind to determine the effects of feedstock variability on biological conversion of streams arising from multiple pretreatment/deconstruction operations, driving development of validated modeling tools that can predict performance of new organisms on variable sugar and lignin streams from corn stover.



COMMENTS

- Having a baseline process is valuable, but it would also be extremely informative to utilize a variety of enzyme cocktails to better understand and optimize based on the feedstock input. This task should also consider other potentially viable pretreatment processes (steam explosions, ammonia fiber expansion, etc.). I appreciate that the task, at least visually, showed the interconnection between this task and others on Slide 4. I would have appreciated TEA information and any support on whether there is actual viability in lignin utilization beyond heat/power.

- This presentation was difficult to follow. The approach and progress came across as scattered, and the impact vague. The third bullet point on the impact slide claims that the results of this task “enable sustained high levels of production in low-temperature conversion processes,” but it’s unclear what exactly this means or if something like it has been accomplished. The goals as described on the project overview slide are similarly vague, so perhaps the researchers would benefit from more specific goals to begin with. The presentation mentioned crosscutting/TEA in places, but costs were never mentioned.

- It’s excellent that the team works across multiple consortia and among five different organizations. The narrow focus is acceptable and is likely needed to best leverage resources. It isn’t clear why the team only focused on MSW. The presenter mentioned that the team looks forward to working with bioproducers, but it probably would have been better to do that in an earlier phase. Opportunities for commercialization are far too attenuated at this stage. The team could benefit from industry engagement. The team appears to be diverse in terms of gender, age, and ethnicity. There was no mention of DEI efforts.

- This presentation focused on the impacts of feedstock variation on low-temperature processes for the conversion to SAF. The focus was on drought-stressed versus non-drought-stressed corn stover. The team tested with deacetylation and mechanical refining (DMR) versus diluted acid versus reductive catalytic fractionation and found no substantial difference between drought-stressed and non-drought-stressed stover, irrespective of processing method. Thus, the main conclusion is that drought stress is not really a concern. Although this appears to be a significant relief, it does not show that this research approach can highlight differences in feedstock variability and recommend differences in processing when a real differentiation occurs. This unfortunately dulls the impact of the work. DMR is touted by the federal labs but appears not to be taken up by industry.

- The team has continued to evaluate material attributes for corn stover, focusing on drought-stressed versus non-stressed stover. The results to date show insignificant impact on the utilization of lignin or sugar in product formation, thus de-risking this source of variability for biorefineries. They have continued to use artificial intelligence to “train” their metabolic models to study the effect of material variability on conversion variability, developing significant interaction networks. The team continues to study the impact of corn stover material variability as well as process variability by focusing on understanding the operating ranges of bioprocesses. They are also beginning to characterize MSW. The team states that they will expand DEI outreach through presentations to MSIs and farming communities. Creating some specific end-of-project DEI milestones and goals would strengthen the commitment to this activity. The shift to studying the impact of material variability on operating ranges of the conversion processes would appear to be a valuable next step. The intent to use CRADA and other BETO projects to validate the model predictions, as well as working with industry to evaluate feedstock variability on SAF precursors, would provide the most benefit from this program on downstream processes. Using an industry survey to gather information about which feedstocks are being pursued could be used to expand the work of this task. Engaging industry partners who are developing biorefineries at demonstration or commercial scale should be a priority task for the next phase of this project and should be included as part of the end-of-project goal and milestone. Corn stover, forest residue, and MSW are becoming the standard suite of feedstocks for a number the FCIC tasks. Further development of low-temperature conversion should include forest residues in addition to corn stover and MSW.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the review team for their interest in the work of FCIC’s low-temperature conversion team. We appreciate both their recognition of the success of our approach and their suggestions for improvement.

We agree that this consortium activity should be kept as industrially relevant as possible using a variety of outreach approaches (including new ones like the potential use of an industry survey). We note that (1) the current experimental strategy toward evaluating feedstock variability was supplemented by crosscutting discussions with industrial entities at meetings or in one-on-one interviews at venues (identifying DMR approaches as unrelatable), and (2) these discussions continue routinely with interactions at various institutions (e.g., persistent demonstrations and technology transfers at the Advanced Biofuels and Bioproducts Process Development Unit at Lawrence Berkeley National Laboratory) to inform our technical strategy. We will also use our recently completed report on the impact of feedstock variability in outreach efforts over the next 18 months to increase awareness of our findings and better gauge adjustments to our approach and collaborations (including intergovernmental agencies and academic research teams). We share the reviewers' interest in expanding as much as practicable into additional pretreatment and deconstruction processes (as well as new enzyme cocktails)—especially those that are most recognized and relatable to the biomanufacturing community. These experiments, where possible, will continue to gather data for predictive modeling within Task 7, as well as techno-economic evaluations and LCAs via collaborative FCIC tasks. We also agree that increasing the number of different feedstocks and pretreatment chemistries, including work on sugar and lignin streams from MSW, will strengthen our outreach messages and better position the FCIC for more discussions with a larger audience. We will need to work with FCIC and BETO leadership to evaluate the feasibility of studying forest residues within our current resources.

TASK 8 - CROSSCUTTING ANALYSIS

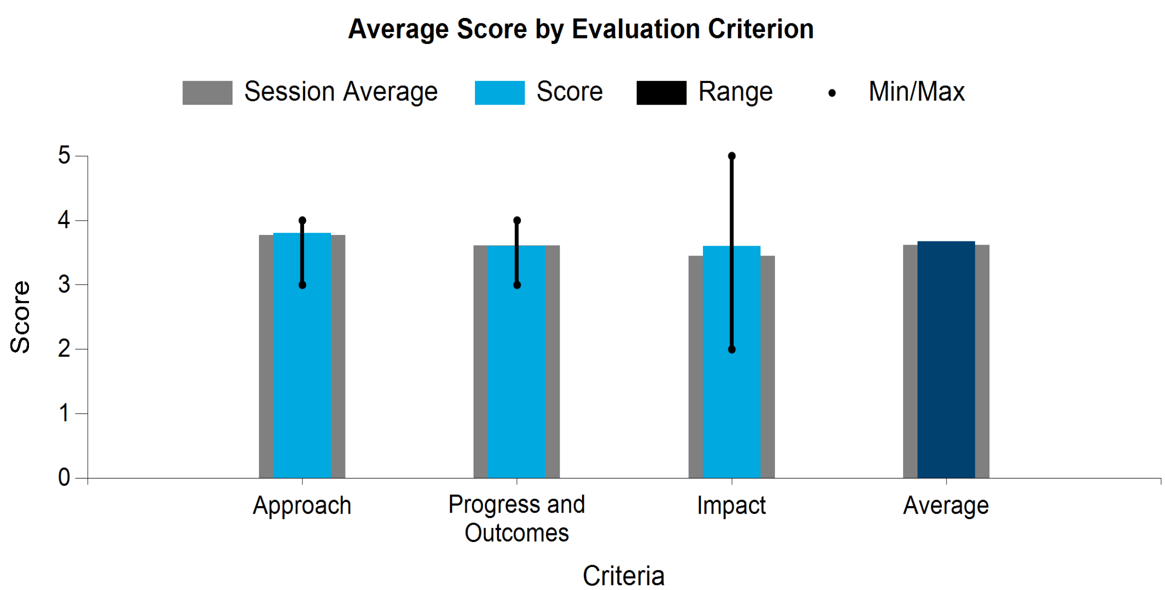
Feedstock-Conversion Interface Consortium

WBS:	Task 8
Presenter(s):	Steven Phillips
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$3,750,000

PROJECT DESCRIPTION

The objective of the Crosscutting Analysis task is to quantify and communicate industrially relevant, system-level cost and environmental impacts for FCIC's discoveries and innovations. TEA and LCA tools are used to evaluate how feedstock variability affects economics and sustainability metrics throughout the biomass-to-fuel value chain. Case studies incorporating information from FCIC experimental research, computational models, and literature into analysis models are used to estimate the impact of process changes and feedstock variability on process economics (e.g., biomass and fuel prices) and life cycle metrics (e.g., greenhouse gas emissions). The scope of work encompasses the field-to-fuel value chain for high-temperature conversion of forest residues by *ex situ* catalytic fast pyrolysis and low-temperature corn stover deconstruction to cellulosic sugars and subsequent biological upgrading to multiple products.

The case study results provide economic and sustainability information to equipment manufacturers, biorefinery owners, and operators to enable them to make informed decisions about feedstock collection and processing, conversion process design, equipment selection, and business feasibility, including key mitigation steps to minimize or control feedstock variability.



COMMENTS

- This is likely the most valuable task of the overall consortium. The case studies in this task and other tasks largely use TEA to examine the results of work that has already been completed. When used well, TEM is like Google Maps for technology development. Initially, it can help you estimate where you are and how far you are from your destination, and it can help you anticipate the best path to get from one to the other. Then, during the development process, it can be used to assess progress and adjust plans accordingly. I think that the top TEA priority for FCIC (or whatever the right part of the organization is) should be to develop baseline TEMs for a representative set of processes. These need to be models, not reports or "assessments." Initially, the models could be used to develop diagrams and sensitivity analyses to help direct and justify R&D resources. Tornado diagrams would be especially useful for understanding the relative impact of process and economic parameters. When using tornado diagrams in this way, it is important to use actual estimates for worst-case, expected, and best-case values, rather than constant percentage variations. The worst-case/expected/best-case values could be based on data analysis or expert judgment. Ideally, these models should be living documents, representing the best current understanding of the technology. As that understanding evolves, so should the models. Part of the "best current understanding" involves the uncertainty in economic and process parameters. These should be addressed explicitly via sensitivity analyses, e.g., tornado diagrams and the Monte Carlo method. With a more quantitative understanding of the sources of uncertainty, researchers can then make efforts to reduce it by collecting data, making process changes, or seeking out industry input. An additional use of these baseline TEMs would be to test new ideas. If a researcher has an idea for a particular process improvement, the first step might be to mock it up in the TEM. They might then "test" the potential impact of their ideas before ever setting foot in a lab, and in this way, focus their resources on the ideas with greatest potential. If it is possible, I tend to think that these models would be more useful in Microsoft Excel/Visual Basic for Applications. A well-built Excel model is so much more transparent and accessible than an Aspen simulation. The researchers could even make them open source, and perhaps solicit input from the public or other institutions. That said, Aspen simulation or CFD modeling might still be used to inform the coarser parameters used in the Excel models.

- This is a strong collaboration between four organizations, which diversifies approaches and thereby improves depth and breadth of engagement. The team is admittedly less comfortable communicating work to stakeholders. In that case, they should consider hiring or partnering with organizations that are comfortable doing that. Presentations to biorefinery stakeholders are important, but it is equally important to communicate work and share case studies with feedstock suppliers. The cost comparison case study for forestry feedstock is an example of key information that can inform industry decision-making. It is very good that the team is assessing systems and not just individual pieces of equipment. The presenter said that some industry feedback has been that scenarios studied don't represent real-world setups. This suggests a need for this team to engage with industry earlier on and explore opportunities to study real-world systems.

- TEA analysis was a critical parameter that was absent from most of the FCIC presentations. I understand that it wasn't a requirement, but the absence was noted. The TEA analysis of the cost/value of various anatomical fractions (Slide 15) was important and would have been a driving force/double-check on many of the papers presented outlining air-driven fractionation and performance of biomass, notably, that an MFSP of $8.76/GGE is a nonstarter! Given the time allotted for presentation, a comprehensive review of individual projects was not possible. A more generalized vision of how the TEA can be applied consistently across multiple platforms was desired. I believe the TEA should be applied earlier in a research project ("presume success"), and the cost predictions should be allowed to help drive early decision-making among various options—then validate!

- This task has developed an alternative approach to TEA/LCA that focuses on demonstrating the impact of feedstock variability on biorefinery design and operation using knowledge generated by other FCIC tasks. The case studies allow for the opportunity to test different process approaches. For instance, the case studies comparing wet milling to dry milling demonstrate the economic effects on the drying process of changing the preprocessing sequence in the biorefinery. The case studies will be disseminated through FCIC technical reports as well as a two-page summary and lessons learned available on the FCIC Data Hub. The case study on Slide 15 shows the difference in MFSP of processing individual fractions of corn stover compared to processing whole stover. However, it is unclear what impact this approach has on the volume of fuel produced for each fraction. An overall economic impact should consider the volumetric impact from discarding hard-to-process fractions versus processing whole stover, or the total cost of processing each fraction separately and then combining the total volume of fuel. It is difficult to assess progress because the end-of-project milestone only says that the team will publish the TEA/LCA lessons learned. There should be a goal for the number of case studies completed as well as the number of case studies that have gone through FCIC review. There is not a clear path for engaging industry except through publishing the two-page summary on the FCIC Data Hub. There should be a more proactive way of directly engaging biorefineries and equipment manufacturers by demonstrating this approach directly to industry. The team should consider financial measures in addition to MFSP to encourage industry partners to utilize the case study method. The end-of-project goal should include a DEI component.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for the valuable feedback recognizing the value of TEA in technology development. We agree that TEA serves as a valuable tool for estimating progress, guiding decision-making, and optimizing resource allocation. The reviewers' comments are helpful in clarifying our strategy moving forward. We agree with the need for more agile and transparent models, industry guidance, and consistent sensitivity analyses. Within BETO, there have been more in-depth models for specific pathways from biomass (stover and forest residues) as part of major reports called design cases. The design cases serve as baseline performance based on n^{th} plant TEA with annual periodic "State of Technology" updates to assess the progress toward the n^{th} plant performance. (See https://bioenergykdf.net/content/beto-biofuels-tea-database for a database of models that have been developed.) The design reports use tornado diagrams and sensitivity analyses to understand the impact of process and economic parameters in the models. We will explore opportunities to improve our use of sensitivity analysis in a case study. To the extent that funding is available, we agree that maintaining living documents that follow the evolving technology understanding is crucial. We appreciate your feedback on stakeholder communication and agree that communicating our work to both biorefinery stakeholders and feedstock suppliers is important. We will explore your suggestion of hiring or partnering with organizations experienced in stakeholder communication as a boost to our outreach efforts. We will work on expanding our communication efforts and engaging with industry partners earlier in the process to study real-world systems and improve the relevance of our work. We acknowledge the importance of applying TEA early in research projects and using cost predictions to guide early decision-making. Typically, these early estimates are done by other programs using the design report approach for each of the key areas of the field-to-fuel value chains. We will investigate ways for our TEA/LCA, done in support of FCIC research, to be used as guidance to researchers on key areas of concern and cost drivers in the value chain. We appreciate your input on the comprehensive review of individual projects and will work on providing a more generalized vision of how TEA can be consistently applied across multiple platforms. We agree that considering the volumetric impact and total costs of processing different fractions is important in evaluating economic impacts. We will ensure that we provide a more comprehensive assessment in future case studies. We also acknowledge the need for a clearer path for engaging industry and will explore more proactive ways to directly engage with biorefineries and equipment manufacturers. We will seek assistance in formulating a valuable DEI component to our research.

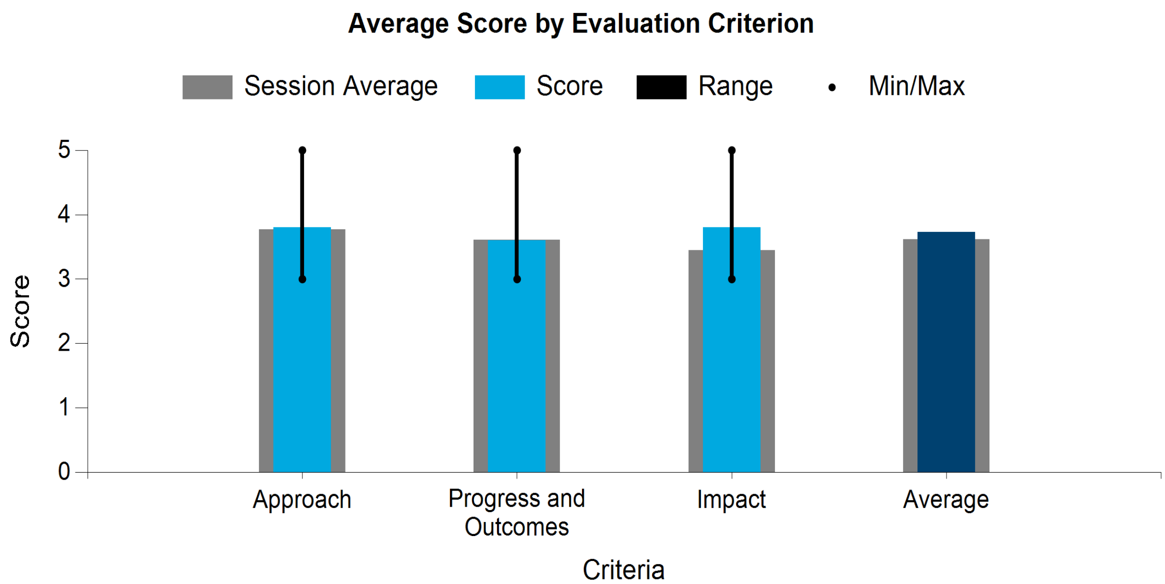
TASK 9 - FAILURE MODES AND EFFECTS ANALYSIS

Feedstock-Conversion Interface Consortium

PROJECT DESCRIPTION

WBS:	Task 9
Presenter(s):	Rachel Emerson
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$450,000.

The objectives of this FCIC task are to (1) implement QbD approaches by applying a systematic criticality assessment methodology using failure mode and effect analysis (FMEA), a robust and well-accepted quantitative risk analysis approach, to evaluate preprocessing and conversion unit operations and systems, and (2) develop a framework to track and quantify the criticality of critical material attributes (CMAs), critical process parameters (CPPs), and critical quality attributes (CQAs). This approach will use subject matter experts (SMEs) from Task 5 (Preprocessing), Task 6 (High-Temperature Conversion), Task 7 (Low-Temperature Conversion), Task 8 (Crosscutting Analysis), and industry for FMEA interviews. A semiquantitative scoring system based on the generation of risk priority numbers is used to assess the CMAs, CPPs, and CQAs for key unit operations within the technology configuration pathways of FCIC. The impacts of this research are (1) the development of a systematic methodology for biorefinery risk assessment using a QbD approach, and (2) generation of a database for risk assessment of future simulated system configurations.



COMMENTS

- I appreciate the effort to utilize not only a consistent but also an industry-accepted framework. The task will need to continue to ensure industry input throughout the assessments. This task seems to be right on point in the way it transforms semiqualitative input into a clearly prioritized and actionable list of risks. A strength of this task is engaging with and obtaining information from subject matter industry experts. The downside that there could be bias is a given that is likely outweighed by the collective analyses and insights gained by industry. This task appears to be much more engaged with industry stakeholders than the other tasks, which is much needed. This excellent industry engagement will generate synergies far beyond the scope of this project. This task seems to be a much better investment and return for federal funding than many other tasks.

- Failure Modes and Effects Analysis (FEMA) is well-known to suffer from decision bias from preformed opinions or evaluation conflicts. It is a practiced risk-assessment tool that is continually looking for ways of improving the method. The value of a FMEA depends not only on the SMEs, but also on how well the system being analyzed is defined and the skills of the data collection individual. A postanalysis review is needed to see whether the guidance provided by the FMEA was useful. I was unable to determine whether such a postanalysis was done. Because FMEA is highly dependent on a very specific operation, clear progress to commercialization is not highly transferable, in my opinion.

- The team has developed an excellent survey process for gathering CMAs, CPPs, and CQAs using SMEs for the material and preprocessing operations. They have demonstrated how to use this information to generate a risk priority number to the preprocessing system (material/preprocessing unit operations). They have developed preprocessing system risk priority numbers for pine residue and corn stover using SMEs from the national labs. They are adding SMEs from industry as they expand the FMEA tool to MSW. The abstract for this task and the project goal in the quad chart call for developing a FMEA analysis of preprocessing, high-temperature conversion, and low-temperature conversion. However, the end-of-project milestone calls for completing FMEA on 90% of the material/preprocessing operations. The end-of-project milestone should include the conversion systems as well. Moving forward with the risk-assessment survey for biorefineries is needed to complete the project goal. A specific metric tracking the percent of operations with currently completed FMEA evaluations is needed to track the progress of this task in meeting its end-of-project goal.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' positive feedback on the use of FMEA as a standardized methodology providing a framework for capturing operation- and system-based risks and their associated critical properties. The concerns regarding potential bias of FMEA and dependence on the knowledge of the SMEs are completely accurate. We acknowledge these as risks and challenges of using this approach and identify these risks within our presentation. We are addressing these risks by using multiple SMEs for each unit operation and/or system and incorporating SMEs from national lab researchers and industry to reduce bias input. We agree with the reviewers that industry engagement is an important and necessary component of this work that we will continue to incorporate into our project. One reviewer identified that our end-of-project goals focus only on completing FMEA analyses on operations and systems in feedstock preprocessing. We acknowledge that conversion should be included in our efforts along with preprocessing. Currently, we have completed FMEA interviews on a select number of conversion area unit operations, and we plan to incorporate more conversion-focused FMEA interviews in the next potential funding cycle.

FEEDSTOCK TECHNOLOGIES

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Feedstock Technologies Program is one of 12 technology areas that were reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 32 presentations were reviewed in the Feedstock Technologies session by 4–5 external experts from industry, academia, and other government agencies. Of the 32 projects reviewed, 26 were reviewed by the Feedstock Technologies panel and six were reviewed by the Feedstock-Conversion Interface Consortium (FCIC) panel. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks, which can be accessed at the Peer Review website: www.energy.gov/eere/bioenergy/2023-project-peer-review.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $59.9 million, which represents approximately 11% of the BETO portfolio reviewed during the 2023 Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Elizabeth Burrows as the Feedstock Technologies Technology Area review lead, with contractor support from Andrew Zimmerman of Lindahl Reed Inc. In this capacity, Elizabeth Burrows was responsible for all aspects of review planning and implementation.

FEEDSTOCK TECHNOLOGIES REVIEW PANEL

Name	Affiliation
Dr. Jingxin Wang*	West Virginia University
Dr. Sally Krigstin	University of Toronto
Dr. Bhima Vijayendran	Redwood Innovation Partners LLC
Dr. Kevin Kephart	U.S. Department of Agriculture

* Lead Reviewer

FEEDSTOCK TECHNOLOGIES REVIEW PANEL SUMMARY REPORT

Prepared by the Feedstock Technologies Review Panel

INTRODUCTION

The Feedstock Technologies area is an integral component of the overall BETO portfolio of projects. It addresses the research and development (R&D) essentials of biomass feedstock development and establishes the foundation for the success of any biorefinery project. A robust industry producing advanced biofuels and bioproducts with biomass requires economical, high-quality feedstock with minimal variation in feedstock quality. This is the subject matter of this program area. The review panel for the Feedstock Technologies program had a cross section of representatives with diverse backgrounds and expertise. Industry, government, and academic perspectives were all represented. This made for strong and varied viewpoints, which became evident in the review comments and the numerical evaluations of the projects.

The Feedstock Technologies Peer Review process occurs every 2 years and addresses progress since the previous review. In the 2019 review, BETO unveiled its plan to adopt a quality-by-design process for its projects. This process is favored by the pharmaceutical industry. The 2021 review (in which 18 projects were reviewed) was conducted virtually due to the COVID-19 pandemic.

In 2023, the review panel evaluated 26 project presentations within the Feedstock Technologies program. Each of these projects is funded by BETO, either through a funding opportunity announcement (FOA) (nine projects) or as part of BETO's annual operating plan (AOP) (17 projects). Of these 26 projects, eight are on supply chains and process modeling, seven address municipal solid waste (MSW) processing and artificial intelligence (AI)/sensing technologies, three focus on cover crops, four are on carbon impact analysis, two concentrate on feedstock production, and two focus on value-added bioproducts. Nine projects were ending, 13 were ongoing, and four were in their beginning stages.

The review process was straightforward. The panel listened to an oral presentation by the principal investigator (PI) of the project. The presentation was accompanied by a slideshow, with a Q&A period following the presentation. Each project was allocated the same amount of time and used the same format for its presentation. Each individual on the panel rated the project numerically and made comments with their assessment based on the following criteria:

1. Approach – Did the project performers develop an approach that has:
    - Significant merit to advance the state of the art of technology, relevance to BETO program and technology area goals, and significant potential for innovation in its application?
    - A clear management plan and successful implementation strategies for identification of project risks and mitigation of those risks?
    - An adequate approach to address diversity, equity, and inclusion (DEI) in the project plan?
2. Progress and Outcomes – To what extent:
    - Has the project made appropriate progress toward addressing the project goal(s)?
    - Have the accomplishments been completed on schedule with the planned approach—and, if needed, have risk mitigation strategies been used to maintain project progress and schedule?
3. Impact – Does the project and its presentation:

- Demonstrate a clear connection between the project approach and the potential for significant impact and outcomes?
- Demonstrate a clear commercialization potential or use or have plans to use industry engagement to guide project deliverables?

Each of the panelists was also asked to provide a written assessment of each project based on the above criteria to rationalize the evaluations. There is no doubt that the panel feels that BETO's Feedstock Technologies program is an important area for their involvement and support. The Peer Review process is an essential step for determining whether the projects are beneficial and addressing the barriers to the industry's success. The biomass harvest, logistics, handling, preprocessing, techno-economic analysis (TEA), and life cycle analysis (LCA) have been problem areas, and the portfolio of BETO Feedstock Technologies projects is addressing a number of these. Below is a collection of comments from the panel addressing several of the areas above in terms of strategy, strategy implementation and progress, and recommendations.

STRATEGY

The program has a clear strategy, supporting the industry by setting a near-term cost target for biomass delivered to the throat of a conversion facility of $84/dry ton, or $3/gallon gasoline equivalent (GGE) for the sustainable aviation fuel (SAF) markets. In the 2023 BETO Multi-Year Program Plan (MYPP), BETO set six key performance goals to achieve by 2030, including enabling commercial production of SAF and renewable chemicals capable of >70% greenhouse gas (GHG) emission reduction. These goals will help researchers and developers from academia and industry work together to achieve the deliverables and generate long-term impacts.

The Feedstock Technologies program has been well managed. The panel was impressed by the projects in the BETO Feedstock Technologies portfolio. BETO has set a clear pathway and goal of producing high-quality, economical feedstocks to support the growth of a healthy bioeconomy. For the most part, the projects had clear targets and go/no-go decision points and were supportive of the BETO goals and MYPP.

The panel agreed that to meet the goal of producing biofuels and bioproducts for the national bioeconomy from sustainable feedstocks and renewable resources, we need a diverse supply of feedstocks, such as agricultural and forest residues, MSWs across the nation, willow and switchgrass in the Northeast, energy cane along the Gulf Coast, miscanthus in the upper Southeast and Midwest, and clean corn stover all over the Midwest. The development of diverse feedstocks is supported by the portfolio funded through BETO and is central to BETO's multiyear plan in support of a robust national bioeconomy.

The Feedstock Technologies program's priority topic areas were determined through extensive stakeholder input from groups such as industry stakeholders, federal advisory committees, interagency working groups, workshops, and professional organizations. Some of the projects reviewed have been in progress for over ten years, whereas others started just a few months ago. Some projects are led by scientists at national labs, others are led by private-sector entities, and still others are led by university scientists. There are several themes that run throughout the BETO Feedstock Technologies project portfolio. There are projects that are investigating and developing state-of-the-art methodologies and advancing the state of technology through the following areas:

- Feedstock handling and preprocessing
- Feedstock quality
- Renewable carbon resources
- MSW

- Coproducts and preprocessing
- Feedstock logistics and storage
- AI and sensing technologies
- Data, modeling, and analysis of the supply chain.

The related FOAs were published to address these topic areas and included several specific objectives within each of the above topics. For example, feedstock supply chain analysis includes the continued development of the *Billion-Ton Report*, DOE's Bioenergy Feedstock Library (BFL), and computational modeling and predictive systems. Additionally, the overall MSW portfolio includes projects that address characterization and MSW separation/sorting/decontamination/blending/processing to improve feedstock quality and consistency. The Feedstock Technologies portfolio also includes requirements for TEA, and more recent projects must include long-term DEI goals.

The panel believes that several projects, especially some MSW projects, could benefit more from stakeholder input, especially from industry involvement. Communications with MSW disposal professionals and agriculture and forestry practitioners seem essential for PIs to improve project performance. Important stakeholders that were notably absent included critical members of the local farming and forest community, including county extension agents and members of local governing boards. If involved in the early stages of a project, these groups might be able to help with advice, logistics, and local issues. Field practitioners are always known for their innovation and problem-solving skills. Although some projects had varied and meaningful stakeholder input, others seemed to be quite deficient in the Feedstock Technologies area. A number of presenters were asked to identify the "customers" for their projects. Often, the PI was not able to succinctly identify who would make use of their project results. It is important for all projects to have their end user in mind and to make sure they are connecting with these stakeholders throughout the project and even beyond.

The panel agreed that Idaho National Laboratory's (INL's) BFL and Oak Ridge National Laboratory's (ORNL's) *Billion-Ton Report* are significant resources and accomplishments. They are beneficial to all who are working in the field nationwide and are much needed. The panel recommends a general guideline for conducting TEA and LCA and calculating dollars-per-hour operating costs and dollars-per-dry-ton unit costs for commercially available biomass harvest or processing under certain site, machine, and feedstock species conditions. This guideline can be used for the cost analysis required for all BETO projects. This would provide PIs and future reviewers with a common starting point for cost analysis and comparisons.

The Feedstock Technologies gaps are well identified and are valid for increasing the mobilization of biomass resources. One panelist noted a lack of projects focused on the biomass depot idea and the biomass by design component in this review. If there has been a shift in direction away from these concepts, there could have been an explanation given in the overview presentation. Another panelist commented that the economic modeling on a few projects seemed unrealistic and not as well thought out as it should be. We hope that by the next review, PIs will have time to consider this and make suitable adjustments.

The Feedstock Technologies program's funding mechanism seems to be working well, although there might need to be an increase in the proportion of FOA projects or a shift in the mix of FOAs versus AOPs to roughly 50/50. Collaborations among academia, DOE labs, and industry could be further promoted through this innovative funding mechanism, especially through commercialization and scale-up programs and activities. Better and more effective communications between this program and the U.S. Department of Agriculture's (USDA's) National Institute of Food and Agriculture and DOE's Advanced Research Projects Agency–Energy through joint FOAs and workshops would be promising. The panel knows that this is up to the appropriations process, but they are supportive of BETO seeking greater funding.

STRATEGY IMPLEMENTATION AND PROGRESS

Overall, the programs are reasonably well structured to monitor progress. It may be helpful to further tighten the milestone deliverable metrics so they are more transparent to measure. In this review cycle, the Feedstock Technologies area funded a wide range of projects addressing all areas of the supply chain, from feedstock harvest and handling to processing to LCA and TEA. The topic areas investigated included:

- Feedstock supply chain analysis and modeling
- Cover crop valuation for biofuels
- AI and sensing technologies
- MSW characterization, decontamination, and processing
- Value-added bioproducts.

The panel believes that BETO is funding a strong portfolio of projects supportive of BETO's objectives. The projects that impressed the panel in providing strong support for this vision are:

- DoKyoung Lee's project, "Next-Generation Feedstocks for the Emerging Bioeconomy," is an excellent project with impactful results. The panel appreciated the project's work on evaluating ecosystem services with diverse field trials and machine learning (ML) modeling. Their approaches and findings can be considered for other applicable projects.
- Rachel Emerson's project, "Bioenergy Feedstock Library," hosts characteristic data from over 70,000 biomass samples representing over 90 crop types, providing tools to store, record, track, retrieve, and analyze data to help researchers and industry overcome challenges posed by biomass variability. It is an impactful project for a variety of audiences nationwide. DOE should continue to support this effort that will benefit the national biomass for energy strategy.
- Matt Langholtz' project, "Supply Scenario Analysis," updates the *Billion-Ton Report* with new additions, such as oilseed and cover crops. It is an impressive and impactful project with more than 4,000 citations of the report, providing important information to a wide variety of stakeholders. DOE should continue to invest in this effort to further improve the data accuracy, regional field data collection, and validation.

Although the panel has singled out the above projects, there are several others that could have been mentioned, and the readers are encouraged to review the entire portfolio. The BETO management team is clearly managing their portfolio of projects toward their near-term/mid-term and final goals of providing high-quality feedstock at an economical cost to support existing and emerging conversion projects.

The panel also noticed that there was a substantial number of projects focused on MSWs, especially on preprocessing (sorting). Although these MSW projects were well done, using different sensor technologies to measure critical characteristics, one panelist indicated that this focus may not be able to achieve cost-effective utilization of MSW biomass, and perhaps industry partners may be better suited to work in this area.

The panel also noticed that some of the legacy-type projects were still targeting chemical molecules such as levulinic acid that have shown very little commercial traction despite numerous attempts with significant venture capital funding. Projects of this nature need to clearly articulate why the particular molecule is being targeted and what the market justification is.

The panel agreed that the implementation of the project associated with the designated technology readiness level (TRL) at the beginning and the end of the project should be encouraged, while a graphical presentation of the project's progress with color coding would be helpful. The panel noticed that some of the projects need to proceed to the next TRL for scale-up or demonstration.

RECOMMENDATIONS

To further improve the impacts of the Feedstock Technologies portfolio, the panel thinks the following recommendations will be helpful for future reviews and funding cycles.

Recommendation 1: Integrate data from various projects and ensure accessibility.

There are a couple of excellent initiatives focused on data collection and cataloging. It would be helpful to all stakeholders in the field if easily deployable tools, such as AI/ML-driven ChatGPT search engines, could be implemented by integrating diverse data from various projects funded in this area.

Recommendation 2: Optimize Feedstock Technologies subprogram investment in computational modeling.

There are quite a few modeling and analytical-based projects in this review. Feedstock Technologies may be overinvested in computational modeling. Future solicitations may focus on data and model generation from lab and field studies that are the foundation of the modeling work. Some of the initiatives in this area seem to have the flavor of modeling for the sake of modeling with no clear path toward integrating the results with downstream tasks, such as pilot-scale demonstration and commercialization. Modeling can provide an acceptable range of production rates and costs, but some performance-related variables, such as equipment delays and utilization rates, are needed from actual studies. Some of the models are being field tested, but some are not. It should be a requirement that all models are field tested; this would give a higher confidence in their accuracy and results.

Recommendation 3: Develop general guidance for future TEAs and cost analyses.

Each of the projects reviewed has a TEA/cost component. There seems to be some inconsistency in these analyses, with some superficial and confusing results. General guidance is essential for future TEAs and cost analyses. Data sharing and uses among completed and ongoing projects could be further enhanced via ORNL's Knowledge Discovery Framework (KDF) and INL's BFL. More dissemination workshops should be conducted. It would be helpful to accelerate R&D and commercialization tasks in making funding decisions.

Recommendation 4: Expand focus on forest logging residues.

At least one panelist mentioned that research on diverse feedstocks, such as forest logging residue, should be considered in the Feedstock Technologies portfolio. Forest logging residue is abundant nationwide but suffers from a costly supply chain system. A key concern is the economics of logging residue collection and harvest. Future FOAs could focus on the logistics of forest residue and the blending and utilization of both agricultural and forest residue biomasses for the production of uniform feedstocks, development of emerging technologies, advancement of equipment, engagement with industry, and commercialization. Work in this area to reduce the cost of this resource's collection and delivery direct to a biorefinery or to a depot for blending would provide at least two major benefits: (1) providing another economical feedstock to support the continued growth of the bioeconomy, and (2) providing an economic incentive and support for cleaning and reducing fuel loads of both public and private forest lands, which would make for healthier forests while also helping prevent natural disasters such as forest fires.

Additional observations from the panel are as follows:

There is extensive investment in MSW characterization. Some projects also entail sorting, and yet others focus on final chemical characterization. As these projects conclude, the results need to be captured in the *Billion-Ton Report*. An important addition to the portfolio is the use of cover crops to enhance the sustainability of feedstock production systems. One panelist stated that these projects are among the best implemented.

The panel understood that DEI was introduced in this review cycle. There appear to be differences in DEI implementation among projects. There needs to be greater clarity on what the higher-level goals are for DEI in future reviews of projects. The involvement of students from underserved communities is laudable, but stakeholder input and direct benefits to the underserved communities should be considered.

To better understand the evolution of the Feedstock Technologies program and to strategize about the program's long-term impacts, the panel thinks that keeping a historical perspective on changing or introducing new goals and/or objectives in the Feedstock Technologies portfolio would be beneficial. It would be helpful to have a map of past goals and major findings followed by the evolution to new goals, whether determined through program results or political forces. It was positive to see a more holistic approach being taken for complete biomass utilization focused on achieving the best value for each material component. A more comprehensive and practical approach can be considered in future funding cycles with respect to carbon sequestration and decarbonization.

FEEDSTOCK TECHNOLOGIES PROGRAMMATIC RESPONSE

INTRODUCTION

BETO would like to thank the review panel for their careful evaluation of the Feedstock Technologies projects and subprogram overall. The panel's dedication to improving BETO is sincerely appreciated by both the Feedstock Technologies team and the broader stakeholder community. Recommendations by the Peer Review panel are referenced regularly when making decisions about the program.

The Feedstock Technologies team appreciates the positive comments made by the review panel regarding program management, strategy, goals, and implementation. We will continue to work to maintain a high level of success in these areas. The Feedstock Technologies team particularly appreciates the recommendations to improve the program. Our comments about these recommendations are as follows.

Recommendation 1: Integrate data from various projects and ensure accessibility.

Ensuring data availability is one of the most important ways to maximize the value of government-funded R&D. DOE already requires that all data collected through its projects be published on osti.gov, which is linked to data.gov, but we realize that this is not enough. We will leverage ORNL's Bioenergy KDF and INL's BFL to further integrate data from multiple projects, especially projects from the same funding opportunity. Special emphasis will be placed on integrating data from the MSW funding opportunities (see below) as well as data on purpose-grown energy crops. The review panel noted a lack of attention to the "customer" when considering the outcomes and impact of applied R&D projects, and this is especially important for data availability. When making integrated data available, we will ensure that the users of the data drive the content and format of the data provided.

Recommendation 2: Optimize Feedstock Technologies subprogram investment in computational modeling.

BETO researchers have developed many models. BETO recognizes that models are only as good as the data used to generate/validate them, and moreover, that models need to be used by stakeholders to realize their full benefits and to enable supply chain design and process equipment operation that do not rely on empiricism. We will focus more heavily on these aspects to increase the value of existing models. Our immediate plans for funding opportunities indeed focus on lab and field experimental data generation in the most promising areas identified by BETO-funded models, such as feedstock resource and supply chain analysis for deploying purpose-grown energy crops for SAF, as well as first-principles-based computational modeling of material handling and feedstock quality improvement for integration with downstream processes. BETO routinely uses sensitivity analysis (e.g., tornado charts) from supply chain modeling efforts to identify future R&D needs and topics for future FOAs, and we will pay special attention to making sure this link is apparent to external stakeholders. BETO models are continuously improved by leveraging new data from the lab and the field that can inform and validate the accuracy of models. BETO researchers have made progress by integrating industry data with the company name removed to protect proprietary information, and we will continue to encourage this type of information sharing while protecting the intellectual property of our project partners.

Recommendation 3: Develop general guidance for future TEAs and cost analyses.

BETO is committed to developing BETO-wide uniform TEA guidance. One of the first steps will be to host a workshop on the challenges of harmonizing these data before issuing standardized guidance; the Data, Modeling, and Analysis subprogram has made plans to hold this meeting. Additionally, as suggested, we will work to put integrated TEA data into the Bioenergy KDF. The idea to hold data dissemination workshops is a good one.

Recommendation 4: Expand focus on forest logging residues.

The subprogram agrees with this recommendation and acknowledges that a similar recommendation was made in the 2021 Project Peer Review summary report. In the past two years, BETO has:

- Funded at least three Small Business Innovation Research projects on forestry residues or woody biomass
- Coauthored a chapter on forest restoration in a report to Congress on carbon dioxide reduction
- Held a breakout session on forest management during BETO's workshop titled "Bioenergy's Role in Soil Carbon Storage"
- Included forest fire mitigation in BETO's MYPP, released in March 2023, and added salvaged material from natural disasters and invasive species as renewable carbon resources of interest
- Made a strategic hire with expertise in forest biomass logistics.

Additionally, thanks to a collaboration with the USDA Forest Service, the updated *Billion-Ton Report* will include estimates for biomass from fire reduction treatments. Projects reviewed by the FCIC review panel include forestry residues, but we agree that more emphasis is warranted, especially in the areas noted by the panel: logistics, equipment advancement, industry engagement, and commercialization. Forestry residues are listed second in the list of renewable carbon resources in the MYPP, and BETO will continue to support this important resource in coordination with the U.S. Forest Service.

Response to additional observations from the panel:

Regarding the suggestion to incorporate data from the MSW projects into the *Billion-Ton Report*: new data on wastes will be incorporated in the next *Billion-Ton Report*, including the addition of county-level fats, oils, and greases, and mature-market price competition will be accounted for. Furthermore, a nationwide MSW characteristics database will be created, focusing on quantity and quality and considering spatial and temporal variability. BETO's MYPP, released in March 2023, specifically mentions this effort, and a workshop is being planned for fall 2023 to discuss and coordinate the three cohorts of MSW funding opportunities and related national lab projects. As recommended in the strategy section of the panel's summary report, the workshop organizers will emphasize outreach to MSW industry stakeholders across the supply chain to inform database development.

The idea to create a map of historic goals and major findings followed by the evolution to new goals is a great one. We will keep this project in mind and ensure that it is accomplished prior to the next Peer Review. At a minimum, the map will be provided as a resource for the next Peer Review panel. Additionally, more clarity on DEI goals and implementation will be provided to the next panel; this is an ongoing DOE-wide effort, and much progress is being made.

Lastly, to address a comment in the panel summary's strategy section, we will emphasize engagement with members of the local farming and forest community, including county extension agents and members of local governing boards. BETO's Small Business Innovation Research program took initial steps in this direction by piloting a unique set of topics (fiscal year 2021 [FY21]–FY23) focused on community-driven bioenergy development. After the first pilot, eight other DOE applied offices adopted the idea. The BETO-funded projects include engagement with farmers, foresters, tribal nations, local community groups, and many others. Our upcoming efforts on deploying purpose-grown energy crops for SAF will also have a strong focus on farmer engagement.

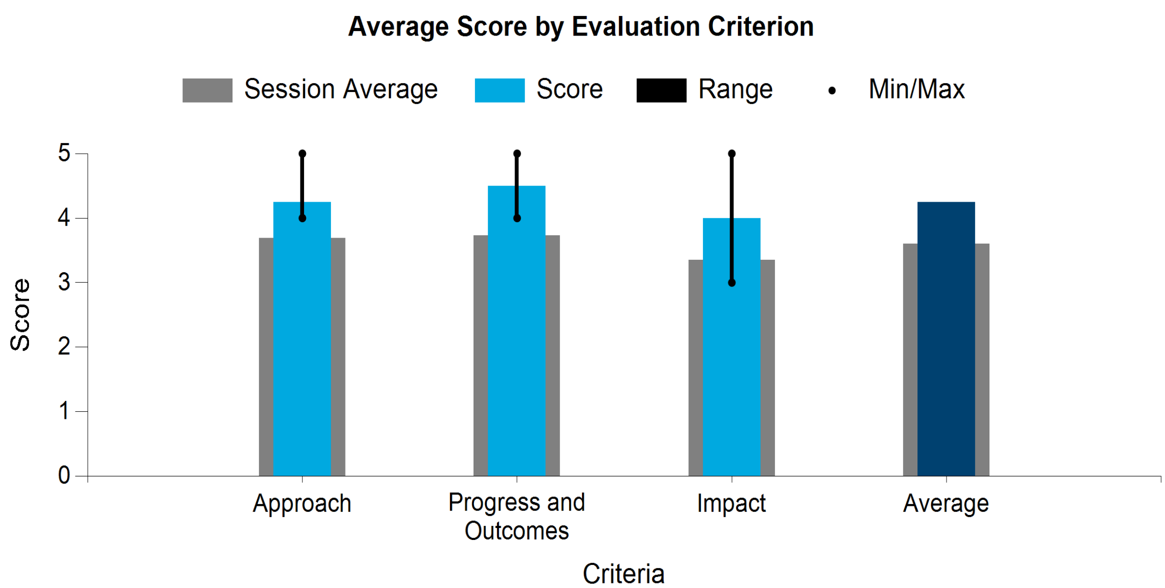
NEXT-GENERATION FEEDSTOCKS FOR THE EMERGING BIOECONOMY

University of Illinois at Urbana-Champaign

WBS:	1.1.1.105
Presenter(s):	DoKyoung Lee
Project Start Date:	10/01/2018
Planned Project End Date:	09/30/2024
Total Funding:	$6,251,399.00

PROJECT DESCRIPTION

Perennial bioenergy crops like switchgrass can supply feedstock for sustainable bioenergy production and improve ecosystem services on marginal croplands. Biomass and associated ecosystem services for high-yielding switchgrass cultivars (i.e., Liberty and Independence) were evaluated on marginal fields in Iowa, Illinois, Nebraska, and South Dakota. Biomass was determined by commercial harvesting and baling, and ecosystem services examined soil quality, GHG emissions, water quality and quantity, and biodiversity. In harvest years 2 and 3, new cultivars Liberty and Independence produced 13%–32% and 10%–36% more yield, respectively, depending on location, when compared to previous cultivars, and nitrogen fertilization was important for maintaining sustainable yields. Compared to corn, switchgrass had 15%–70% lower N_2O emissions and 4–10 times lower NO_3-N leaching, but higher water use due to higher total biomass. Bird diversity was greater in corn, but total bird number was higher in switchgrass. Feedstock composition differences were related to location and cultivar. This project provides a template for growing feedstocks that could lower biofuel cost by using detailed yield, harvest logistics, fuel use, and field capacity data to perform TEA. These results meet the BETO goal of developing productive, cost-effective, and sustainable bioenergy feedstock systems on marginally productive croplands across geographic locations in the U.S. Midwest.



COMMENTS

- This is a very strong team with a well-laid-out approach and execution of the tasks needed to meet the major milestones and deliverables. The project seems to have met the key milestone. I'm not clear on the commercialization path—who are the potential commercial partners? On Slide 6, some of the risks—weather, breakdown of machinery—are noted. These types of things are bound to happen. What is being done to estimate/project rolling average type data? Slide 7 shows variation of crops in different states, plots in a given state, a given year, and the results. Are the variations understood?

- This is a very good project with lots of results and accomplishments. On Slide 6, several challenges were discussed for the project. Some of them have already happened, whereas others are just potentials. It is not clear how the team has handled or mitigated these challenges. I'd like to revisit a couple of questions I raised in the previous review. First, best management practice (BMP) development is being used as a major success factor. It is not clear which BMPs will be developed. This may be planned in Budget Period 4 and 5. I think BMPs can be developed earlier, and the BMPs' application and effectiveness can be accessed in Budget Period 4 and 5. Has there been any progress on BMP implementation in the project? Second, there are many different ways to do the modeling work in ag/forest ecosystem services. Using ML is appropriate but challenging, especially in the algorithm selection and data set preparation, for consistency and robustness. Can you explain more about how the model has been trained for improvement and how tract size and machine type would affect the field harvest performance?
- Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. This is a very expansive field-based research project on switchgrass and corn production systems in several Midwestern states. Their approach is to obtain extensive field data on switchgrass cultivars, nutrient management, and harvest management to develop carbon uptake models. An interesting, repeated observation was that switchgrass systems had considerably greater soil CO_2 efflux than corn systems. They attributed this to switchgrass having greater root mass and thereby greater production of CO_2 through root respiration. This observation calls for much greater investigation. This project will have a major impact on soil carbon sequestration research.
- This is a valuable and very well executed project. The data gathered is comprehensive and will lead to a much better understanding of switchgrass as a feedstock. This was one of my favorite presentations of the session. The presenter provided a lot of information, but the slides were well laid out and easy to see, and the whole presentation told a very meaningful story. One slide outlining the roles of the contributors would be beneficial.
    - Approach: The technical objectives are well laid out. The PI specified what they were going to do and accomplished what was set out. This project was well designed and has significant potential to develop BMPs for this application.
    - Progress and Outcomes (P&O): Even though a significant portion of this project was carried out through a difficult period (COVID), the team managed to keep the project on track. The challenges identified on Slide 6 are generally unpredictable and uncontrollable (i.e., weather-related). However, this provided an opportunity for real-life learning that can be applied to future work. Nice work on the modeling, especially the remote sensing models; this was novel and very useful.
    - Impact: There is a plethora of meaningful data that will continue to be synthesized to answer important questions related to switchgrass crops. This project is contributing to other BETO projects, such as the biomass sample library and Bioenergy KDF. The BMP guidelines and their introduction to local stakeholders will be a very important outcome of the project. Working with seed partners will improve biomass commercial opportunities. The largest question will be whether switchgrass makes sense in the long term when used as a large commercial crop.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: This is a very strong team with a well-laid-out approach and execution of the tasks needed to meet the major milestones and deliverables. The project seems to have met the key milestone. I'm not clear on the commercialization path—who are the potential commercial partners? On Slide 6, some of the risks—weather, breakdown of machinery—are noted. These types of things are bound to happen. What is being done to estimate/project rolling average type data? Slide 7 shows variation of crops in different states, plots in a given state, a given year, and the results. Are the variations understood?

- Response: We thank the reviewer for the comments. The target market for the project is cellulosic ethanol producers and biorefineries, including stand-alone facilities and facilities co-located with grain ethanol production facilities situated across the country. Moreover, the target production market area for the switchgrass varieties is the marginally productive croplands in the Midwestern region. The regional farmers, who have marginally productive croplands and environmentally degradable lands, will have the greatest interest in adopting these new switchgrass varieties. The possible competitor crops will be corn, soybeans, and perennial forage crops, but the economic benefits from the higher yield potential of switchgrass compared to the low yield of these crops will mitigate the perceived barrier to market penetration. One of the biggest challenges with perennial energy crops is stand establishment under unfavorable weather conditions. Flooding delayed the stand establishment; however, all sites were successively established, and we did not have much problem with data collection even though biomass yields were low during the establishment year. Switchgrass cultivar and site differences influenced biomass yield for both the field-scale and small-scale field trials. Site differences at the field-scale level were evident with high biomass yields in Brighton, Illinois > Urbana, Illinois > Nebraska > Iowa > South Dakota for yields averaged over the three years (2020–2022). Biomass yield was marginal in the establishment year (2020) for all cultivars in the five sites, but the yield increased immensely in the second and third years after the establishment. Lower yields in 2022 in Urbana, Illinois; Iowa; and Nebraska are attributed to drought. The newly introduced Liberty and Independence cultivars produced higher biomass on average when compared to local cultivar Shawnee. Likewise, biomass yield of Carthage, a new cultivar, averaged 9% greater than Sunburst, despite the stand damage due to winter injury. Moreover, nitrogen fertilization with 50 pounds of nitrogen per acre increased biomass yield by 10%–15%.

- Comments: This is a very good project with lots of results and accomplishments. On Slide 6, several challenges were discussed for the project. Some of them have already happened, whereas others are just potentials. It is not clear how the team has handled or mitigated these challenges. I'd like to revisit a couple of questions I raised in the previous review. First, BMP development is being used as a major success factor. It is not clear which BMPs will be developed. This may be planned in Budget Period 4 and 5. I think BMPs can be developed earlier, and the BMPs' application and effectiveness can be accessed in Budget Period 4 and 5. Has there been any progress on BMP implementation in the project? Second, there are many different ways to do the modeling work in ag/forest ecosystem services. Using ML is appropriate but challenging, especially in the algorithm selection and data set preparation, for consistency and robustness. Can you explain more about how the model has been trained for improvement and how tract size and machine type would affect the field harvest performance?

- Response: We thank the reviewer for the insightful comments. The challenges faced in the project were mostly weather-related. Spring flooding resulted in establishment challenges during the first year and delayed weed control and fertilization. Cold winters in South Dakota during the second and third growing years caused stand damage (winter kill) and delayed harvesting, whereas drought in the third growing year in Illinois and Nebraska affected the biomass yield. Spring flooding was mitigated by replanting all affected plots, and harvesting (delayed due to early snowfall and cold) was performed in the early spring in South Dakota. The project evaluated biomass productivity under typical rainfed conditions; thus, irrigation was not included to mitigate the drought. The technical challenge encountered with machine breakdown, especially in Nebraska and Iowa, was mitigated by conducting prompt repairs and rescheduling operations. We have made progress in the field-scale feedstock production practices, including estimating feedstock chemical quality and mineral composition. We are now working to produce a switchgrass management guide summarizing the BMPs specific to the new high-yield bioenergy-type switchgrass cultivars produced on marginal lands to reduce variability in yield and quality, generate economic return for producers and processors, and provide environmental services. The BMPs being developed include establishment practices, weed control, fertilization regimes, and biomass harvest management and logistics, as well as storage systems and their economics and energetics. We hope to publish the BMPs in late 2023. The application of ML in predicting the agronomic and environmental attributes of perennial bioenergy crops grown on marginal croplands has not been widely explored. Thus, ML model development tasks for this project focus on foundational efforts, particularly finding (1) an algorithm or set of algorithms that are well suited to predict end-of-season biomass yield of multiple bioenergy switchgrass cultivars under U.S. Midwest conditions, and (2) the most important predictors or explanatory variables. Data used for training the model were collected as part of the study (yield, weather, and other publicly available data), which allows some control over the quality, quantity, and availability of the data. Using data from three cropping years (2020–2022), we evaluated a wide range of algorithms that have been applied for commodity crop production applications, including traditional (ordinary and partial least regression), ensemble (random forest, gradient boosting machines, and AdaBoost regressor), K-neighbors regressor, and artificial neural networks. We found that random forest and gradient boosting machines proved to be the most accurate algorithms, although artificial neural networks could be further tested as more data become available from upcoming growing seasons. We also found that the top predictors are climate and topographic variables. This particular work has been peer-reviewed and was recently accepted in the *Energies* journal. Factors that affect field harvester performance, such as tract size and machine type, are outside the scope of this current project, and thus are not included as part of the model capabilities. However, they can be included as part of future model capabilities funded by future projects and can build on the final model outcomes of the Affordable and Sustainable Energy Crops project.

- Comments: Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. This is a very expansive field-based research project on switchgrass and corn production systems in several Midwestern states. Their approach is to obtain extensive field data on switchgrass cultivars, nutrient management, and harvest management to develop carbon uptake models. An interesting, repeated observation was that switchgrass systems had considerably greater soil CO_2 efflux than corn systems. They attributed this to switchgrass having greater root mass and thereby greater production of CO_2 through root respiration. This observation calls for much greater investigation. This project will have a major impact on soil carbon sequestration research.

- Response: We thank the reviewer for the insightful comments. We observed higher soil CO_2 flux from the switchgrass field in the second and third growing seasons compared to the corn fields. We have embarked on several studies to ascertain the CO_2 source, as the soil CO_2 flux is the sum of soil organic matter mineralization, heterotrophic respiration, and root respiration, as well as autotrophic root respiration. We hypothesized that the greater root mass of switchgrass contributes to the higher CO_2 flux under switchgrass production. We have already sampled 0–15 centimeters depth of root biomass to quantity the total root mass at this depth. We are also planning a more comprehensive root biomass sampling campaign up to 100 centimeters in autumn 2023. Moreover, a preliminary field study is underway to assess the root contribution to total CO_2 emissions.

- Comments: This is a valuable and very well-executed project. The data gathered is comprehensive and will lead to a much better understanding of switchgrass as a feedstock. This was one of my favorite presentations of the session. The presenter provided a lot of information, but the slides were well laid out and easy to see, and the whole presentation told a very meaningful story. One slide outlining the roles of the contributors would be beneficial.

- Approach: The technical objectives are well laid out. The PI specified what they were going to do and accomplished what was set out. This project was well designed and has significant potential to develop BMPs for this application.
- P&O: Even though a significant portion of this project was carried out through a difficult period (COVID), the team managed to keep the project on track. The challenges identified on Slide 6 are generally unpredictable and uncontrollable (i.e., weather-related). However, this provided an opportunity for real-life learning that can be applied to future work. Nice work on the modeling, especially the remote sensing models; this was novel and very useful.
- Impact: There is a plethora of meaningful data that will continue to be synthesized to answer important questions related to switchgrass crops. This project is contributing to other BETO projects, such as the biomass sample library and Bioenergy KDF. The BMP guidelines and their introduction to local stakeholders will be a very important outcome of the project. Working with seed partners will improve biomass commercial opportunities. The largest question will be whether switchgrass makes sense in the long term when used as a large commercial crop.

- Response: We thank the reviewer for the generous comments. The present project targets marginal lands. The viability of switchgrass as a commercial crop depends on the market demand for the biomass, ecosystem service benefits, and its profitability. Switchgrass biomass is primarily used for biofuel production and as a feedstock for bioproducts. We expect the market demand for biofuels to increase and stabilize and to provide long-term viability for expanded switchgrass cultivation. Moreover, switchgrass has potential ecosystem service benefits that include nutrient cycling, carbon sequestration, reducing soil GHG emissions, improving soil and water quality and quantity, and providing a habitat for birds and insects. The increased environmental concerns faced today will likely persuade policymakers to shift policy and encourage switchgrass cropping in large areas. For instance, the Conservation Reserve Program and related marginal lands are currently targeted for long-term switchgrass production. In addition, the release of groundbreaking research and technological advancements that can enhance switchgrass productivity, biomass quality, and processing efficiency, such as breeding (new high-yield switchgrass cultivars), improved agronomic practices (establishment, fertilization timing, harvest methods), and processing techniques, can contribute to making switchgrass a more attractive option for large-scale commercial cultivation. Whether a crop makes sense at the commercial scale depends on market availability and profitability. We evaluated the profitability of switchgrass in the project by comparing the farm-gate prices with corn and soybeans, and found that switchgrass competes favorably with soybeans at the high price of $88 per megagram and with corn at $66 per megagram. In addition, switchgrass had lower production costs (land preparation, seed acquisition, establishment, management, harvest, and transportation) but higher income compared to the row crops (https://doi.org/10.1002/glr2.12017).

SUSTAINABLE HERBACEOUS ENERGY CROP PRODUCTION IN THE SOUTHEAST UNITED STATES

Texas A&M AgriLife Research

WBS:	1.1.1.108
Presenter(s):	Ted Wilson
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2024
Total Funding:	$6,251,605.00

PROJECT DESCRIPTION

This project develops a comprehensive assessment of the economic viability and environmental sustainability of producing advanced energy cane and biomass sorghum in the Southeast United States. Field experiments are being conducted in seven sites for energy cane and six sites for biomass sorghum across five states (Texas, Louisiana, Mississippi, Georgia, and Florida), involving five institutions (Texas A&M University, USDA Agricultural Research Service [ARS], Mississippi State University, University of Florida, and Tennessee State University). Comprehensive data on agronomics, off-season storage, and sustainability have been collected from 2020–2022. Major findings include:

Agronomics:

- Stem and root biomass increase through the season, while leaf biomass decreases toward the middle of the season.
- Energy cane yielded more than biomass sorghum, and southern sites produced higher yields.
- There was almost linear biomass loss during storage, and higher biomass loss for aerobic storage.
- Cellulose, hemicellulose, lignin, and ash all increased during the first 3 months of storage.

Sustainability:

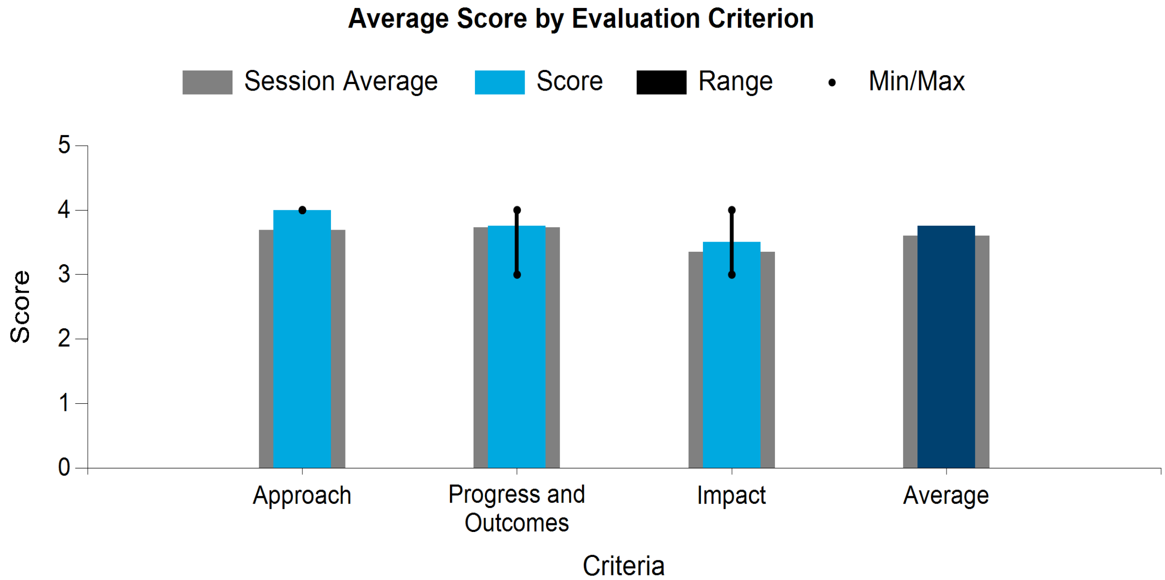
- Soil organic carbon (SOC) was, on average, higher post-harvest than pre-planting.
- Higher nitrogen rates had significantly greater N_2O emissions.
- Surface runoff water: Total nitrogen spiked after nitrogen application and decreased thereafter.
- Deep percolation water: Nitrogen application did not affect total nitrogen concentration.
- There was higher soil microbial diversity post-harvest compared to pre-planting.
- There was considerable variability in ground-active invertebrate diversity across sites and crops.

Enterprise budgets of energy crop production:

- Field operations account for the largest cost component in enterprise budgets.
- The total cost for biomass sorghum is higher than for grain sorghum.
- The total cost for energy cane is higher than for biomass sorghum.

Comprehensive integrated analysis (field-fuel economic viability and sustainability, site-specific BMPs, and operational plans) will be carried out in 2023 to the end of the project.

The current project complements existing studies on energy crops and assesses the economic viability and sustainability of cellulosic energy crop production in the Southeast United States. Outcomes from the project will accelerate adoption of cellulosic bioenergy development in support of BETO's strategic goal to reduce the price of biofuels to <$3/GGE and reduce the cost of feedstock to less than $84/dry ton.



COMMENTS

- This is a well-laid-out and well-executed project. The team is strong and has a proven track record. The project appears to have met all major milestones. It is not clear what the next steps toward commercialization are. Slide 6 mentions organizational and operational risks. What are the proposed mitigation steps? On Slide 20, what is the unit on the y axis?
- (1) In addition to the organizational risks you identified, are there any technical risks you have encountered over the last two years, and what measures you have taken to mitigate them? (2) Why is the Weslaco site's yield significantly higher than other sites for biomass sorghum, or lower for energy cane? (3) I raised a similar question in the previous review. The data analysis and interpretation can be further enhanced and improved in the coming years based on more data collected, such as the number of observations for each measurement and the number of replications. Some details are also needed to explain analysis of variance (ANOVA) and principal component analysis (PCA) data and results. (4) It is not clear how labor cost was considered in the cost analysis, and how these cost factors will be able to achieve the target of <$84/dry ton or <$3/GGE. (5) Any BMPs will be helpful for farmers and practitioners.
- Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. This project is evaluating energy cane and high-biomass sorghum as feedstocks in the Gulf Coast region and Southeastern states. The primary intent of the work is to provide production information for siting biorefineries. They have made excellent progress on the production aspects of the project and have reinforced that these two species can reliably produce very high yields of biomass. The project also revealed, however, that no significant increases in SOC occurred. Although these species are excellent candidates to support biorefining, they do not seem to have great potential for soil carbon sequestration in production systems that remove all of the herbage.

Determination of dry matter losses associated with harvest timing and storage was listed as an objective; however, no results were presented.

- Presentation comments: Black font and standard font type would improve the presentation.
    - Approach: There was a clear definition of objectives, and an excellent slide (4) showing the roles of the collaborating team members. The project shows links with other BETO projects. Only two operational risks were mentioned. I'm sure there are many more; however, if these were the most severe, then the project has good prospects to proceed with little difficulty. Slide 7 was very helpful in understanding the technological approach used. This project is nearing its end date of 2024 and is a long-term, 5–6-year project.
    - P&O: On Slide 7, I have a question about the dry biomass loss chart. It shows dry biomass loss for sorghum at 25% in storage for 3 months, and 50% at 6 months. If this is the case, then how can it possibly be economical? What is the field of storage losses? It seems like this system would not be practical. The energy cane shows a similar trend, but storage losses are a little lower. On Slide 15, you should use percent increase or decrease of carbon so scales are comparable. On Slide 20, a stacked bar chart for each site would be better for comparison. The project shows some good data but is not presented in a way that would provide uptake for stakeholders.
    - Impact: The impact slide (21) is good, but I didn't see the metrics presented in such a way that it would be easy for a farmer to decide whether this would benefit their land and practices. I think what I am missing is a deliverable for 2023—the integrated analysis, as mentioned on Slide 22. I would have expected, with less than a year left in the project, to see some of this important analysis. The plan for disseminating results was not clear.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: This is a well-laid-out and well-executed project. The team is strong and has a proven track record. The project appears to have met all major milestones. It is not clear what the next steps toward commercialization are. Slide 6 mentions organizational and operational risks. What are the proposed mitigation steps? On Slide 20, what is the unit on the y axis?
- Response: Steps for commercialization will include (1) potential biorefinery site selection based on a comprehensive analysis of land availability, biomass productivity, and environmental sustainability; (2) identification of BMPs for growing bioenergy crops that optimize profit and environmental benefits; (3) development of year-round biomass supply plans; and (4) provision of large-scale funding from DOE to (a) create a minimum of three biorefineries and associated storage facilities and transportation equipment for the Southeastern United States; (b) fund low-cost loans to support farm land purchases, equipment for bioenergy crop production and harvesting, and buildings for feedstock storage to support the production of a year-round feedstock supply sufficient to meet the needs of a biorefinery; and (c) establish a bioenergy commodity check-off system to ensure a research infrastructure to support necessary genetic, agronomic, insect, weed, and disease management research improvements to address evolving production and management needs. Wide-scale establishment of the bioenergy industry will rely on government incentives to promote commercialization of biomass sorghum and energy cane and national networks of biorefineries. Number 4 is beyond the scope of the current project, but our team would very likely play a major role in its implementation. Mitigation steps for organizational risk include (1) development of detailed sampling schedules for individual tasks; (2) monthly project updates on task implementation status; (3) frequent communication via email, phone, and video to resolve emerging issues; and (4) cross-training of project personnel for potential staff changes. Mitigation steps for operational risk include (1) production of biomass sorghum seed or energy cane stalks for commercial-scale planting/replanting; (2) appropriate seed bed preparation to minimize excessive moisture caused by

poor drainage in some soils to promote an aerobic environment for root health; and (3) sufficient land and equipment preparation to guarantee smooth and timely field operations. On Slide 20, the y-axis unit should be dollars/acre.

- Comments: (1) In addition to the organizational risks you identified, are there any technical risks you have encountered over the last two years, and what measures you have taken to mitigate them? (2) Why is the Weslaco site's yield significantly higher than other sites for biomass sorghum, or lower for energy cane? (3) I raised a similar question in the previous review. The data analysis and interpretation can be further enhanced and improved in the coming years based on more data collected, such as the number of observations for each measurement and the number of replications. Some details are also needed to explain ANOVA and PCA data and results. (4) It is not clear how labor cost was considered in the cost analysis, and how these cost factors will be able to achieve the target of <\$84/dry ton or <\$3/GGE. (5) Any BMPs will be helpful for farmers and practitioners.

- Response: Technical risks: Please see response above on "mitigation steps for operational risk." Weslaco's yield: Welasco's higher biomass sorghum yield is thought to be due to double-row beds (two rows per 40-inch bed instead of one row per 30-inch bed for other sites) and the use of drip irrigation (most other sites did not apply irrigation). We mistakenly used the average of low and optimal nitrogen levels for Beaumont and Starkville, which lowered the yield for the two sites. The low yield for Tifton was due to damage from nematodes. A main factor in lower energy cane yield is probably the very late harvest (early March instead of December) due to a combination of equipment breakdown and wet weather. We are also examining other factors that might have contributed to differences in yield among different sites. A comprehensive analysis of the factors impacting biomass yield across sites and years will be included in the final report. Data analysis and interpretation: We are in the process of integrating data from multiple years and sites and will provide improved comprehensive analysis, including ANOVAs and multivariate analyses (PCAs and others). Labor cost and target yield: An enterprise budget for each crop was built based on variable costs (material costs, labor costs, custom service costs, etc.) and fixed costs (machinery depreciation, equipment investment, management fees, land charge, etc.). Comprehensive economic analysis through enterprise budget, biomass yield, transportation logistics, and conversion processing will determine whether the target of <\$84/dry ton or <\$3/GGE can be achieved under different biomass pricing and biorefinery-scale scenarios. BMPs: Please see response above on "steps for commercialization."

- Comments: Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. This project is evaluating energy cane and high-biomass sorghum as feedstocks in the Gulf Coast region and Southeastern states. The primary intent of the work is to provide production information for siting biorefineries. They have made excellent progress on the production aspects of the project and have reinforced that these two species can reliably produce very high yields of biomass. The project also revealed, however, that no significant increases in SOC occurred. Although these species are excellent candidates to support biorefining, they do not seem to have great potential for soil carbon sequestration in production systems that remove all of the herbage. Determination of dry matter losses associated with harvest timing and storage was listed as an objective; however, no results were presented.

- Response: Lignocellulosic feedstocks have two potential ways to reduce atmospheric CO_2: through soil carbon sequestration and as a renewable and replacement resource for fossil fuels. Soil carbon sequestration is a relatively slow but very important process. A small change in the percent carbon concentration equates to a very large change in terms of megagrams/hectare. Soil to a depth of 15 centimeters has an average mass of 2,260 megagrams/hectare. One tenth of a percent increase of soil carbon sequestration is equal to 1.13 megagrams/hectare. We expect to see a significant increase in soil carbon with additional growing seasons for the energy cane. Because biomass sorghum is a rotational crop, its rate of increase of soil carbon will be less. The other benefit of lignocellulosic feedstock is its renewable nature. Atmospheric CO_2 is captured by plants through photosynthesis, released through biofuel combustion, and then captured again in a cyclic renewal way. Burning fossil fuel is a one-way release of CO_2 into the atmosphere. Our scheduled LCA will quantitatively address this topic. Biomass loss during storage is included on Slide 13 in the BETO review presentation. Biomass loss from harvest timing will be assessed through seasonal biomass as early harvest penalty and as standing biomass loss post maturity.

- Comments: Presentation comments: Black font and standard font type would improve the presentation.
    - Approach: There was a clear definition of objectives, and an excellent slide (4) showing the roles of the collaborating team members. The project shows links with other BETO projects. Only two operational risks were mentioned. I'm sure there are many more; however, if these were the most severe, then the project has good prospects to proceed with little difficulty. Slide 7 was very helpful in understanding the technological approach used. This project is nearing its end date of 2024 and is a long-term, 5–6-year project.
    - P&O: On Slide 7, I have a question about the dry biomass loss chart. It shows dry biomass loss for sorghum at 25% in storage for 3 months, and 50% at 6 months. If this is the case, then how can it possibly be economical? What is the field of storage losses? It seems like this system would not be practical. The energy cane shows a similar trend, but storage losses are a little lower. On Slide 15, you should use percent increase or decrease of carbon so scales are comparable. On Slide 20, a stacked bar chart for each site would be better for comparison. The project shows some good data but is not presented in a way that would provide uptake for stakeholders.
    - Impact: The impact slide (21) is good, but I didn't see the metrics presented in such a way that it would be easy for a farmer to decide whether this would benefit their land and practices. I think what I am missing is a deliverable for 2023—the integrated analysis, as mentioned on Slide 22. I would have expected, with less than a year left in the project, to see some of this important analysis. The plan for disseminating results was not clear.
- Response: The results on biomass storage loss from seven study sites consistently indicate high biomass loss during both aerobic and anaerobic storage. This poses a major challenge for year-round biomass supply, and the reviewer's concern about the practicality of off-season storage is well justified. This is an area that is understudied but critical to the economic viability of a biorefinery operation. Our integrated analysis in Budget Period 4 will examine best options to address the year-round biomass supply challenge. Regarding Slide 15, we will include the percent change in the final report. On the stacked bar chart: A stacked bar chart would make it difficult to visualize different cost components for each site. In terms of information for stakeholders: Please see the response under "steps for commercialization." Deliverables for 2023 were included on Slide 22: Comprehensive integrated analysis (field-fuel economic viability and sustainability, site-specific BMPs, and operational plans) will contribute to accelerating cellulosic bioenergy development in the Southeast United States. In terms of disseminating results: We have established an effective and well-attended outreach program in conjunction with the annual rice field day at the Texas A&M AgriLife Research Center in Beaumont. On the field day in 2022, we had a tour of our energy crop field experiment in Beaumont. We have also presented our results in the annual meetings of The American Society of Agronomy, the Crop Science Society of America, and the Soil Science Society of America International Annual Meeting in 2021 and 2022. Manuscripts are being prepared for publication in bioenergy-related journals. Results will also be provided to DOE's Bioenergy KDF.

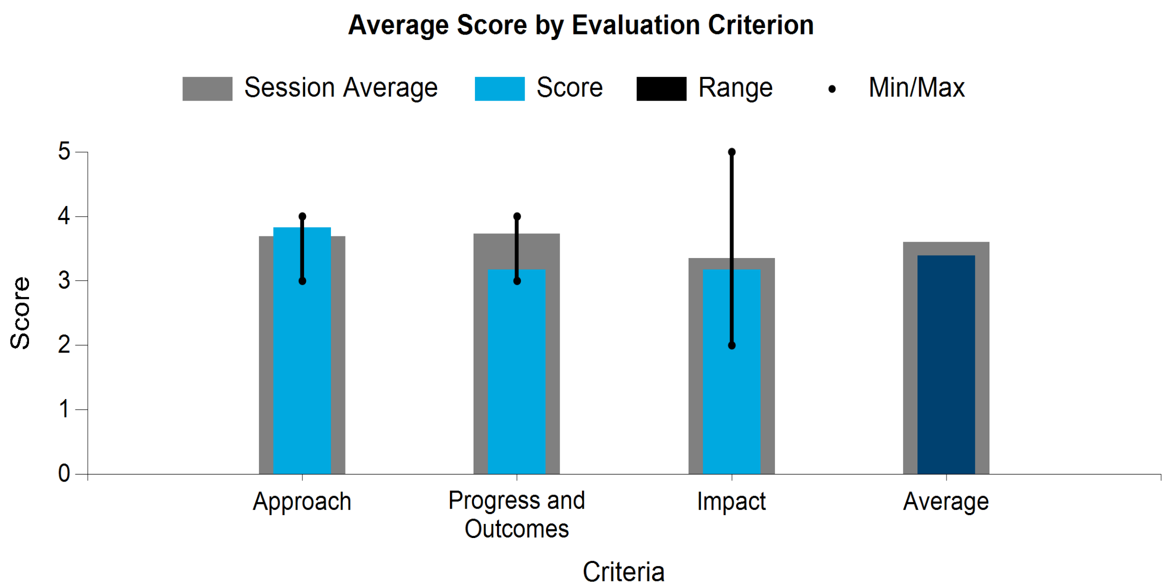
CHARACTERIZATION OF MECHANICAL BIOMASS PARTICLE-PARTICLE AND PARTICLE-WALL INTERACTIONS

Pennsylvania State University - University Park

PROJECT DESCRIPTION

WBS:	1.1.1.114
Presenter(s):	Hojae Yi
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2024
Total Funding:	$907,658.00

Forest residue feedstocks include a mix of particles from bole wood, bark, needles, twigs, etc. Similarly, corn stover is a complex bulk material with properties influenced by anatomical content such as cob, husk, leaf, and stalk. The resulting feedstock flow behavior varies due to differences in the anatomical origin and percentage of each fraction in the bulk feedstock. It is because the bulk feedstock behavior is the manifestation of responses of particles and their interactions at the underlying scale. Friction and adhesion are thought to be the two dominant interactions between biomass particles or particle-wall surfaces affecting the flow, which is a key mechanical phenomenon describing feedstock handling. This project aims to develop micro-mechanical test devices and protocols to characterize biomass particle and interparticle properties that are sub-millimeter to several millimeters in size typical to ground biomass. Upon successful completion, this project will result in a novel knowledge of values and variabilities in the friction and adhesion between (1) biomass particles and (2) biomass particles and a common wall material in biomass handling systems. This novel knowledge will enable innovative design and manufacturing of engineered biomass supply systems to handle, store, and deliver conversion-ready feedstocks consistently through innovative biomass handling modeling such as discrete element modeling (DEM).



COMMENTS

- The feedstock tested with the device has been particularly limited. Southern pine from a single location and time is not likely representative of the feedstock in question. As other projects noted, there are differences between years, ages of trees, harvest locations, etc. There was a broad statement made that this information could impact biomass handling, including modeling. However, no information is provided on *how* this will be accomplished. Will the PI be working with modelers, equipment designers, etc.? The impacts that are outlined are largely qualitative. A significant amount of data is being generated as a part of this work, but it's not clear where it's going and how it will ultimately be used. I agree with risk #4 as listed (limited day-to-day applicability). Risks and mitigations were laid out and realistic but did not include impacts or likelihoods. The validation and reproducibility of this novel piece of equipment was not clearly laid out. In terms of progress, a nice Gantt chart was provided, but it does not align with the dates on the quad chart.

- The team seems to have made good progress toward developing a characterization device with unique and important applications in feedstock handling. Their industry partnership with Forest Concepts indicates that there is a need for this device; however, the presentation did not clearly articulate any specific use cases, so it is difficult to evaluate the potential for impact on industry. I would recommend asking the following question: "If this device worked perfectly, what would that look like, and how could one quantify the potential benefit to industrial practice?"

- The slides are well organized, detailed, and adequately explained. The strength of this project is academia partnering with a private-sector industry company that has strong expertise in feedstock issues. It wasn't clear from the presentation why the given particle size was chosen and what specific commercial applications would benefit from a better understanding of characteristics at that size. The live presentation explained size selection. How this project advances feedstock handling beyond the status quo for commercial applications is general but not specific. The project will need to validate the reliability of the tester devices with an acceptable test standard. Graduate student recruiting efforts toward DEI are not explained, nor is any success toward achieving that intended outcome demonstrated.

- The approach of first-principles measurement of fundamental biomass mechanical properties (particle-particle and particle-wall interactions) is intriguing; however, the PI seems to be fundamentally developing a novel mechanical apparatus ("interparticle mechanics tester") and using results from this novel tester to correlate to observed bulk behavior. However, the novel mechanical device has not been tested against materials with known properties (elastic modulus, friction, adhesion) to calibrate or test the validity of the device. I suggest that the PIs test the device against polymer samples of the correct size and shape where these properties are well established. For instance, one can use polymer nibs from acetal polymers, atactic or syndiotactic polypropylene, polybutylenes, polyesters, etc. Because these materials are well characterized with known properties, one could calibrate the instrument and validate the measurement capabilities of the device. Additionally, the bulk handling characteristics of these materials are well-studied; how they behave in screw extruders and other flow characteristics is well known. One could develop and test the bulk property correlations of a model on simplified systems prior to tackling the models on biomass materials. Because of the lack of calibration and testing against known standards, I don't feel that one can claim the interparticle test has been successfully developed. That remains to be seen. Additionally, it is claimed that the device is "quick and accurate"—quick is a relative term, and listing a more precise cycle time for measurement is preferred. The "error bars" around the measurements presented are quite large, and I can't tell if that is due to mechanical property variation or measurement variation by the instrument, or even operator dependence. I think the approach has great promise, but the mechanical device development has not been demonstrated. Once it is calibrated against known standards, it could be useful in determining other material handling challenges, such as the influence of particle shape and entanglement of particles on flowability characteristics.

- The interparticle mechanics tester is a novel device with potential for patentability. The statistical approach and consideration of appropriate sample size and environmental controlled testing mitigate the identified risks. The project has met its milestones for Budget Period 2. The project has potential to provide impact in the flow of materials in hoppers, screw conveyors, and other material handling devices. However, the current testing to correlate the friction and adhesion of particles to wall material may not be sufficient to determine the performance in material handling equipment. Also, the review does not discuss the FOA metric of achieving an R-squared value of >80% relating the characteristics to feedstock handling. Adding a partner to evaluate material handling process performance as a function of particle-wall and interparticle properties would provide further verification of the correlation to bulk material handling as well as the commercialization potential of the interparticle mechanics tester.
- In terms of approach: The team has a well-thought-out approach to begin to characterize particle-level interactions of biomass, and they provided a nice outline of mitigation strategies as well as implementing feedback from previous peer reviews. The team does not currently have estimating impact in their plan, but are looking to do this in the future, which would be excellent. A full TEA is not required, but some estimate of impact would be beneficial. Specifics of the involvement and integration of forest products into the project were not presented. In terms of P&O: The team exceeded their initial mechanical property milestone with 20 replications rather than the requisite five, and so the subsequent milestone was increased in difficulty to 20. One significant issue is that the system has no reference materials for the equipment and correlation development. A reviewer suggested using plastic polymers, as they have extensive data and correlations. While this may help address this issue, plastic is not the same as biomass, and the researchers should have identified potential remedies for this issue. In terms of impact: A potential patent and commercialization of the interparticle tester would be a significant achievement and a real help to all solids industries, not just biomass. The ability to evaluate data on the particle level when other research is only on bulk and/or numerical modeling/analysis without aid of data will be especially helpful. The team has already started on patenting and commercialization of the tester.

PI RESPONSE TO REVIEWER COMMENTS

- Many thanks to the reviewers for their time and effort in evaluating various projects and providing insightful comments. We firmly believe that incorporating your comments strengthens this project and broadens its impact. In terms of project impact: This project has designed and constructed a novel first-principals-based interparticle mechanics test. The friction and adhesion between particles have long been hypothesized to be fundamental mechanisms of particulate materials' mechanical behavior. As pointed out by the comments, issues in biomass handling include the large variability in flow behavior and the lack of understanding of the cause of such variability. Significant portions of the FCIC and BETO FOAs on biomass handling have produced knowledge and tools to address these issues. Most notably, DEM is a promising computational tool to investigate and predict particulate material handling, including milled biomass. For example, the INL group has active research programs on developing and using DEM. However, no existing experimental device or protocol exists to measure the parameters of the DEM framework, forcing fields to rely on secondary measurement protocols. The device and experimental protocol developed under this project produce key parameters of DEM at the particle scale, which provides a pathway to understanding the cause and magnitude of the variability in biomass handling. Therefore, the immediate use of the product of this project is to advance the understanding and prediction power of biomass handling through computational simulation. To this end, we are actively working on follow-up collaborations with the INL group. The limited number of sample species and batches of biomass feedstocks in this project was set to keep the number of experiments achievable with the given resources and timeframe. While the representativeness of species and batches is bounded, this project includes four different tissue types and two different moisture content levels. The friction and adhesion measurements between particles of different tissue types demonstrate different variabilities between species and anatomical origins. These findings can be readily used in developing fractionation strategies for improved biomass handling for southern pine residue and corn stover. We are looking into collaboration opportunities with FCIC to this end as well as disseminating the findings to the field. We particularly appreciate the suggestion on validation. Because there is no referential material, experimental device, or standard to determine friction and adhesion between particles, the appropriate validation of this novel device is a crucial component. Following up on the suggestion, we are identifying and procuring appropriate polymer materials to conduct the validation experiments. In the meantime, we have acquired a precision steel ball bearing with a known surface specification and experimental measurements of friction coefficients using a conventional tribometer. The validation test with the metallic surface compared to the tribometer resulted in a negligible magnitude of variation between measurements. This validation result indicates that the observed variations of biomass particles are innate to biomass particles. We will include further validation of the device in the remainder of the project. We aim to achieve an R-squared value greater than 80% relating to the characteristics of feedstock handling, based on the bulk mechanical property measurement carried by Forest Concepts with the Cubical Triaxial Tester, which is another novel analytical device developed through a BETO-sponsored project. Comingled corn stover (4 millimeters) is one of the feedstocks that Forest Concepts routinely processes, and we do have data on handling with an industrial-scale hopper, which we will use in validation of the established correlations between friction/adhesion and bulk scale biomass handling.

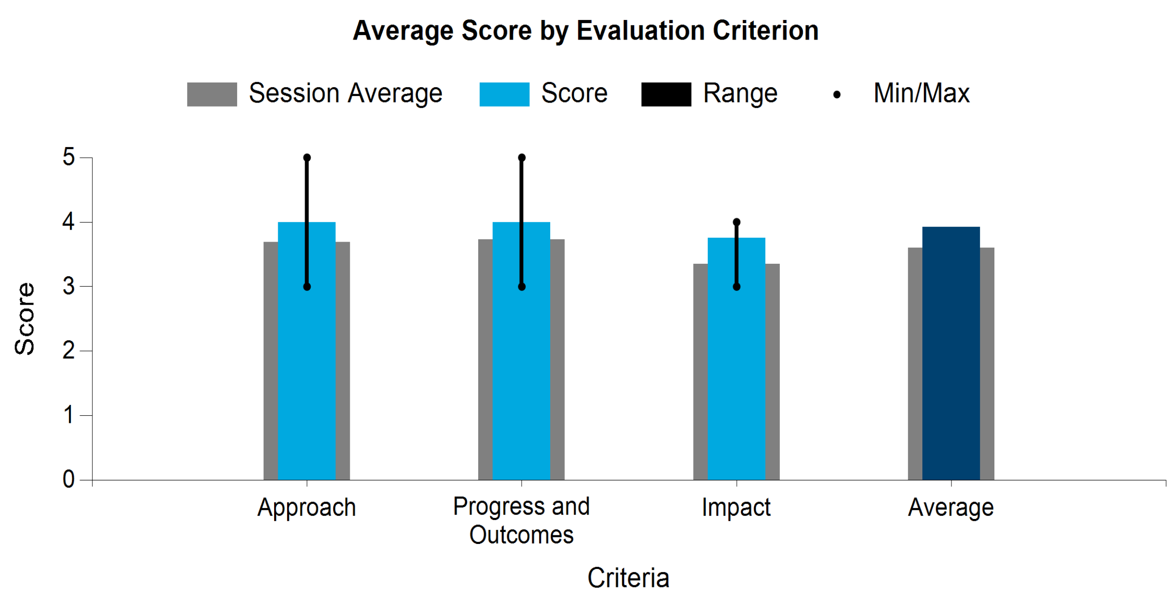
FEEDSTOCK SUPPLY CHAIN ANALYSIS

Idaho National Laboratory

WBS:	1.1.1.2
Presenter(s):	David Thompson
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$3,000,000.00

PROJECT DESCRIPTION

The geographic distribution, low bulk density, and wide variability of biomass types, moisture levels, and compositions making up the billion tons of biomass potentially available for bioenergy create a unique challenge to the development of reliable, cost-effective biorefineries to provide low-cost, high-volume biofuels that can compete with petroleum-based fuels. This foundational project led the development of the pathway to the 2022 MYPP targets for development and verification of feedstock supply and logistics systems that can economically and sustainably supply industrially relevant quantities of herbaceous feedstocks for biochemical conversion at a delivered cost no higher than $85.51/dry ton (2016 dollars). The project also contributes to meeting a delivered feedstock cost target of $71.26/dry ton, in support of achieving the $2.50/GGE minimum fuel selling price (MFSP) target for 2030. This project investigates both conventional feedstock supply systems and a number of advanced (active quality management) feedstock supply system strategies, including blending and commoditization of biomass to meet the modeled cost, quantity, and quality specifications required to meet long-term BETO targets for biofuels production, cost, and volume. Beyond design case development and annual state of technology (SOT) tracking, this project performs high-impact forward-looking analyses toward enabling the development of an advanced feedstock supply system. The project was last merit reviewed in FY20, and its current 3-year cycle runs through FY23.



COMMENTS

- The team is strong and has the proven experience and track record in the needed skill sets to execute the work plan. The project seems to have met the deliverables. The team needs to articulate the results delivered versus the original plan more clearly. Slide 16 shows that overall operating effectiveness value increased steeply from 2019 to 2021, then declined in 2022? Why? Is this projected trend moving forward? Was there any feedback from Exxon/Shell on the report presented to them?

- The project was initiated in 2006 and has evolved over the last several years, including the addition of advanced supply chain management in FY14 and the design of the n^{th} plant in FY18. A major piece of supply chain resilience can be considered in the future study. In terms of approach, the number of milestones was mentioned. However, they need to be clearly defined. Two major project risks were discussed. However, their mitigation plans are not convincing. In terms of P&O, it is not clear how to estimate downtime on Slide 14. Furthermore, more explanation is needed on how this analysis can help real production for industry partners. In terms of impact, there are good results and publications. Any outreach and commercialization efforts would further enhance the project's impact. Specifically, the lessons you have learned since 2006 should be able to help for scale-up of the project.

- Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable, climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending.

- This is a very important project, as it attempts to answer economic feasibility questions surrounding fractionated biomass. The methodology and approach allow for testing of permutations related to the amount of biomass recovered versus the amount of fractionation and resulting quality. These are very important questions that can help optimize the resource but also balance processing costs. I hadn't seen failure and downtime considered in operations prior to this presentation, and thought it ties the feedstock quality to mill operation. The costs and efficiencies can now be balanced. I have had reservations about the value added by fractionated materials, and this model should hopefully help elucidate the value through the whole supply chain and bioconversion process. The presentation contained a lot of information in a short time. It is difficult to fully comprehend all aspects of the project.

PI RESPONSE TO REVIEWER COMMENTS

- This project has a very diverse work scope. In previous BETO Peer Reviews, this led to confusing the reviewers by presenting multiple accomplishments in a very short presentation. Those reviewers indicated a pressing need to understand how we accomplished the analyses and used the results to advance the feedstock supply system SOT, rather than outlining individual analysis accomplishments toward project milestones. Hence, for this review, we focused on analysis approach, methodology, and how the results are used to advance the SOT. We developed new analysis tools and carried out the annual SOT assessments. The results presented for this review covered SOT assessments for FY21 and FY22; during late FY22, BETO announced a shift of program focus to carbon intensity and SAF volume targets rather than delivered feedstock cost. Accordingly, we have adjusted the focus of our future assessments to region-specific analyses that identify available supplies of individual conversion-ready feedstocks based on regional characteristics that impact feedstock quality and carbon intensity. The utility of the first-plant analysis to industry is in identifying the feedstock properties that have the most significant impacts on preprocessing operation and ultimate product yields from the conversion. We showed total operating time and total downtime as well as the percentages of downtime occurring due to the various biomass properties, which can be used with the total downtime to estimate downtime attributable to individual properties over the course of a year of operation. We compared first-plant and

n^{th}-plant costs for the volume of biomass preprocessed; the difference is the cost incurred by decreases or interruptions of system throughput due to biomass properties and losses of biomass from the system. We showed a comparison of the first-plant time on stream and the assumed n^{th}-plant time on stream. Finally, we provided comparisons of total delivered cost due to the enforcement of compositional specifications, as well as overall operating effectiveness for supply logistics (harvest through storage) and preprocessing systems. This clearly identified losses of convertible organics during storage as a significant underlying issue that must be solved for the supply system to consistently meet yield requirements. Finally, with regard to risks, as an analysis project that projects performance for large-scale systems, our primary risks are a lack of sufficient scale-relevant data to adequately model the systems and understanding cost/quality trade-offs between aspirational n^{th}-plant assessments and the realities seen in first-plant projects. In the absence of large-scale data, we align with BETO feedstock R&D projects, utilize industry outreach and stakeholder engagement, and, when possible, utilize experiential information from industry preprocessing operators to inform the economics for larger-scale systems.

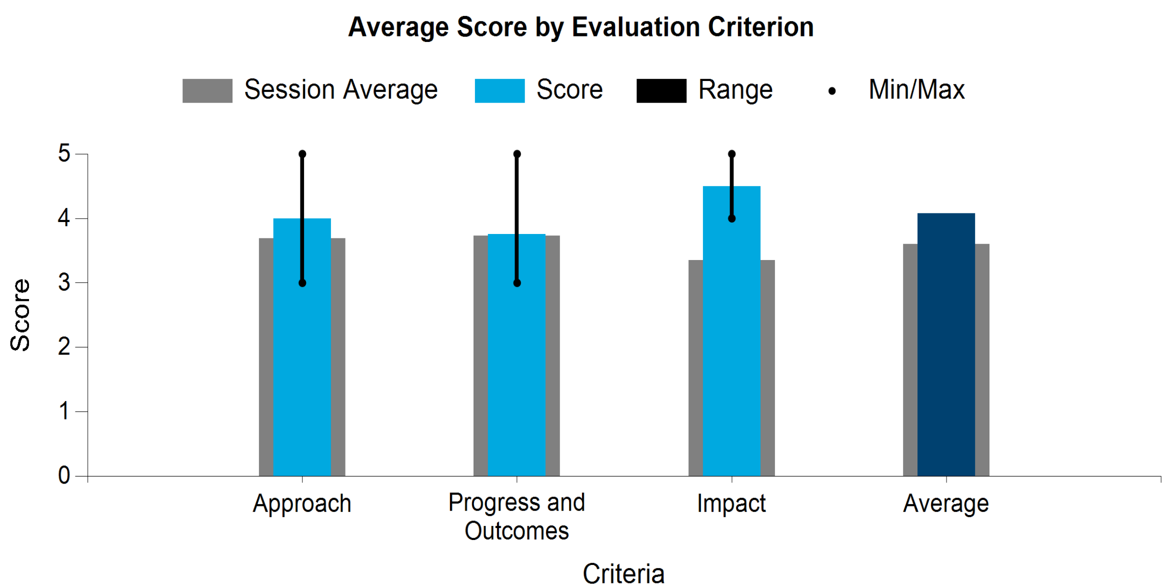
SUPPLY SCENARIO ANALYSIS

Oak Ridge National Laboratory

WBS:	1.1.1.3
Presenter(s):	Matt Langholtz
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$2,025,000.00

PROJECT DESCRIPTION

The goal of this project is (1) to provide DOE and bioeconomy stakeholders with the biomass feedstock data needed to develop strategies to grow the bioeconomy (2023 *Billion-Ton Report*), and (2) to determine the optimal allocation of national biomass resources for decarbonization (best use of biomass [BUoB]). This project provides data including biomass feedstock quantity, cost, and spatial distribution. Previous *Billion-Ton Reports* (e.g., https://www.energy.gov/eere/bioenergy/2016-billion-ton-report; https://www.energy.gov/sites/prod/files/2015/01/f19/billion_ton_update_0.pdf) have identified ~1.2–1.5 billion tons of biomass potentially available annually in the United States in a base-case scenario. However, changing economic conditions, updated data, and interest in new feedstocks warrant an updated analysis, expected to be completed in 2023. *Billion-Ton Reports* and associated data support and inform government, research, and industry. Data from the *Billion-Ton Reports* are being used in a spatially explicit analysis of bioproduct pathways, including pyrolysis, Fischer-Tropsch, fermentation, and alcohol-to-jet, to assess BUoB for decarbonization based on minimization of carbon abatement cost.



COMMENTS

- This program is highly relevant and potentially impactful by advancing the prior pioneering work in the field. The team is very strong and has a proven track record and credentials. The proposed plan and milestones are well discussed. The project seems to be on track, and the 2023 report is expected shortly. The team has addressed the suggestions/comments raised in the previous Peer Review. It looks like a fair amount of emphasis is placed on energy crops like camelina. The cost is estimated at $0.15/pound. Is this the final cost delivered to the seed crushing plant? Is there enough infrastructure for harvesting, processing, etc.? As the team knows, the USDA has done some extensive work in this area. Is there much coordination between these efforts?

- This is a good project, with two tasks focusing on the billion-ton study and BUoB. DOE should continue to invest in this effort. To further improve data accuracy, regional field data collection and validation can be considered. In terms of the approach, I did not see that mill residue was considered as a part of forest biomass. Regional variation in logging residue tonnes per acre, the available amount of logging residue, and quality degradation over 1–3 years after harvest can be considered in the future report. Input-optimization-output was discussed in the modeling process. However, exactly what and where optimization was employed is unclear. In terms of P&O, results were good. In terms of impact, the number of citations of the *Billion-Ton Report* is very impressive. I look forward to reading the upcoming 2023 *Billion-Ton Report*.

- Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable, climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending. The project leader described the objective of this project as pushing the frontier of feedstock R&D. This team has led the production of two *Billion-Ton Reports*, with the second edition occurring in 2016. They are now concluding work on the *Billion-Ton Report* for 2023 and have added other feedstocks, including oilseed crops, forest thinnings, macro-algae, and CO_2 to e-fuels. I don't understand the addition of the latter, as CO_2 is not a biological feedstock. The group has expanded to also develop a decision tool on BUoB; however, this effort has had difficulty because of the absence of clear markets for feedstocks. I recommend that valorized ecosystem services be included as a considered BUoB.

- This is a very good project. The approach for the *Billion-Ton Report* is tried and tested. Additional feedstocks have been added to the report, which looks at future biomass resources. Progress is on track. The impact is very high, as this is a widely used and cited report. The information in this report is used extensively by those involved in the biorefinery industry, and as long as the intent of the report and the availability of biomass are clearly stated, this is an excellent, impactful project. It should be noted that on all presentations, there should be a minimum font size. The charts and tables pasted into the PowerPoint often have very small font, and at times this makes following the presentation difficult. Questions: Is there thought given to mapping other related production facilities (i.e., chemical/materials/pulp mill, etc.) in the biorefinery mapping? Also, are biomass depots being considered in the mapping for the BUoB?

PI RESPONSE TO REVIEWER COMMENTS

- Regional field data collection and input data are based on the Regional Feedstock Partnership (https://www.energy.gov/sites/default/files/2016/07/f33/regional_feedstock_partnership_summary_report.pdf). Mill residues are included in the analysis but are largely in use for hog fuel and may provide limited additional resource potential in a national context. Regional variation in logging residue and potential quality degradation will be considered. CO_2 is a non-biomass resource of interest to BETO. We agree that ecosystem services should be considered in downstream analyses. We agree that mapping of existing production facilities should be considered. Biomass depots have been and should continue to be considered in modeling and mapping of biomass resource use. The Biomass Supply Analysis Team thanks the reviewers for their comments and constructive feedback.

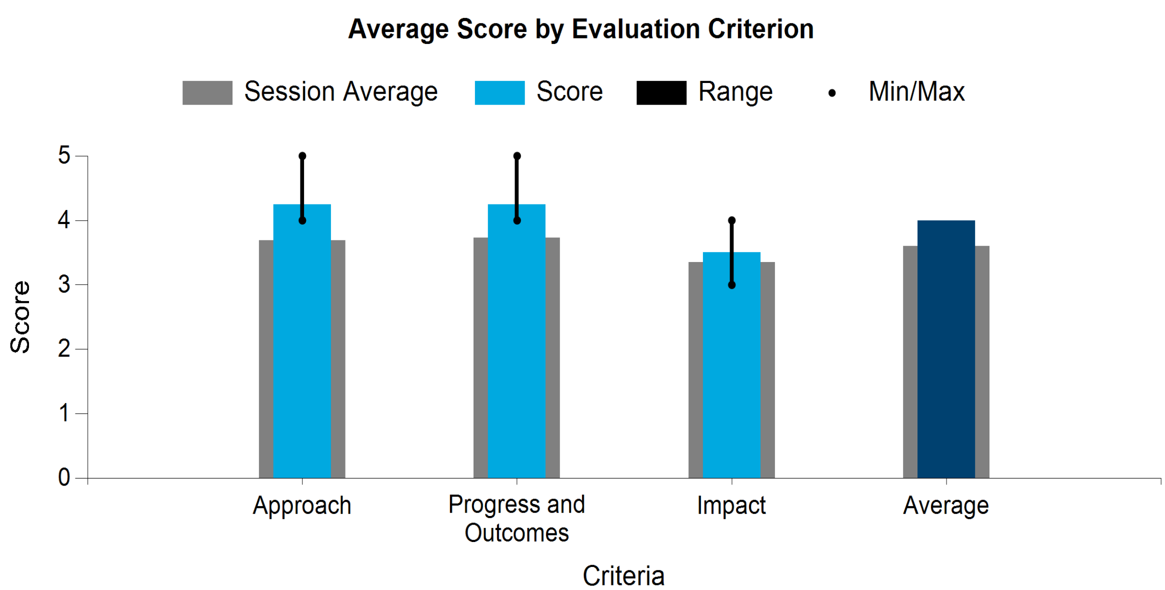
TRIPLE BOTTOM LINE SUSTAINABILITY INDICATORS FOR SPATIALLY EXPLICIT, MULTI-FEEDSTOCK, MULTI-TECHNOLOGY WASTE-TO-ENERGY SUPPLY CHAINS

Pacific Northwest National Laboratory

WBS:	1.1.1.6
Presenter(s):	Andre Coleman
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,125,000.00

PROJECT DESCRIPTION

There is broad public support for sustainability concepts, but defining and tracking progress toward multi-objective sustainability goals has proven to be challenging amid complex social, environmental, and economic interactions across geographic and jurisdictional boundaries. To address these gaps, Pacific Northwest National Laboratory (PNNL) is coupling state-of-the-art analytical methods (e.g., resource assessment, TEA, and trade-off analysis) with novel research in sustainability accounting to develop new standardized tools for the public that provide credible guidance to the waste community in support of regional waste-to-energy planning. PNNL is developing a unified sustainability assessment methodology to define, measure, and track sustainability goals for waste resource supply chains and evaluate the long-term trade-offs of different waste conversion strategies. Importantly, these tools will ultimately consider the local waste "diet," community goals, and nontraditional benefits (e.g., health, environment, equity). Stakeholder engagement is explicitly integrated into all aspects of the project. The completed sustainability framework could be used by federal, state, and municipal decision makers to identify and compare regionally relevant waste conversion pathways in a transparent and consistent manner.



COMMENTS

- This is a strong team with a proven record in the field through prior BETO-funded projects. The skill sets and organization of the team members are well articulated. The team has proactively reached out to potential end users and has started work with one of them. The project has made good progress against milestones. It looks like municipal waste is ubiquitous and well dispersed across the United States. How consistent in quality/supply is this source? Are there any synergies/economies of scale to treat this as one and develop the required quality, conversion, and equipment metrics? The project needs to address the lack of interest risk with stakeholders.

- This is a good waste-to-energy project. In terms of approach, the top potential project risks were well identified. However, the corresponding risk mitigations need to be clearly addressed. The roles and responsibilities of each project participant are not clear. In terms of P&O, good progress has been made. In terms of impact, the project mentions that social equity and environmental justice are a centerpiece of the model implementation. It is not clear how they have been implemented in the model applications.

- Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable, climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending. The project leaders pointed out that local governments and community leaders have difficulty understanding the organic waste streams in their communities, and even more difficulty understanding how to capture value from these wastes. This project has built significant momentum in meaningful stakeholder engagement, and I encourage them to continue with more outreach to rural, underserved communities. The project's geospatial analysis of underutilized waste streams is excellent. This project provides the strongest work reported for ongoing biomass R&D to achieve environmental justice in addition to circular bioeconomies. I recommend that they partner with other federal agencies to build awareness and build partnerships with minority-serving institutions.

- As far as the approach, there is significant merit to this project. Often, these models are for larger jurisdictions, but are equally or more important for assisting municipalities with decision-making, because they may have ownership of the waste. The communication routes could be improved by increasing the number of collaborators on the project. The presenter stated that they will be looking to link with more partners in the future. This is a vital component of the project that can affect success, but I didn't see risk mitigation outlined. Inclusion of environmental justice metrics is to be commended. Slide 4 is very informative; it shows who is doing what and points to a clear implementation strategy. There was a thoughtful analysis of challenges. Municipalities are motivated by ratepayers and their priorities, and it is difficult to get them to understand and plan for the future (outside of politicians' terms of office). In terms of P&O, excellent progress has been made to date. The project is midway and has already made some very good progress and produced some valuable results. Slide 9 gives a snapshot of indicators and an idea of the template. This will be easy to expand as new indicators come to light. Slide 12 breaks down the waste producers to the region—this is very nice information. As far as impact, risks to this project may be large. However, the project is still extremely valuable, as this will become a priority sometime in the future—even with disinterested stakeholders and short-term thinking by politicians.

PI RESPONSE TO REVIEWER COMMENTS

- Reviewer 1 Response: In terms of feedstock supply variability, because most markets and waste management services in the United States are highly consolidated and specialized, the wet organic wastes they ultimately produce are reasonably consistent in quantity and quality (including contamination). Some wastes, like wastewater solids and food waste, are steady year-round and correlate well with population growth. Depending on geographic region and animal type, manure supplies can be highly seasonal or year-round. Despite careful farm product price management, manure supplies are sensitive to market conditions, as animal herds are actively managed to address supply and demand (e.g., culling when prices crash). Similarly, depending on the region and crop, agricultural residues may be seasonal or year-round, and despite careful management of the food supply, crop harvest, and subsequent crop residue, supplies are often impacted by rising costs (especially fertilizer), severe weather, or drought, or all three, as was the case with historically low crop harvests in 2022. Historical variability is not always a good predictor for future conditions, but we can learn the key drivers that impact feedstock supply and enable the model to represent changes over time. Currently, the model evaluates average annual conditions to maximize profit for an average year. This approach meets our current need for rapid analysis. However, as a future development option, modulating waste flows, prices, and performance variables can improve our ability to model realistic impacts from population growth, waste policies, market dynamics, climate, risk management, etc. Also, there are several ways we can address input variability in the future, but they will require additional investigation and testing. In terms of economies of scale, the model does indeed account for economies of scale in relation to the total capital investment and annual operating expenses. An important feature of the model is the ability to model blended waste scenarios to achieve larger facility capacity. To accomplish this, we rely on scaled cost data provided by industry and experimental analysis teams modeling emerging technologies. We can quickly update our cost data as the TRL improves, providing better cost estimates. Additionally, as new technologies or processes become available, these can also be incorporated. As far as stakeholder interest—the involvement of stakeholders has been a key pillar in the project design to (1) understand the current gaps, challenges, practices, and aspirations from the perspective of multiple entities; (2) provide the foundation for case study design; and (3) provide a critical review and understand the practicality of sustainability metrics and measures and the modeling process as a whole. A key objective of this work is to build a capability that is useful, insightful, and impactful at the community, city, county, and state level. Building out stakeholder groups is a lengthy and involved process. The messaging in the presentation wasn't intended to convey that there is no interest, but rather that there is significant work involved. The process our team has used to establish stakeholder interest has been effective, receiving official endorsement of the work. Through our stakeholder interactions, our team has also realized that there is a significant lack of knowledge in new technology options for waste-to-energy conversion. Thus, an education component is advocated for, but there is much more that needs to be done that will need to happen at more programmatic levels.

- Reviewer 2 Response: In terms of risk mitigation, we apologize for not clearly summarizing our major risks and mitigation strategies. This information is presented below.
    - Price and policy uncertainty: We cannot accurately predict future market or policy conditions, and emerging technology cost and performance data are experimental. We mitigate this by (1) using the best available data; (2) applying sensitivity analysis to model a range of market and policy futures; (3) using statistical methods to assess long-term historical market and policy behaviors; and (4) eliciting external review.
    - Stakeholder interest: Municipalities may not have the policies, budget, or expertise to initially engage with a Waste to X (W2X) platform for trade-off analysis in this opportunity space. We mitigate this with direct stakeholder interaction, development of technology education materials, and demonstration of the modeling platform.
    - Unknown rate of technology adoption: We cannot predict technology readiness (commercialization) timelines or municipal/industry interest in new technologies. We mitigate this by adopting an enabling assumption that emerging technologies become commercially available in <10 years and are socially acceptable.

  - Roles and responsibilities: We apologize for not clearly communicating the individual contributions of our team members beyond a high-level role/title. The following summarizes the roles and responsibilities of each team member. Andre Coleman and Timothy Seiple serve as the PIs, project managers, and task leads for the project. They also perform all the data management and spatial analysis. Craig Bakker provides operations research support and is responsible for selecting and implementing the optimization approach. Chrissi Antonopoulos serves as the lead economist to guide implementation of the sustainability indicators. Saurabh Biswas serves as an expert in sustainability science to provide a sound theoretical foundation for framework design and indicator design and interpretation, including potential feedback and bias. Michael Walsh and Dallase Scott are key performers for our subcontractor responsible for managing and facilitating stakeholder engagement. Andrew White serves as an expert in environmental, social, and governance; energy equity and environmental justice policy; and practice for energy systems. Bethel Tarekegne is an internal project reviewer with experience in policy research on building equitable, sustainable distributed energy systems.

  - Indicator implementation: Given the limited presentation time, it was not possible to go into depth about how sustainability indicators are implemented in the model, so we appreciate the comment and opportunity to explain! The W2X Pathways model is designed to rapidly simulate and compare impacts from various waste management strategies. It is essentially a two-step process. First, we use a techno-economic optimization model to partition available waste resources among competing technologies for conversion to various energy endpoints (i.e., electricity, biofuels, biogas, etc.). The optimizer seeks the “best” overall waste utilization strategy by maximizing the systemwide net present value—profit. The siting game can be controlled to represent a wide range of scenarios. Second, based on the proposed optimal mix of technology locations, types, scales, and feedstocks, we can calculate various economic, social, and environmental impacts as the basis for performing trade-off analysis to understand the pros and cons of each waste strategy from a sustainability perspective. In other words, the impacts are calculated after the W2X facility siting process. Depending on how we run the model, we can evaluate the impacts of just the winning technology at a given location, and/or we can compare the relative impacts of building different technologies at the same location. In our software, sustainability indicators are represented as formulas or functions that accept input about relevant facility properties to calculate the magnitude of a particular impact. For example, based on the size of a facility, we can estimate the required number of employees, which is used to estimate economic impacts, but also safety-related impacts, such as injury and illness rates and total incidents per year. The facility size also gives us enough information to estimate air quality impacts such as GHG emissions, and even total residuals and effluent. The most difficult part of the project is developing a formula and gathering supporting data to adequately represent an impact indicator in a model with the appropriate units of measure that are relevant to stakeholders. The inclusion of sustainability scientists and human geographers on the team helps define metrics, measures, and supporting data related to social aspects, such as energy equity, environmental justice and health exposure, and social vulnerability, providing a critical component beyond the more traditional economic and environmental sustainability. Additionally, working with and eliciting feedback from community-level environmental justice stakeholders is key in this process. Even after this current project concludes, indicator development and interpretation will remain an active area of research within sustainability science. Our hope and objective is that the work completed under this project helps provide a foundation for future development in this space.

- Reviewer 3 Response: We are grateful for the positive comments, but also for raising several points of action beyond what our team has been discussing. In terms of supporting climate-smart systems, a major project objective is to perform and produce actionable analytics to generate multiple possible solutions that are possible within a defined geographic area. This will provide leaders with salient information to make informed decisions on further investigation, policy development, planning, investment, and actions beyond the status quo. We recognize that every community and jurisdiction will have a differing set of priorities, which the model supports. We further recognize that most leaders and decision makers will not have the capabilities to self-perform this type of multi-objective optimization analysis for current conditions, let alone quantify how a given scenario could impact/contribute to state or local-level climate goals, social sustainability, and economies. Driving toward climate-smart systems requires an adaptation to the business-as-usual process, and the utilization and conversion of wastes to numerous possible energy products is part of the solution. In terms of feedstock variability and blending, we agree that the inclusion of feedstock variability is a necessary part of the modeling process. We have several options for representing variability in the model. Please refer to our previous response on feedstock supply variability. We also address feedstock blending, a process that we believe helps stabilize variability, in the previous response on economies of scale. As far as stakeholder engagement, outreach, and coordination, with the help of our subcontractor who specializes in stakeholder engagement, we have successfully developed and maintained a focused partnership with the Boston metro area, including representatives of the various cities, nongovernmental organizations, and public advocacy groups, totaling ~30 different entities. We acknowledge that Boston represents a limited range of perspectives, and we plan to expand our outreach in the future. Our experience with the Boston stakeholder group has allowed us to build a process and gather lessons learned, and we will bring these experiences to future stakeholder groups. Our current level of stakeholder engagement is deliberately limited to be consistent with our project goals and available resources. For us, Boston serves as an incubator to help us learn how to adapt and tune our national-scale modeling techniques and deliverables to regional and local contexts, which admittedly is new for us. We view our work under the current project to be an important stepping stone to expanding the work in the future. Moving forward, we plan to complete the development and documentation of a robust functional prototype that can represent a broad range of pathways and impact quantifications. Once we accomplish this, we will be better positioned to present the concept to many more stakeholder groups and more effectively incorporate their feedback to operationalize the model. We also intend for future engagement to focus on rural and underserved communities and will look for alignment between this effort and the recently announced Empowering Rural America and Powering Affordable Clean Energy programs. Another BETO project (WBS 2.1.0.113) is planning to perform analysis specifically designed to characterize waste impact on underserved communities to identify synergistic opportunities for waste conversion, energy equity, and environmental health. We intend to use the results of that analysis to directly influence our future outreach and model development activities, which will certainly involve partnering with minority-serving research institutions. We also plan to expand our federal and nongovernmental organization partnerships and awareness, but again, we don’t feel ready to advertise yet. After the sustainability model is published and operational, we plan to work with entities such as the BETO Technical Assistance Program to deploy the methods for the public.

- Reviewer 4 Response: We thank the reviewer for their insightful comments and recommendations. Regarding increasing communication and collaboration, please see our previous response on stakeholder engagement, outreach, and coordination. Another reviewer also noted the lack of risk and risk mitigation elements in the presentation. Please refer to our previous response on risk mitigation.

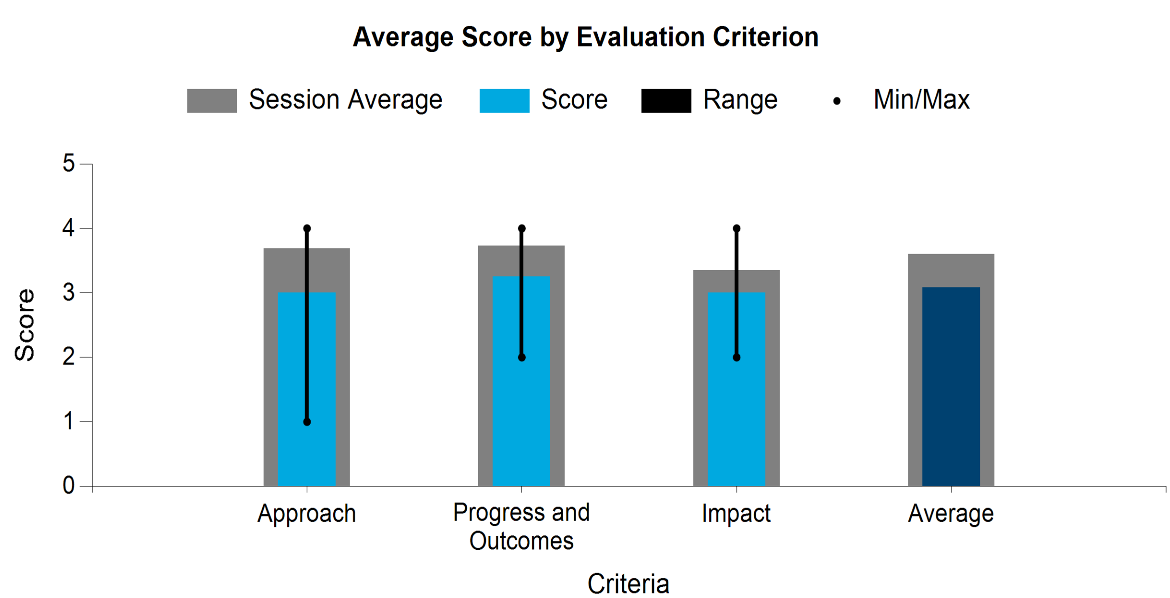
GLOBAL IMPACTS OF ENHANCING DOMESTIC ECOSYSTEM CARBON SINKS

National Renewable Energy Laboratory

WBS:	1.1.1.7/1.1.1.8
Presenter(s):	Patrick Lamers
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2023
Total Funding:	$1,450,000.00

PROJECT DESCRIPTION

The United States has set a target to accomplish a net-zero carbon economy, including a net-zero agriculture sector, by 2050. Initial assessments suggest that 30%–50% of the carbon removals required to achieve this target may (need to) come from terrestrial carbon sinks. The expansion of terrestrial ecosystem carbon sinks aboveground and belowground will inevitably result in resource competition, including for land. Land competition might reduce U.S. commodity outputs (e.g., corn, wheat, lumber), and, given the global trade balance of such commodities, might shift global production to other world regions. Thus, the potential expansion of U.S. carbon banking strategies needs to be assessed in a global, multisector context to quantify potential leakage and land use change effects, which may dampen the domestic efforts from a net global carbon perspective. Here, we use a biogeochemical model to quantify the net GHG and yield effects of terrestrial carbon banking strategies, including no-till agriculture, cover cropping, and biochar application on U.S. cropland, to parameterize respective options in a global, multisector carbon model, the Global Change Analysis Model (GCAM). GCAM will quantify the potential impacts on global agriculture production, land use, and emissions. This supports decision-making at the federal level, e.g., the viability of a net-zero 2050 U.S. economy, potential domestic feedstock competition to support the SAF production target, and the Office of Energy Efficiency and Renewable Energy decarbonization of agriculture pillar. It also advances the state of science in modeling carbon dioxide removal strategies in integrated assessment models.



COMMENTS

- The project plan is well documented, with detailed tasks, deliverables, and go/no-go milestones. The team is well rounded and has a proven track record and capabilities in the field. The team has addressed the comments/suggestions from the last review. The project is on track.

- This is a good project and is worthy of more investment for further investigation. In terms of approach, the project uses DayCent, Daymet, GCAM, and other models for analysis. However, the model integration and the inconsistency of data from different sources need to be addressed. In terms of P&O, the project needs to explain biochar application more, especially the two biochar app rates, three carbon prices, and any interaction between them. As far as impact, substantial efforts are needed for the project to deliver more impact. Some analyses are domestic, while others are global. They should be consistent.

- Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable, climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending. This project uses DayCent as a modeling platform to predict carbon sequestration rates in agricultural soils and production systems. I believe this project would benefit from increased collaboration with the USDA Office of the Chief Economist or the USDA Natural Resources Conservation Service. In the presentation, the team used a comment in a webinar from the USDA Office of the Chief Economist as their strongest example of stakeholder input, indicating a weak approach to stakeholder input.

- The slides for this presentation were not adequate for proper review. The font size was very small on some slides, and the addition of tiny figures where neither the data, axis, nor title could be seen just detracted from the project, rather than helping explain it. There was too much information on a number of the slides. See Slide 7 and Slide 4 as an example. In terms of approach, the roles of the seven people listed on the project were not clear. I didn't see a risk analysis or mitigation strategy. The internship program to target DEI is commendable. As far as impact, no clear communication paths to the stakeholders were identified on the slides. There are only two project partners mentioned on Slide 17. The practical benefit of this project is difficult for me to determine. The PI should consider how this can be synthesized to be useful for policymakers. This needs a story that can be relayed to the layman. It was difficult to evaluate this project.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their constructive feedback. The project team plans to reevaluate the biochar treatment analysis in FY24 using new insights from ongoing literature review and meta-level analyses. The project performs national-level analyses in the context of global developments, all modeled in a single, integrated framework (GCAM). Thus, there is no disconnection between the geographic regions. Rather, U.S. practices are put in context of global commodity markets, and our results thus account for potential indirect effects. Feedstock variability is acknowledged but impossible to address at the level of resolution and aggregation of industries and supply chains in our model. We appreciate the suggestions of additional stakeholder input and plan to seek input from other federal offices in future efforts. We refer to the appendix/additional materials provided in the slide deck for roles and responsibilities within the project teams, stakeholder input and outreach plans, and risks and mitigation plans.

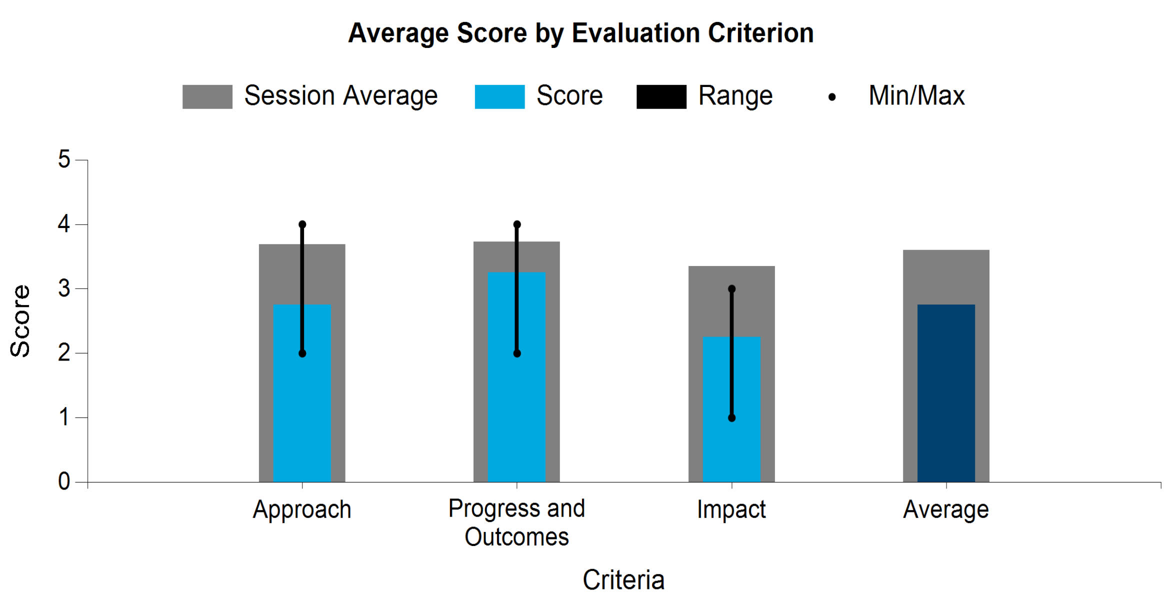
BENEFITS AND LAND USE EFFECTS OF U.S. ENERGY CROP-BASED CARBON BANKING

Oak Ridge National Laboratory

PROJECT DESCRIPTION

WBS:	1.1.1.9
Presenter(s):	Debo Oladosu
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,398,000.00

Carbon banking can help accelerate the production of energy crops in the United States by valuing the associated increases in SOC. Although SOC sequestration has received significant attention, details of national land transitions, potential land use changes (LUCs), and other effects are not yet well understood. However, these are essential to energy crop carbon banking. These LUCs and other "off-farm" impacts have already been identified as potentially limiting the role of carbon sequestration in agricultural soils for reducing GHG. Therefore, as with using food crops to produce biofuels, LUCs and other effects must be addressed when transitioning U.S. soils to energy crop carbon banks. In addition, SOC is highly dynamic and spatially heterogeneous, requiring detailed assessments to reduce uncertainties and carbon banking risks. This project supports DOE, BETO, and private industry by providing national/global-level information and analyses to address these issues to enable energy crop carbon banking in the United States. The project will examine scenarios for SOC sequestration, the national benefits, and the LUC effects of global interactions in the economy's agricultural, energy, and other sectors. The project will seek to identify opportunities to maximize the complementary benefits of land use for agricultural production and energy crop carbon banking in the United States, as measured through environmental, social, economic, and equity sustainability indicators.



COMMENTS

- The project objectives, work plan, and deliverables are well documented. The team is well balanced and has the needed skill sets and capabilities to deliver the results. The project is on track. The required infrastructure to plant, harvest, and crush the seeds needs to be developed to have the projected impact on SAF. Slide 12 on economic analysis is not clear and needs further explanation.
- In terms of the approach, the challenges and risk mitigations are not clearly defined, and the data from many different sources and the conditions of the model development need to be further addressed. The project includes an analysis of growing energy crops for carbon banking versus growing forests of shorter rotation. In terms of P&O, the land use types range from existing cropland pasture (cotton crop) to miscanthus and sorghum, but other land types may be considered, such as marginal land and abandoned mine land. Analytical results from the three scenarios are confusing and inconsistent. In terms of impact, the project needs to address how its findings can help farmers implement more climate-smart agricultural practices.
- Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable, climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending. This project examined carbon banking for prospective cropping systems in Georgia. The project employed computational models aided by AI and ML. Satisfactory progress has been made with respect to AI development; however, a lack of understanding of agriculture became evident in the presentation. The project would benefit from increased collaboration with cropping systems experts in USDA ARS or a regional land-grant university.
- I find it difficult as a reviewer to grasp some of the project information when the slides are overloaded and the fonts are very small, i.e., Slides 4, 6, 7, 10, etc. This is a fairly high-level project that uses a number of models to arrive at some predictions for carbon soil banking. I am not clear on the project's approach, progress, or impacts. There were many terms and acronyms that I was not familiar with, and I didn't feel that an adequate explanation was given to help non-expert-level reviewers. There were a number of significant risks, including scarcity of data and the dynamic nature of soil carbon. I'm also not sure how impactful the large-scale predictions will be; it is more important to have more spatially explicit information for landholders to apply. The uptake of this project will be very difficult unless the results are translated into a more common language that a farmer or landholder could easily understand.

PI RESPONSE TO REVIEWER COMMENTS

- Comments 1: The project objectives, work plan, and deliverables are well documented. The team is well balanced and has the needed skill sets and capabilities to deliver the results. The project is on track. The required infrastructure to plant, harvest, and crush the seeds needs to be developed to have the projected impact on SAF. Slide 12 on economic analysis is not clear and needs further explanation.
- Response 1: Many thanks for your comments. Slide 12 presented key scenarios highlighting the main results of our simulations on the effect of SOC incentives on carinata adoption. We are preparing a paper that presents the other scenarios and puts the key scenarios in context with a more detailed discussion.
- Comments 2: In terms of the approach, the challenges and risk mitigations are not clearly defined, and the data from many different sources and the conditions of the model development need to be further addressed. The project includes an analysis of growing energy crops for carbon banking versus growing forests of shorter rotation. In terms of P&O, the land use types range from existing cropland pasture (cotton crop) to miscanthus and sorghum, but other land types may be considered, such as marginal land and abandoned mine land. Analytical results from the three scenarios are confusing and inconsistent. In

terms of impact, the project needs to address how its findings can help farmers implement more climate-smart agricultural practices.

- Response 2: Thanks for your comments. Given that this is an analytical project, the challenges and risks are mainly related to data availability, tools, and personnel. The presentation highlighted the complexity of estimating SOC changes and efforts under the project to address the associated issues. We will examine the role of different land types in SOC accumulation with energy crops more closely. The three scenarios discussed during the short presentation highlighted the key results of evaluating SOC incentives for carinata production. We are preparing a paper that presents the other scenarios and puts the key scenarios in context with a more detailed discussion. We also plan to work with stakeholders to present these results and to better understand their perspectives on climate-smart agricultural practices for SOC accumulation.

- Comments 3: Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable, climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending. This project examined carbon banking for prospective cropping systems in Georgia. The project employed computational models aided by AI and ML. Satisfactory progress has been made with respect to AI development; however, a lack of understanding of agriculture became evident in the presentation. The project would benefit from increased collaboration with cropping systems experts in USDA ARS or a regional land-grant university.

- Response 3: Many thanks for your comments. We have made some progress under this effort, but there is much to do. In this context, we appreciate the suggestion to collaborate with USDA ARS or land-grant universities and plan to pursue this as part of our stakeholder engagement.

- Comments 4: I find it difficult as a reviewer to grasp some of the project information when the slides are overloaded and the fonts are very small, i.e., Slides 4, 6, 7, 10, etc. This is a fairly high-level project that uses a number of models to arrive at some predictions for carbon soil banking. I am not clear on the project's approach, progress, or impacts. There were many terms and acronyms that I was not familiar with, and I didn't feel that an adequate explanation was given to help non-expert-level reviewers. There were a number of significant risks, including scarcity of data and the dynamic nature of soil carbon. I'm also not sure how impactful the large-scale predictions will be; it is more important to have more spatially explicit information for landholders to apply. The uptake of this project will be very difficult unless the results are translated into a more common language that a farmer or landholder could easily understand.

- Response 4: Thanks for your comments. Yes, the dynamic nature of SOC, the scarcity of data, and the lack of a standard model present significant risks to this analytical effort. We have made some progress in addressing these issues, but much remains to be done. Although the preliminary results of the SOC simulations we presented were at the state level, the simulations were performed at the soil map unit/cropland use level—the most detailed level available from different data sources. Additional results of our efforts will be presented as maps at this more granular level. Yes, it is important as suggested for farmers and landholders to understand our results, and we plan to engage with these stakeholders as part of the project.

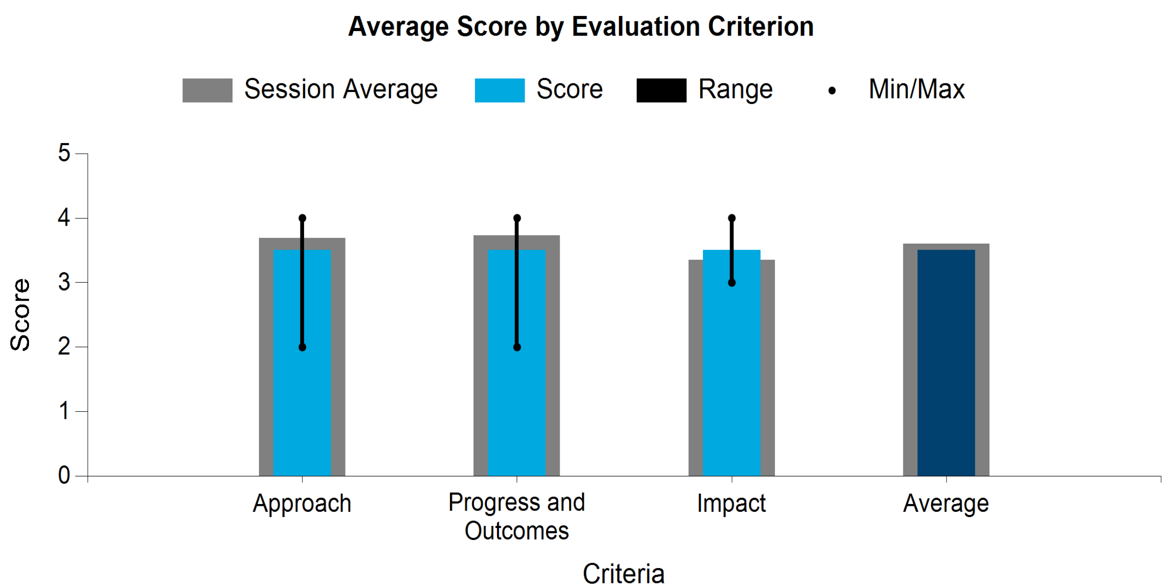
COVER CROP VALORIZATION FOR BIOFUELS AND PRODUCTS

Idaho National Laboratory

WBS:	1.1.2.1
Presenter(s):	William Smith
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,250,000.00

PROJECT DESCRIPTION

This task identifies technically feasible but currently underutilized cover cropping systems with the potential to decarbonize agricultural activities associated with corn stover harvest as a feedstock for conversion to sustainable fuels. The project focuses on the economics, biogenic carbon use, and biomass quality impacts of using cover crops where the stover residues are used as feedstock for fuel production. The novelty of this work is that it goes beyond traditional ecosystem services and uses existing consensus values of those services as a baseline monetary value from which to measure success. Objectives include (1) economic evaluation of combining cover crops with agricultural residues to improve on-farm economics with and without cover crops, (2) decarbonization potential of combining cover crops with residue removal relative to conventional agrichemical application and field operations, (3) laboratory-scale evaluation of cover crop materials, (4) evaluation of economically advantaged biochar to modify soil carbon, and (5) testing of INL's bale probe to measure soil carbon. Results will be used to populate and expand INL's feedstock logistics models. The outputs will be used to show how cover cropping, residue removal, and integrated land management have the potential to provide growers with a sustainable additional income stream and supply biorefineries with a high-quality and sustainable biomass resource.



COMMENTS

- This relatively new 3-year project is making good progress in the area of GHG emissions, which are a serious problem associated with farming. The team is well balanced with active participation from industry. The potential partner companies are good and active. Slides 11–13 have interesting data on zeta potential for the heavy and light fractions. It looks like the light faction is better suited for biochar. Are there any estimates on the contribution to reduction in GHG emissions from this use?

- This is a good project involving collaboration with Antares Group and Continuum Ag. On Slide 7, how do you plan to mitigate and handle these uncertainties in the coming year? The diversity, equity, and inclusion plan (DEIP) can be further developed to serve underserved communities. Cost analysis can be incorporated into biochar applications. BMPs can also be developed for farmers for cover crop practices.

- Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. The focus of this project is on examining trade-offs between cover crop management decisions and the inclusion of biochar. The work includes significant involvement of subcontractors for field demonstrations and stakeholder input. The highlight of the project in 2022 was participation in a field day event near Washington, Iowa. The necessity of measuring grain yield was emphasized as a key finding; however, that is already known for cropping systems R&D. They also reported results showing the benefits of using biochar, but no results were obtained or reported. No publications were reported, but the project is early in its implementation.

- Liked the use of the "farm budget" as the metric for measuring success, as the decision to carry out this practice will be based on specific farm operational costs and trade-offs with soil carbon. Because yield is the key variable for good farming profits, this should be a priority of the measurements. For better uptake by farmers (removal of corn stover for biomass), the questions posed in this project need to be answered. Relating to farmer operations is key information that will be needed by farmers to make the best decision. Chart 2 is not an adequate size to view the labels, etc. The font on many slides is very small and difficult to read. The blue color is also not ideal. In terms of approach, the study involves a case study of one farm. It will provide insights into what should be considered in an assessment, but the results themselves are of limited value. The questions asked (3) are highly relevant and need to be answered in order to make this a relevant and impactful process to allow for better utilization of corn stover residues. Modeling, while identified as challenging, is important for the real-life application of these findings. The partnerships with agricultural companies were good. In terms of P&O, the section on biochar was not well presented. Nothing about the costs/supply/sustainability of biochar—or the carbon footprint of biochar itself—was mentioned. Is it locally supplied? How is it brought to the site, spread, etc.? I don't fully understand the supply chain for the product and therefore whether it might make sense. In terms of impact, I have concerns about the limited number of sites/systems that will be analyzed in this project. Should preliminary BMP be included in this project?

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive and productive comments regarding the scope and progress that we've made thus far. The reviewers have recognized that our approach of using producers' on-farm budgets as our economic target comes with certain challenges and opportunities. Opportunities include analyses showing the potential revenue stream generated by stover residue removal and sale, which can offset the additional operational costs incurred by cover cropping, especially when working with a single producer over several years. Challenges—as specifically noted by our reviewers—include showing how those site-specific budgets can be extrapolated to other producers' conditions. Multiple reviewers reminded us that as we learn more about cover cropping and biochar application for sustainable residue removal, we need to distill our knowledge into BMPs that we can share with our collaborators for broader dissemination among producers. We believe that this communications strategy is important, as it also addresses a DEI concern: that the products of our research enable economic opportunities for rural economies as bioconversion technologies scale up. We have much to learn about the uncertainties surrounding soil carbon, the role of cover crops as a replacement for organic carbon removed during stover removal, and whether cover crops positively or negatively impact grain yield. First, although cover cropping and grain yield have been described in the literature—as stated by a reviewer—the added factor of residue removal is a relative unknown. We view cover cropping as a soil carbon replacement strategy with the potential to increase the amount of stover that can be removed sustainably. However, as we showed in our presentation, grain yield plays a larger role in producer profitability than either residue value or carbon credits. There is uncertainty in the literature about whether cover cropping and reduced tillage practices have a positive, negative, or neutral impact on long-term grain yields. We can make assumptions about how residue removal may impact the producers' budgets based on a range of modeled removal rates and sales values, but we need to understand how this additional operation impacts the row crops' yields to have a clear picture of whether residue removal is sustainable to the grower.

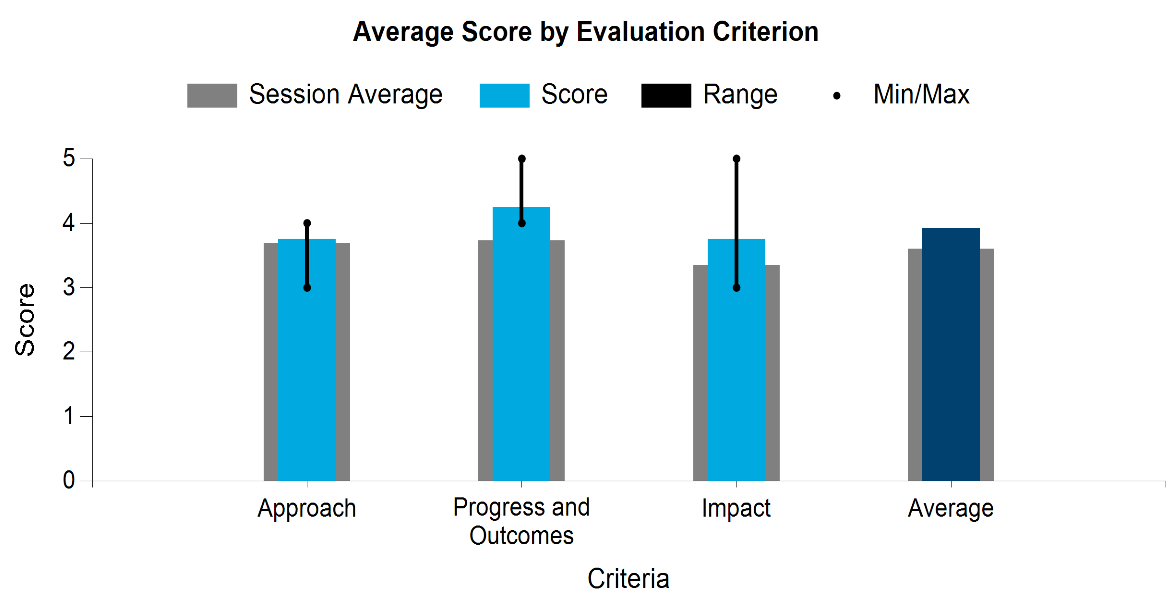
MAXIMIZING THE VALUE OF LATE YEAR COVER CROPS IN THE PACIFIC NORTHWEST

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	1.1.2.2
Presenter(s):	Daniel Santosa
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,470,000.00

This work highlights the potential of cover crops for use in biofuels from the perspective of the whole supply chain and life cycle to benefit farmers, biofuel producers, and the overall bioeconomy. In terms of utilization, cover crops equaled only 3.9% of all U.S. cropland in 2017. In addition, in Washington state, cover crop utilization is even lower, at <1%. Increased usage of cover crops provides an opportunity for producing biofuels and improving agricultural sustainability by improving soil health, thus enabling decarbonization efforts for both the agricultural and transportation sectors. The project objective is to provide a deeper understanding of the wide variation in cover crop use—in particular, the relative roles of climate, soil type, production practices, and application of cover crops as a feedstock for biofuels production. Typically, cover crops are grown for soil health only; however, biofuels production requires understanding trade-offs of harvesting optimal levels of cover crops to understand the impacts on soil quality. The first-year experimentation demonstrated promising results for the overall net benefit of cover crops in three different weather systems (wetland, irrigated, and dryland). We observed a net revenue due to the cash crop yield gain, with no observed loss of or impact on soil health. Moreover, improved revenue and sustainability is achieved when cover crops are blended with other wet waste, such as sewage sludge. The outcomes of this work are a deeper understanding of (1) an underutilized feedstock for fuel and (2) how to improve agricultural and agronomic practices, achieve biofuel production at a modeled cost target of $3.15/GGE, and achieve >70% GHG reduction by 2030.



COMMENTS

- This is a well-structured project with clear and specific, measurable, achievable, relevant, and time-bound milestones. The team is strong, with a proven track record and credentials. The focus on quantifying minimum technical achievements at this early stage is highly relevant and useful. I am wondering, with several projects funded by BETO, whether there are reliable guidelines/metrics for what minimum technical achievements are needed for operations like high-temperature air, gasification, Fischer-Tropsch, etc. (i.e., operations that are needed for biofuel and high-value chemical production). Such a guideline would be useful in focusing on early promising candidates.

- It is not clear how these three locations were selected and whether soil type was considered. DEI needs to be implemented in underserved communities. It is not clear whether any pretreatment was done on wastewater sludge for contamination. The cost of decontamination should be factored into the cost analysis.

- Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. This project is early in its implementation, but is perhaps the best executed of the cover crop projects. It has a diversity of three locations in Washington state, several cover crop types, and several primary crops that are appropriate for the Pacific Northwest region. The team is obtaining data to conduct LCAs for the various cropping systems. The PNNL team is collaborating with research and extension staff at Washington State University. Excellent impactful work is underway, and they have yet another growing season to obtain data.

- The project has valuable objectives: to produce information on the costs and benefits of using cover crops directly as a fuel source, which also reduces the overall carbon intensity of agronomic practices. In terms of the approach, there was a good slide (4) showing the partners and their role in the project. However, the slide is very wordy and was hard to read or absorb during the presentation. The project is sound and has a good chance of being very successful. There was good identification of risks and mitigation strategies built into the project. Missing from the project structure is who will be doing the outreach to the farming community. As far as P&O, there were some good initial findings related to the association between cover crops and the improved yield of a main cash crop. How will the information be shared and in what form? Is the intent to write scientific papers and/or extension bulletins? In terms of impact, is there sufficient market demand for the residue to warrant this extra step? The regionality of biomass energy plants would limit the viability to specific areas. Field demonstration days and feedback are very important for future implementation.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for taking their time and providing their thoughtful and insightful comments. We agree that the effort to quantify the critical material attribute (CMA) of the biomass is critical for the relevance and usefulness of cover crops and other feedstocks. We used a yield predictive model to estimate biofuel yields based on the hydrothermal liquefaction (HTL) feed compositions (carbohydrate, lipid, protein, ash, and lignin contents). The yield predictive model was developed from an experimental data set generated from the HTL flow reactor systems at PNNL. Examples of HTL yield predictive models can be found in recent PNNL publications, such as https://doi.org/10.1016/j.jece.2023.109706, https://doi.org/10.1016/j.apenergy.2020.116340, and https://doi.org/10.1016/j.algal.2019.101450. We would also like to clarify that the crop locations, soil types, and cover crops were chosen to represent the diversity of farming practices that are amenable to cover cropping in Washington state. The cover crops were selected to represent the varietals of legumes and grasses that are considered the best fit to the crop rotations and that will support the subsequent growth of primary crops that are appropriate for the Pacific Northwest. In addition, soil type is one of many factors that differ among sites, among which are climate and access to water. The aim is to consider different growing regions to inform which cover crops and regions might produce sufficient cover crop biomass and composition for biofuels. This knowledge can be used to incentivize adoption of cover cropping. We also appreciate the comments with regard to sewage sludge pretreatment. The HTL team at PNNL has been collaborating with multiple wastewater treatment facilities and waste management entities. We learned that any additional pretreatment step or decontamination effort for the wet waste feedstock is not necessary. However, a simple dewatering or dilution step may be required to control the viscosity and pumpability of the HTL feed. This is also consistent with the latest PNNL conceptual process design of a wet waste HTL pathway that was extensively reviewed by internal and external experts (https://doi.org/10.2172/1897670). In terms of outreach to underserved communities, we agree with the reviewers on how important this effort is. This project focuses on serving both rural and underrepresented communities across the state of Washington, in partnership with the Washington State University (WSU) Center for Sustaining Agriculture and Natural Resources, by holding annual field days in three farming locations. This is our primary way of demonstrating the growth and economic potential of cover crops for cash crop production alongside a presentation of sustainable agriculture practices. We have conducted outreach in the WSU Puyallup Research and Extension Center Cover Crop Field Day on May 1, 2023, and the field day in 2022. There is another upcoming field day in June 2023 at the WSU Research and Extension Centers across three sites in Washington state. Additionally, WSU will be presenting findings to diverse audiences, including underrepresented farmers, at annual meetings like the Tilth and Hay Growers Association. In terms of publications, we presented our first-year results at the American Chemical Society Spring 2023 meeting in April, and we will be presenting our TEA and LCA methodology and preliminary results at the 2023 American Society of Agricultural and Biological Engineers annual meeting in July. After our third growing cycle in 2024, we will have additional data on seasonal and climate variability, which will impact the overall cover crop production. We will present the results in journals. In addition, there is demand for economically advantaged residues from cover crops, which would not lead to additional land use change—one of the key factors in determining a biofuel's percent GHG emissions reduction. With the cover crops in the off season, the feedstock logistics are enhanced relative to just corn residues, which are harvested solely in August–October. It is clear that the price of cover crops for biofuels would have to be better than the price of using the cover crops as fodder or bedding.

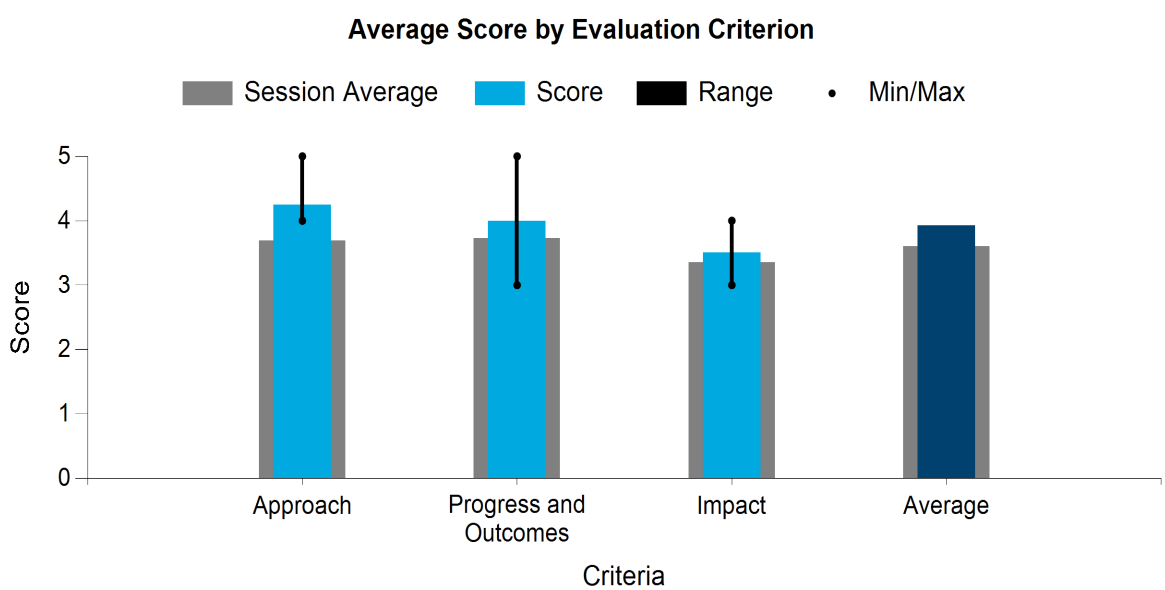
NATIONAL AVAILABILITY AND COSTS OF COVER CROPS MANAGED AS BIOFUEL FEEDSTOCKS

Oak Ridge National Laboratory

WBS:	1.1.2.3
Presenter(s):	Esther Parish
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,740,000.00

PROJECT DESCRIPTION

Cover crops—grasses, legumes, or small grains grown between the harvest and planting seasons of cash crops—offer many ecosystem benefits, including reduced soil erosion and increased soil organic matter. These benefits of planting cover crops during the off season help improve the conditions of the primary crop. More importantly to farmers, these cover crops may be harvested and utilized as biofuel feedstocks. Early studies suggest that cover crops could produce 2–3 tons/acre of biomass, comparable to higher-producing corn stover collection rates, or up to 65 gallons/acre of oil for oilseed crops. This is not always the case, however, as there may not be adequate time between the desired harvest and planting dates of the primary crop for the cover crop to reach maturity and viability as a biofuel/bioproduct feedstock. The feasibility of creating a double cropping system depends on the selection of appropriate cover crops, the determination of optimal harvest/planting dates, and the weather during the cover crop growing season. Because the maximum environmental benefit from cover crops comes when the biomass is not harvested, missed opportunities for ecosystem services must also be considered. Currently, cover crops of any type have very low adoption rates. However, adding a revenue stream for these secondary crops will incentivize adoption of cover cropping systems and could significantly expand adoption of this conservation practice. This project will elucidate the environmental and economic competitiveness of cover crops compared to other cropping options. This information will contribute to an understanding of potential cover crop adoption and oilseed crop production at a national scale with relevance for the potential development of renewable aviation fuels.



COMMENTS

- This is a well-laid-out project focused on secondary oilseed-based cover plants. Progress to date seems to be on track. The price/cost projected in one of the slides seems to be optimistic. Does this include collection/crushing costs of the seed oil? Compared to soybean/palm, the yield per acre is quite low, and hence the cost of crushed oil from these sources could be higher. Some of the oils, such as camelina, have fairly high omega 3 fatty acid content and other beneficial constituents and will have higher value in nutraceutical and pet food applications. It is worth focusing more on these higher-value products than on SAF. A Canadian startup has some interesting camelina-based products. The project needs to engage potential industry stakeholders.

- As far as approach, the project addresses the use of cover crops for SAF. Specific pathways from cover crops to SAF should be considered for analysis. In terms of P&O, on Slide 9, there may not be sufficient data points to develop a model in that case. In terms of impact, the income from ecosystem service benefits is not clear. Some field trials would be helpful and beneficial to the project. We encourage the team to continue and enhance its collaboration with the University of Maryland Eastern Shore.

- Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. This project is early in its implementation and was recently modified to include oilseed cover crops, including pennycress, carinata, and camelina. These crops were included in addition to rye, winter wheat, and hairy vetch. Results from this project will be included in the forthcoming *Billion-Ton Report*, and this work will obtain information on cover crop ecosystem services such as soil health, pollinator habitat, and synergies with cash crops. The project will support a student intern from an 1890 land-grant institution. A significant impact is anticipated from this project.

- In terms of approach, the project shows a clear understanding of the criteria for success on Slide 2. The approach is well laid out and makes sense. As far as P&O, this is early-stage research for mobilizing a new biomass feedstock, either oil crop or herbaceous. This work is needed to justify the concept of cover crops on a national basis. The preliminary results are good. The impact of the project is well laid out on Slide 15. This will lend information to potential commercialization efforts in the future.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you to the reviewers for this constructive feedback. Our project is new, but we have already been able to make significant progress by incorporating oilseed cover crop production into Policy Analysis System Model (POLYSYS) modeling runs for the forthcoming national bioenergy resource assessment (aka the *Billion-Ton* 2023 report). Our preliminary results indicate that incorporating carinata, camelina, and pennycress cover crops into traditional crop rotations could provide ~22 million tons of oilseeds from across the eastern United States that could be used to produce ~3 billion gallons of SAF. The POLYSYS oilseed price of $0.15 per pound reflects the price of harvesting the seeds but not the cost of crushing or transporting the seeds. We also acknowledge that oilseed crops may be used for a variety of end products that may prove more lucrative than SAF. However, this modeling work shows that there is significant potential for cover crops to contribute toward the SAF Grand Challenge.

- Over the coming years, we will engage with industry through the Commercial Aviation Alternative Fuels Initiative to better understand the information needed to make cover crops a commercial reality without unintended consequences. We will continue to collaborate with the University of Maryland Eastern Shore regarding herbaceous cover crop potential, and we look forward to hosting one of their undergraduate students at ORNL from May–July 2023 through the Undergraduate Research Student Internship program. The scope of this project does not include field trial installation and sampling. However, we will reach out to researchers at other labs and universities to see if data from their ongoing field trials can used to model the potential ecosystem benefits and trade-offs associated with harvesting cover crops for bioenergy production at regional and national scales.

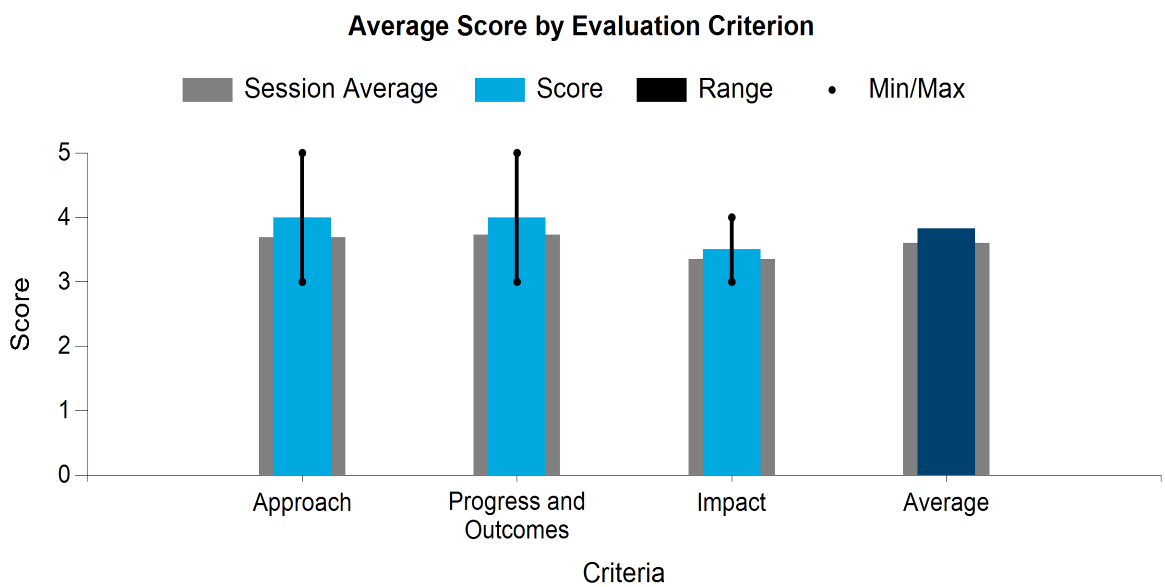
VALUE-ADDED PROCESS INTENSIFICATION IN THE SUPPLY CHAIN

Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.1.1000
Presenter(s):	Bradley Wahlen
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,755,000.00

This project utilizes the necessary unit operation of storage and queuing to address feedstock challenges and add value by reducing downstream chemical and energy input. The long residence time of storage or queuing is used to achieve this through low-severity treatments. Microscale changes to biomass that occur over time in storage lead to macromolecular and tissue-level impacts during deconstruction, fractionation, and conversion. Using in-storage treatment, this project demonstrated a reduction in alkali and alkaline earth metals in a bark fraction from forest product residues, reducing a contaminant that limits its suitability for conversion. In-storage treatment of corn stover with formic acid led to partial breakdown of lignin, observed as a higher pyrolytic efficiency of lignols in pyrolysis gas chromatography/mass spectrometry. These molecular changes led to a lower activation energy required to initiate pyrolysis. Additionally, corn stalk consists of disparate materials—pith and rind—that are tightly bound, and their physiochemical differences reduce pretreatment efficiency. In-storage treatment targeting pectic polymers enabled the separation of pith and rind and the recovery of intact vascular bundles, improving corn stalk processability and enabling the recovery of potentially valuable coproducts. These principles of low-severity treatment over long periods of time to enable molecular changes to impact feedstock performance are being implemented with industrial partners at field scale.



COMMENTS

- This is a very impactful project with a clearly stated work plan, objectives, and deliverables. The team is well seasoned in the field and has very credible experience, a proven record, and strong capabilities. The team also has a good connection for implementation. The project is on track and is expected to focus on further larger-scale demonstration and TEA. Slide 12 shows the pH dropping to 3.2 from 5.3—is there any potential impact on materials of construction in downstream conversion steps from corrosion issues?

On Slide 14, is there any estimate of energy savings based on increased conversion? What is the impact on operating expenditures (OpEx) in downstream operations?
On Slide 16, we see reduced minerals—what is the impact on any catalyst poisoning?

- (1) This is a good project with clearly defined goals and methods. It addresses the value-added opportunities versus reducing costs of process components along the supply chain. However, it should clearly address where and when these value-added and cost-reduction activities should take place along the entire supply chain. (2) I agree that bark biochar is good for soil amendment and carbon sequestration. However, some comparisons are needed for bark char with biochar derived from wood. (3) In terms of impact, POET is a major industry partner for this project. It is not clear whether any major findings from this project have been applied in their production processes, such as storage and pretreatment to improve conversions. Future work can focus on the consistency of TEA data as well as large-scale storage and preprocessing of multiple feedstocks.
- BETO investments in feedstock pretreatment are important for optimization of the use of off-spec materials, stabilization during storage, and preparation for conversion processes toward specific products, such as SAFs, composite materials, or high-value chemicals. Companies that are scaling up the use of lignocellulosic resources for biofuel production often store feedstocks in piles that are exposed to the elements. They have experienced occasional spontaneous fires in these piles, similar to what can occur with silage and hay for animal feeding operations. Fire risks are enhanced with certain combinations of water concentration, such that heating results from anaerobic fermentation. A rapid influx of oxygen can cause a fire or even an explosion. This project is examining the use of acid treatments as an approach to pile management to both reduce the risk of fire and support pretreatment to reduce the recalcitrance of corn stover. Thus far, the team has observed that formic acid treatment achieves these goals and eases separation of stem rind and pith tissues. The industry partner in this project is POET. This project is on track and will be impactful for improved corn stover management.
- This project aims to use long-term (or short-term) storage to positively impact downstream processes through the use of low-severity treatments. The approach is well thought out. The opportunities on page 6 are valid and well defined. In terms of P&O, the results at the lab scale are very promising, and the analysis of the impacts is thorough and valuable. As far as impact, the main concern is the scale-up phase, where you are dealing with large industrial piles with dynamic moisture content/oxygen/temp conditions. It would be good to test a range of conditions for your pretreatments to see what the efficiencies of the treatments are at less-than-optimal conditions. These conditions can be derived from the literature, on testing and modeling done on large storage piles. It isn't clear what the subject matter of the patent or intellectual property (IP) would encompass. How does the PI see the rollout of this to the industry? Are there scale-up projects planned? This is good preliminary work, but it is a long way from commercial implementation.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their time and thoughtful comments. We agree that this project has the potential to positively impact industry and address storage challenges at scale. This project is currently collaborating with POET to study storage stability in large-scale storage piles. Additionally, progress toward commercialization of process intensification in storage can be achieved in the next cycle of the project through a combination of monitoring the storage conditions (temperature, moisture, dry matter loss) of commercial-scale piles and demonstrating mitigation strategies in the laboratory that will result in the desired critical quality attributes under a range of conditions observed at scale. TEA will be used to inform treatment strategies and determine costs. This project has sought to take advantage of the long residence time in storage to perform low-severity pretreatments to biomass that improve critical quality attributes, enable tissue separations, and reduce recalcitrance in conversion. TEA will be used to understand treatment costs and positive benefits to downstream operations. Questions related to the corrosivity of treated biomass, impacts to energy utilization in conversion or OpEx, and the effect of mineral reduction on catalyst poisoning might be best answered through collaborative research with other BETO-funded projects. This project will seek opportunities to work with others to better understand the impact of process intensification in the supply chain on downstream unit operations.

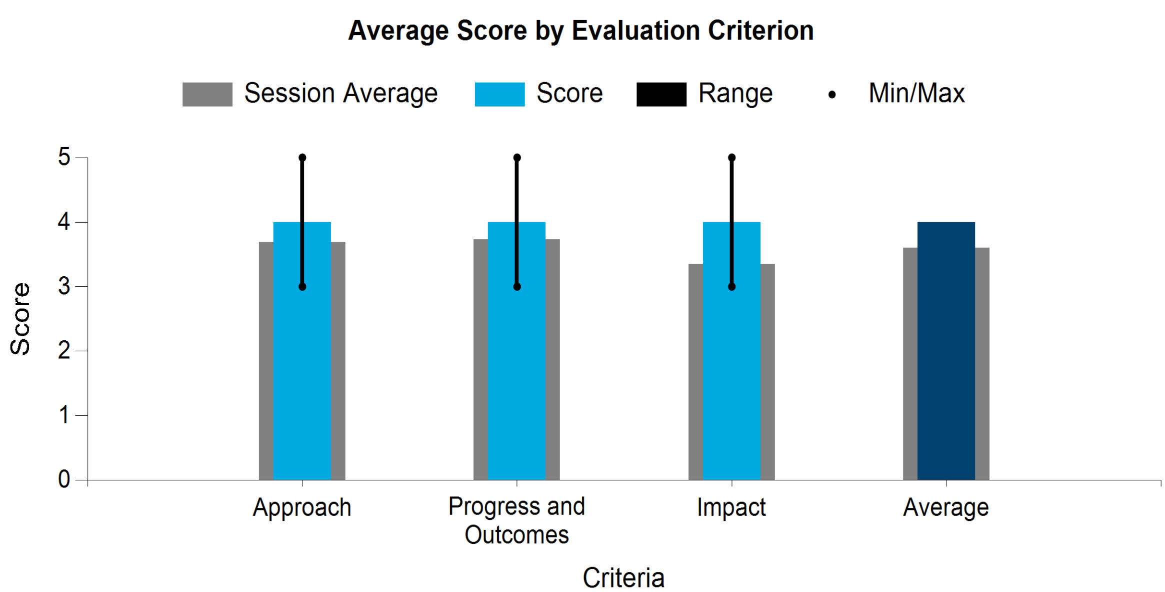
BIOMASS SIZE REDUCTION, DRYING AND DENSIFICATION

Idaho National Laboratory

WBS:	1.2.1.2
Presenter(s):	Neal Yancey
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,922,194.00

PROJECT DESCRIPTION

Variability in feedstocks leads to significant downtime, low production rates, and poor-quality feedstocks. The goal of the project is to understand how process variables for preprocessing unit operations (i.e., milling, drying and dewatering, densification) impact the critical quality attributes of low-value carbon resources and how variables and material properties interact within and impact processes to produce products with the desired critical quality attributes using a quality-by-design approach. The specific objectives of the project are to: (a) take advantage of the Biomass Feedstock National User Facility (BFNUF) process development unit upgrade and grinding process for MSW fractions to understand its impact on the CMAs; (b) identify the impact of shearing process conditions on mechanical dewatering of forest residue fractions, as well as its impact on quality attributes; (c) create at least three MSW blends that meet moisture content, porosity, and density specifications by optimizing process conditions; (d) develop a densification model based on the compression characteristics; (e) analyze the processes tested for TEA to understand the energy and cost savings for high-moisture forest residue and MSW fraction processing; and (f) work with FCIC Task 5 on developing the discrete element method models for the grinding process. This project was successful at developing methods to achieve the required CMAs, including moisture content, porosity, and density. The TEA developed showed that a cost of $16.35/dry ton can be achieved using screening, advanced milling, and high-moisture densification. The resultant feedstock has lower-ash, high-durability pellets, which increase flowability and reduce downtime.



COMMENTS

- This is a well-laid-out project with a clear work plan, objectives, and deliverables. The team is experienced in the field and is working closely with other BETO-funded project teams working on similar topics. It looks like the project is on track. It would be helpful to clearly show the current status versus milestones and what is planned for the remaining performance period. What is the commercialization path? Slide 17 shows a 50% reduction in cost. Is this for a full-scale plant? What is the confidence level?

- (1) No details are provided on the approach. (2) Pellets were made separately from leaf, cob, stalk, and husk for testing. In reality, they can be mixed. It is not clear how pellets made from a mixture of leaf, cob, stalk, and husk affect the pelletizing process and fine reduction. (3) In terms of P&O, it is not clear what moisture content was used for making the pellets. Particle size, moisture content, and temperature will all affect the pellets' formation and properties. (4) On Slide 17, it is confusing how the cost was improved from 2019 to 2020 and 2022. It seems that the comparisons are not based on the same categories each year. (5) As far as impact, in addition to testing advanced preprocessing, a potential commercialization plan should be explored. (6) It is not clear what specific future work on forest residue will be conducted for later budget periods in this project.

- BETO investments in feedstock pretreatment are important for optimization of the use of off-spec materials, stabilization during storage, and preparation for conversion processes toward specific products, such as SAFs, composite materials, or high-value chemicals. This project represents essential continuous improvement for feedstock handling. Typically, feedstocks are ground rapidly in high-horsepower grinders to rapidly reduce particle size, and afterward, high-temperature drying is used. This high-throughput processing often causes systems to be plugged, and equipment damage can cause failure and stoppage, resulting in excessive opportunity costs. This project aims to redesign feedstock preparation by optimizing grinding through milling technologies and using chemical and low-heat drying. The project's initial TEA shows a reduction in prep costs from $33.64 to $16.35 per dry ton. Additionally, feedstock consistency is improved, and ash concentration is reduced. This work will help establish specification standards for biomass and nonrecyclable municipal solid waste (NMSW) feedstocks.

- In terms of approach, the responsibilities of the team were well laid out in the table on page 4. I appreciated that all biomass fractionation was considered, but the focus of the presentation was on MSW. The team demonstrated out-of-the-box thinking. This project was well presented. All slides could easily be read, and the charts were well presented. As far as P&O, the team did nice work on the three milling technologies. The comparison of the technologies for the same MSW produced results beneficial to the processing at the next step. The project looked at challenges in the physical/chemical variability in biomass and how to process efficiently. The actual densification trials look promising. Pellets are a good form for conventional equipment and can be delivered to a process efficiently and at a consistent feed rate; this is a promising direction. Low-temperature drying was out-of-the-box thinking, which is needed in this industry. Forced air ambient drying as a pretreatment may also show promise. We did work in this area for drying woody biomass with good results. Online sensor development should be continued. This gives real-time information and allows for diversion or better process control in subsequent processes. In terms of impact, this project has come a long way through really thoughtful process work and applying real-time monitoring to affect process control. Real-time process monitoring will be very useful for scale-up operations. This information will be very good for decision-making at the mill gate or biomass depot, but it is unclear how the technology transfer will take place. It isn't clear how the project will be commercialized, or what the plans are for industry uptake of the outcomes.

PI RESPONSE TO REVIEWER COMMENTS

- We want to thank the reviewers for their thoughtful comments and assistance in reviewing this project. It is important, as was noted, that the data from projects like this are effectively disseminated to industry as they work through the same types of issues. Just last week, INL hosted a ribbon cutting ceremony to highlight recent additions to the BFNUF capabilities. This ceremony, attendance at conferences, publications, and other outreach efforts are just some of the ways data is shared with industry. In this project, the focus was on fractionation/sorting followed by downstream milling and densification as needed for the individual fractions. Processing of the bulk material has been investigated and will likely continue for some time, but the need to fractionate and clean up feedstocks is becoming more apparent as a necessary approach to control variability in the feedstocks. Regarding the comment on Slide 17, the comparison was made by changing the fundamental approach each year to improve the overall outcome. The original baseline included drying using a rotary drier, hammer milling, and densifying. The next year included high-moisture size reduction and densification. The final approach included fractional milling, high-moisture milling, and high-moisture densification. Although corn stover has long been a major focus of our research, other feedstocks, like forest residues, will continue to be a fundamental part of our research as well. However, there is a growing need for research in other areas, including MSW, waste plastics, e-waste, and others.

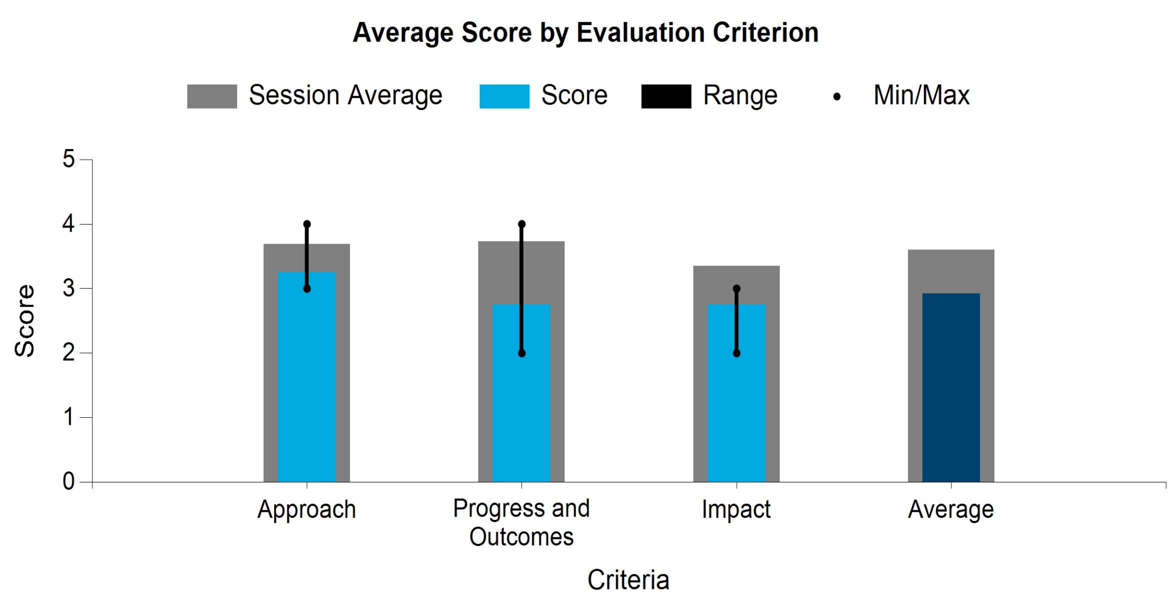
THERMAL CONDITIONING FOR DEVELOPMENT OF CO-PRODUCTS FOR CARBON CYCLE SEQUESTRATION

Idaho National Laboratory

WBS:	1.2.1.4
Presenter(s):	Jordan Klinger
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,800,000.00

PROJECT DESCRIPTION

This project explores pathways to generate coproducts from nonrecycled wastes that are not suitable for SAF production. Materials diverted to such support schemes are not of sufficient quality, are unable to be decontaminated, or have nonbiogenic carbon origins. The goal is to lock this carbon into long-lived goods for sequestration, while simultaneously generating additional carbon offsets and revenue to support SAF generation. Doing so would enable and develop new feedstock streams for commercial products, such as building materials (thermal and acoustic insulation), composites, lightweighting components, and carbon-dense materials, all with potentially lower carbon intensity compared to market alternatives. The main challenges arise from the heterogenous nature of wastes, the degraded quality of materials, and the nature of complex mixtures. To overcome this, the project is structured to investigate the hyperspectral characterization of wastes, including biogenic carbon detection, to direct unsuitable material to a preferred coproduct. In addition, several experimental tasks look at thermal, mechanical, and chemical modification of properties and component formulation. Overarching techno-economic and life cycle assessments are guiding the project through regular milestones, the go/no-go decision gate, and final recommendations. To date, one of the coproducts—building insulation—has been shown to have near-performance parity to commercial products and beneficial economics compared to market prices.



COMMENTS

- This is a well-conceived project to find new value-added uses for municipal waste components that do not meet SAF requirements. The team is well balanced and has the required skill sets and capabilities to carry out the project tasks and milestone deliverables. Work to date has identified and reached the preliminary proof-of-concept stage for developing insulation mats to compete with existing paper and cellulose ones. It isn't clear how and when this opportunity will be handed over to a potential commercialization partner. On Slide 7, it isn't clear what the insert at the bottom left is. On Slide 8/9, it looks like biogenic carbon and total carbon are used interchangeably. It is noted that the experimental insulation mat is within 10% of market value, but it isn't clear what this means. The slide on cost has units in dollars/ton, and the current products are in dollars/square foot. It isn't clear how to compare the two.

- (1) In terms of approach, the go/no-go decision points are not clearly defined, and they do not make a lot of sense. It is not clear whether contamination removal is considered in the analysis. (2) As far as P&O, the project makes progress. However, more explanations on the progress and outcomes will be needed for the coming years' reporting. Unsorted MSWs contain 68% biogenic carbon. It is not clear whether your analysis considers this carbon. (3) In terms of impact, commercialization of this material for residential housing insulation could be significant. The DEIP should be addressed.

- BETO investments in feedstock pretreatment are important for optimization of the use of off-spec materials, stabilization during storage, and preparation for conversion processes toward specific products such as SAFs, composite materials, or high-value chemicals. The potential exists to produce low-carbon-intensity products from thermal conditioned NMSW. Feedstock characterization for carbon isotopic composition will be necessary for products to enter low-carbon-intensity bioproduct markets. This project is developing hyperspectral carbon isotopic analysis of NMSW feedstocks and assessing the effects of thermal and mechanical modification. Coproducts, such as household thermal insulation, are also being examined. Progress has been satisfactory with carbon isotopic analysis of NMSW separated components. Testing for thermal insulation has been done for physical biological composites. The TEA based on the retail process of incumbent products seems unrealistic, however. Outputs include publication manuscripts, an invention disclosure, and a demonstration of home insulation.

- In terms of approach, using radiocarbon analysis for determining biogenic carbon seems like a complicated methodology for determining bio-based carbon content. The waste materials that are made from biogenic carbon are common knowledge. In terms of P&O, on page 8, I didn't see anything surprising in this table, and it could have been estimated without radiocarbon analysis. The difficult materials are those that contain various layers or plies, similar to juice boxes, but I didn't see that in the list. I cannot read the table on page 9. The cost comparison on page 14 was the processing cost of the MSW versus the retail sales price of the competing materials. This needs to be better thought out for a fair comparison. It is unclear what the three columns of "energy usage," "purchase price," and "throughput" represent on the MSW processing. In terms of impact, the IP on page 15 looks interesting but was not discussed in the presentation. Will this project reach a TRL of 5? This project deals with a small component of MSW, which will at best compete with very low-value materials. The TEA should consider the products currently used for these applications for meaningful comparisons.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' expertise, time, and thoughtful comments during this review process. Below are comments and additional details on the common feedback topics of TEA and the development of bio-based carbon detection methods. TEA is an invaluable tool to help guide process optimization and determine economically viable processes. During the BETO Peer Review preparation, we sought to compare the TEA of producing building insulation from MSW to other commercial alternatives. Because the economic details of the commercial products were not known, we compared the production cost of the MSW insulation (including packaging, delivery, etc.) directly, and determined a potential markup/profit from that comparison. The 18-month go/no-go milestone for this project was to demonstrate that, at a minimum, one of the projected coproduct pathways could be produced at comparable (±10%) costs to that of the sales price for market alternatives. Following the Peer Review preparations, we completed the economic analysis for the MSW insulation pathway. This analysis showed that the total cost to producing the product was $16.30/dry ton of product, excluding the addition of chemicals as flame retardants and biological activity inhibitors. This is only a fraction (<1.4%) of the cost of commercial products, such as cellulose insulation, which had a retail price of nearly $1,200/dry ton at the time of the analysis. Although the final insulation cost is dominated by the chemical additives, loadings of up to 10% by mass for each of the compounds still enabled an economic MSW insulation pathway with a production cost more than a factor of four smaller than the alternative product price. The presentation outlined one invention disclosure related to this project, although another patent application is under review at INL related to this concept of MSW insulation. The translation of such a product to market could follow well-known pathways of patent IP licensing from INL, for example. Team members involved in this work are/have identified and engaged potential partners/licensees, pending IP review. The rapid detection and measurement of bio-based carbon in waste materials will be critical for enabling certification or documentation of feedstock streams. These could be advantageous for fuel production pathways such as SAF, or for estimating the bio-based carbon being sequestered into coproduct pathways. Particularly in the case of displaced fossil resources where the carbon is stable and otherwise unsuitable for fuel production, any reduction in GHG emissions (or economic benefit) substantially benefits the primary objective of fuel production toward meeting BETO programmatic targets. Although the proposed hyperspectral methods can be complicated and require large upfront data sets and validation, they are a prime example of how the national laboratories support industrial development. As a near-term target, as a review indicated, categorical labeling as demonstrated in the presentation slides can be used as a proxy for bio-based carbon analysis. Indeed, the challenges will arise from multilayer packaging and more complex composite materials. Future work will drive the incorporation of these materials in rapid assessment techniques.

RESOURCE MOBILIZATION

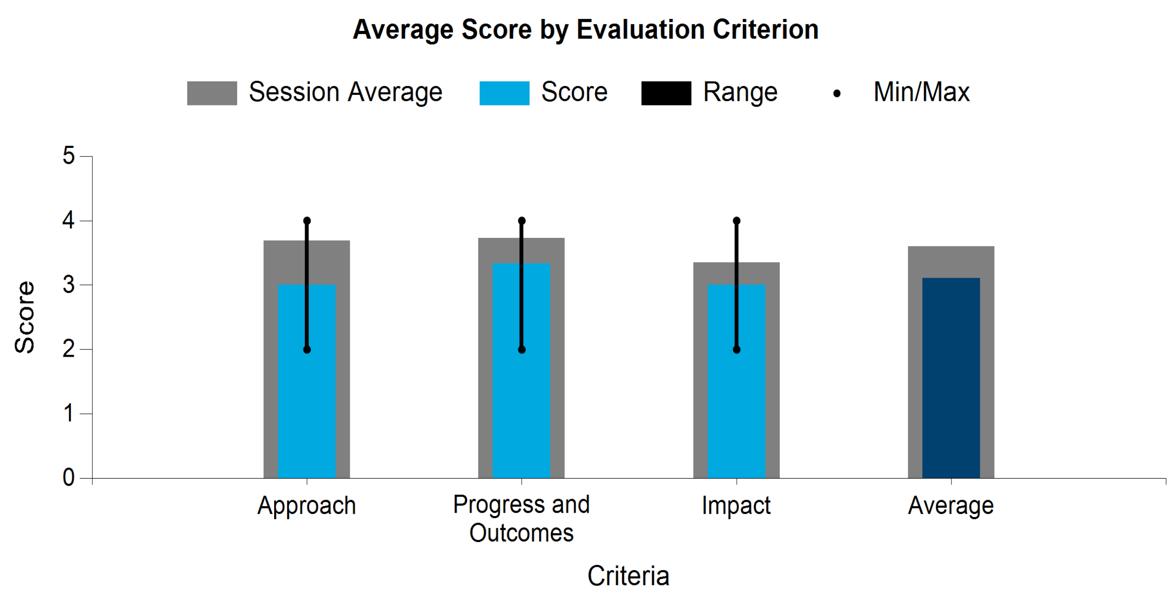
Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.1.5
Presenter(s):	Pralhad Burli
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$765,000.00

The future of the bioenergy industry is linked to the willingness of farmers to participate in the biomass supply chain and supply feedstocks to the market. However, variability in the physical and chemical properties of biomass can be detrimental for conversion processes. Thus, strategies to fractionate the biomass and use it either as blended feedstocks or in alternate bio-based markets can improve the economic viability of the biorefinery. This project focuses on identifying strategies that can lead to higher adoption in the production of herbaceous biomass feedstocks and that use materials that are not suitable for biochemical conversion in alternate midstream markets.

We used agent-based models to simulate interactions between stakeholders to understand prospective trajectories of biomass mobilization and evolution of the supply chain. This modeling approach helps increase our understanding of systems in which the behavior of agents is not known with complete certainty, but is instead dictated by probabilistic decision rules. We developed integrated models to demonstrate the potential for using biomass fractions in value-added markets to increase the use of biomass fractions, identify drivers of increased adoption, and reduce the risk of participation in the biomass supply chain.



COMMENTS

- This is a useful economic-based diffusion model to better understand the practical viability of crop-residue-centric biomass feedstock. It seems to have made good progress in biochar applications. Is this a viable opportunity? Why has the biomass collection area decreased? (Slide 6.) How will buy-in from farmers be secured for the output results for filed implementations?

- Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending. This modeling project is studying how to upgrade off-spec feedstocks through material fractionation and subsequent blending with corn stover. The team noted that corn leaves are a least-favored component of corn stover because of their high ash concentration and low density. They examined the use of blended materials in the production of biochar; however, like most biochar projects, no consideration was given toward the development of the coproduct pyrolysis oil. This project has produced only limited publications, and the team's external outreach needs to be improved to make the work more relevant to industry needs.
- This was a good presentation. However, I'm not sure I could completely wrap my head around what the project goal was and whether this was a meaningful or useful goal. The idea of a biorefinery is to take biomass and convert it into multiple product streams. The biorefinery could potentially separate the material streams ahead of or at any time during the process. The idea is that the most suitable material goes to the most value-added option for it. There should be nothing labeled as "off-spec" material; this should be "on spec" for the alternative product stream. I think that choosing one or two alternative markets is a very limited approach, yet there seems to be a lot of detail around the one alternative "biochar." How and why did the investigators decide this was a viable market alternative over other thermal technologies? It wasn't clear how they developed this approach. I can't join the dots between this work and industry uptake. The flowchart is so small I can't even read it on my computer (white font on green background).

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their feedback on our modeling approach and analysis to evaluate potential pathways for supply chain evolution and biomass resource mobilization. Our model is designed for a representative supply shed, and in its current version, it evaluates the supply requirements and biomass use for a representative biorefinery served by two preprocessing depots. The model demonstrates that the biomass collection area decreases over time in response to increased farmer adoption, whereby the biorefinery agents can contract with farmers located closest to the depots to minimize transportation costs. We agree that choosing one or two alternate markets is a limited approach; however, our intention was to demonstrate different modeling frameworks as a proof of concept that can show how some of the biomass that is not suitable for conversion to biofuels can be utilized in alternate markets. To evaluate the specific viability for biochar adoption, we identified the requirement on farms by developing an index using soil pH, water holding, and cation exchange capacity as indicators and incorporating the associated costs of biochar application and potential yield benefits. The model determined that only some of the farmers in the study region are potential biochar adopters, as the benefits on each farm might vary depending on a variety of underlying factors, and biochar application might not be economically beneficial for all. From an industry perspective, our end-of-project goal is to demonstrate how an integrated supply chain can support the biomass needs of a biorefinery and utilize fractions that are not suitable for conversion to fuels in alternate markets that can help the overall economic viability of the biorefinery by reducing biomass loss. Since the previous Peer Review, we have published one journal article. One manuscript is under review, and one manuscript is in preparation and is scheduled to be presented at the Association of Environmental and Resource Economists 2023 Summer Conference. Research in this project has also contributed to reports published by the International Energy Agency Task 40. We will increase our external outreach efforts and will continue to engage with industry participants to make our insights relevant for their uptake.

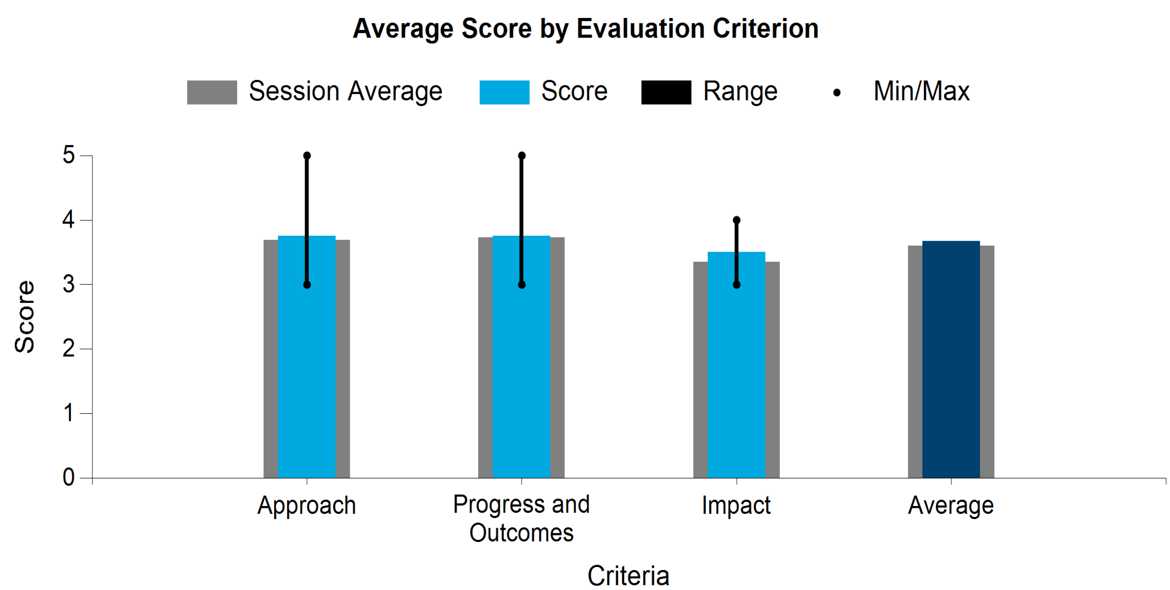
MUNICIPAL SOLID WASTE PREPROCESSING AND DECONTAMINATION

Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.1.7
Presenter(s):	Vicki Thompson
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,850,000.00

This project is developing a suite of preprocessing tools to reduce the variability and improve the quality of the biogenic organic fraction of MSW (excluding wet food waste), either by itself or as a blendstock for conversion to SAFs. The project is working with underserved and rural communities to source MSW streams and characterize the percentage of each MSW fraction and the types of contaminants present. The team is assessing preprocessing tools that can produce consistent feedstocks that meet conversion specifications and remove problematic contaminants. TEAs are conducted in parallel to select the most economic technologies. The project end goal will be preprocessing decision matrices to process and decontaminate MSW streams for fermentation and pyrolysis pathways to aviation fuels. These decision matrices will allow users to develop processes targeted for their waste streams.



COMMENTS

- The full project started recently and has made good progress. The team is well organized and has the necessary expertise, including local municipal waste handling organizations. Slide 6 mentions hazardous waste. What are the key components/their hazards/mitigation? Could this be a showstopper? Slide 8 shows various decontaminating agents. How are they disposed of safely?

- (1) This is a sound project. Some details on the approach should be provided to strengthen the project. (2) In terms of P&O, the project has made some good progress since the last review. The analysis, such as linear regression, could be further improved. (3) The decontamination strategies are not clear. If chemicals are used for decontamination, how will these chemicals be handled after the treatment? (4)

Mitigation strategies for some of the identified risks are not clear. (5) A DEIP needs to be specified to serve the underserved communities.

- Land use change and competition with food production are often cited as concerns for lignocellulosic feedstock production. Development of NMSW as a feedstock is warranted because it does not compete with agriculture for food production, and because the use of NMSW will offset the flow of waste into landfills and mitigate landfill methane emissions. Conversion of wastes into useful products and services is a basic aspect of circular economies. BETO has made significant investments into NMSW research, including the projects reviewed in this report. Some of the challenges of developing NMSW as an economic resource include (1) the extreme heterogeneity of NMSW, and (2) the presence of toxic and undesirable constituents. Therefore, BETO has made significant investments into NMSW characterization, sorting, blending, and milling to overcome these challenges. This project is evaluating (1) four decontamination strategies for NMSW, (2) blending NMSW with corn stover and pine, and (3) feedstock storage. The intent is to develop a consistent in-spec feedstock for SAF and chemicals. The team has made significant progress and has made a good effort on publishing the results. They have also filed one patent application.
- In terms of approach, there is a clear focus on diversity and inclusion, with a focus on underserved communities and rural communities without curbside recycling access. Priority is given to understanding the contamination issues for the material and developing safety procedures for handling. Project goals are very relevant to improving the feedstock and are also relevant to SAF. The presentation should include a slide showing member involvement. One consulting company is mentioned on the quad slide, but I'm unsure of their role in the project. In terms of P&O, the rapid change in the market from plastic (expanded polystyrene) to fiber-based packaging with various additives or layers is obviously changing the characteristics of MSW. It is difficult to keep up as these new materials come online and infiltrate the market. This will be a challenge going forward, as noted by the PI. Storage is an important aspect of the feedstock quality for this type of material. I noted that this milestone was delayed. Contaminants are related to the process. Contaminants for enzymatic hydrolysis/pyrolysis/SAF may be quite different, and perhaps a table showing which contaminants affect which conversion pathways would be valuable and would help target the correct contaminant based on the conversion. Slide 9 is very informative. All the relevant information is presented clearly in one slide! MSW quality mapping shows promising results that will be very valuable for planning by local municipalities and potential MSW users. For MSW storage, do you monitor microbe populations, especially for hazardous bacteria? As far as impact, this is a well-designed project with excellent progress over the last review. The PI presented the results in a clear, concise manner. The information generated in this report will help direct the potential of MSW feedstock.
- This project appears to be well positioned to fill in many questions about handling and preprocessing of MSW. I hope that there are plans for dissemination of the information to relevant stakeholders.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive comments on this project. We believe that this project has the potential for strong impact in the waste industry and will contribute to the goal of a circular economy. The reviewers had comments on decontamination strategies and the wastes that would be generated. Our TEA/LCA does include the wastewater treatment required to mitigate those wastes and models industry standard waste treatments. Other technologies that we are considering include solvent extraction, where the solvent is recovered with very high efficiency. The hazard identified by the reviewer was not hazardous waste, but rather hazardous biological organisms that might be encountered during MSW storage. This will be important for the waste industry to understand the risks of storing MSW for longer periods of time. A DEIP has been developed for working with the Shoshone-Bannock Tribes in Idaho, and an agreement was signed with them recently. INL will work with the tribes to characterize their waste streams and give recommendations for recycling and converting their wastes into fuels and chemicals. Part of our dissemination plan for our MSW capabilities was demonstrated during a ribbon cutting event on May 24 and 25, which introduced government, academia, and industry to the upgraded capabilities of INL's BFNUF. Several demonstrations on handling, processing, and decontamination of MSW were provided to attendees. A number of contacts were made during this event, and we will follow up on these. We also plan to work with Resource Recycling Systems to disseminate our results further.

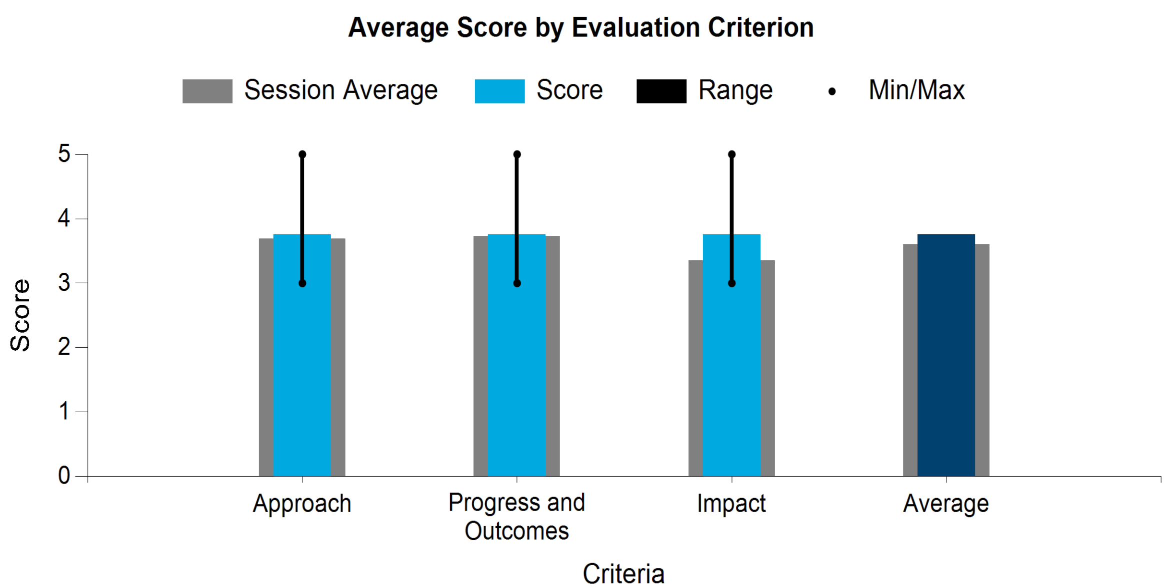
VALUE-ADDED BIOCOMPOSITE PRODUCTION USING OFF-SPEC BIOMASS FROM MECHANICAL FRACTIONATION

Oak Ridge National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.1.9
Presenter(s):	Erin Webb
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,100,000.00

Mechanical fractionation of biomass (e.g., particle size/shape/density separation by air classification) to select the portions that are easiest to handle and most convertible has emerged as a promising strategy to manage variability and reduce biofuel feedstock cost. This approach requires that the remaining biomass be sold to a separate nonfuel market to maintain economic viability. Biocomposite materials could provide such a market. In this project, we aim to better understand how typical characteristics of off-spec biofuel feedstocks—fines, high ash—impact biocomposite performance. We expect this understanding to enable the development of specific application areas for biocomposite based on the attributes of the biomass fiber and extrinsic ash particles and the thermo-mechanical properties of the resulting biocomposite. The proposed project will also identify and optimize surface treatments to improve biocomposite. Thus far, in small-scale screening tests, we have demonstrated strong performance of composites for a wide range of moisture, ash, and particle sizes, indicating broad opportunities for aligning biocomposite applications with biomass feedstock characteristics. In the coming months, we will apply the knowledge gained in small-scale testing to larger-scale printing demonstration(s).



COMMENTS

- This is a worthwhile effort to find high-value applications and markets for biomass waste that is not intended for SAF and thus to improve the overall economic returns for a biorefinery. The target chosen in the project is biocomposites with biofiber reinforcement for use in 3D printing applications. The project plan, approach, and tasks/milestones are well laid out. The team has the necessary technical expertise, skill sets, and capabilities to meet the deliverables. It is not clear what the commercialization path is and who the potential commercialization partners are.

- This is a good project and is worthy of more investment for further investigation. Collaborations among national labs, universities, and industry would help generate more impactful outcomes. Particle size and associated surface area need to be further investigated. The mixture of multiple feedstocks could be a concern in 3D printing due to their heterogeneity. A list of detailed cost components, including logistical and processing costs of multiple feedstocks, should be considered in future TEA.

- BETO investments in feedstock pretreatment are important for optimization of the use of off-spec materials, stabilization during storage, and preparation for conversion processes toward specific products such as SAFs, composite materials, or high-value chemicals. This project is developing value-added biocomposites from off-spec materials. The composites being developed are based on (1) raw off-spec biomass that is not suitable for biofuel production (e.g., corn stover fines and pine), and (2) polylactic acid. Also, 3D printing is being used to produce demonstration products from composites. Observations thus far include the following: (1) Fines from corn stover are preferrable to biomass with relatively long fibers. (2) Ash concentration can be a factor that impacts 3D printer head performance. (3) Switchgrass fiber results in desirable product stiffness. (4) The water concentration tolerance is relatively high at 5%–15%. This work will be impactful to the circular bioeconomy by developing bio-based construction and consumer products from otherwise low-value feedstocks.

- This project uses low-quality biomass from other processes for composite production in a 3D printing application. This was one of the best projects in terms of approach, outcomes, and impact. Some of the charts pasted in the presentations had fonts that were difficult to read. In terms of approach, the roles of the various members were not clear. The approach was well thought out and can be achieved. Some additional effort should be put into identifying products/markets for the material and specifying the quality required for the products. This would ensure uptake once the research proves successful. In terms of P&O, this was a nice research project. It would be nice to see a profile of the ideal properties of the material for the application(s), i.e., the range of important characteristics for 3D printing (e.g., viscosity, ash, modulus of elasticity). Some of the properties tested may not be that important (i.e., tensile strength), but a range for each property would be useful. This is an innovative and cool project! As far as impact, scale-up should be considered at this time. The project is not intended to be a demonstration project, but the next steps for larger production should be identified during this phase.

PI RESPONSE TO REVIEWER COMMENTS

- The project team would like to thank the reviewers for their encouraging and constructive comments. We appreciate the reviewers acknowledging our goals to use “off-spec” biomass (from a biofuel conversion perspective) for biomaterials to create a value-added coproduct for the biofuel value chain. While we are excited about the progress we’ve made to date, reviewers made astute and useful observations and suggestions for the remainder of our project. We agree that it is time to apply the insights we’ve gained in understanding how the properties of biomass particles impact biocomposite preparation and performance to designing large-scale systems. As noted by a reviewer, this is not a demonstration-scale project, but we can begin to consider the steps to scaling up these systems. This should include TEAs and industry engagement, as encouraged by multiple reviewers. Specifically, in the next phase of this project, we will focus on identifying and testing products and markets to better define ranges of acceptable biomass quality and evaluate potential commercialization paths. A reviewer noted challenges associated with mixtures of multiple feedstocks. We haven’t tested mixtures in our experiments so far (we’ve compared batches of different feedstocks, but not mixtures), but this is an interesting idea and one we might try if time allows. Being able to utilize feedstock mixtures, though challenging, would create a very robust coproduct pathway.

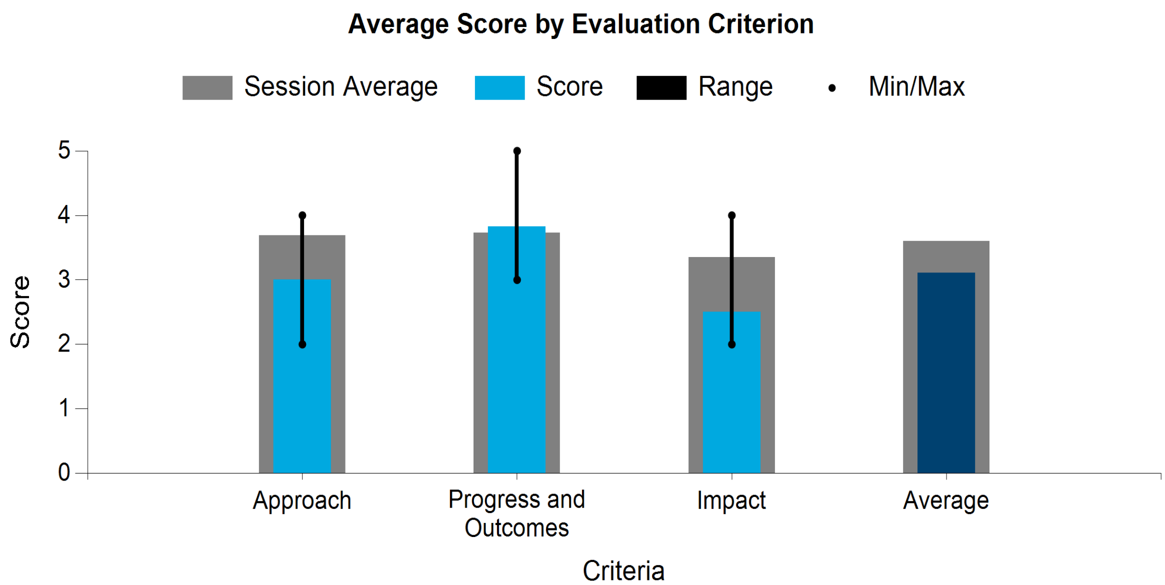
ENHANCED FEEDSTOCK CHARACTERIZATION AND MODELING TO FACILITATE OPTIMAL PREPROCESSING AND DECONSTRUCTION OF CORN STOVER

Montana State University

WBS:	1.2.2.100
Presenter(s):	David Hodge
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2023
Total Funding:	$1,625,000.00

PROJECT DESCRIPTION

This project addresses the challenge of processing compositionally and structurally heterogeneous corn stover through physical fractionation to both streamline processing and generate new potential coproducts. We developed new, field-deployable analytical tools that are coupled with empirical models that can be used to predict feedstock properties and processing performance. The overall scope of this project is to (1) identify conditions for optimal corn stover fractionation using a two-stage physical fractionation; (2) assess how physical fractionation impacts properties, partitioning of biomass, and response to processing; (3) further adapt, develop, and validate several advanced characterization tools for assessing biomass properties that can be linked to processing behavior; and (4) develop and validate predictive models based on measurements that can be performed in the field or at the biorefinery gate to predict feedstock processing behavior (preprocessing and deconstruction). The first objective will employ pre-separation processing (size reduction) of corn stover, which is next subjected to enhanced separations to yield fractions enriched or depleted in select compositional components or properties. For the second objective, fractions will be screened for their response to post-separation processing (pretreatment and enzymatic hydrolysis), and detailed characterization profiles will be developed, employing at least two techniques to assess the state of water association with the biomass (water retention value and low-field, nuclear magnetic resonance [NMR] relaxometry) and dynamic image analysis to assess distribution of particle size and morphology. For the final objective, we will utilize these tools to develop empirical models. These models will enable us to assess the relative abundance of tissue type in order to assess fractionation efficacy and predict fraction performance during pretreatment and enzymatic hydrolysis. A key impact of this project will be the development of the capability to tailor feedstock properties to the conversion process, allowing for more streamlined processing. Another important impact will be the ability to generate lignocellulose fractions enriched or depleted in select properties that could be used in other applications as coproducts. This is an important component of enabling the economics of cellulosic biofuels processes. This technology also has the potential to be employed at the regional depot scale, which addresses the critical challenge of feedstock logistics for low bulk density herbaceous feedstocks such as corn stover. Finally, this project will generate new, industry-relevant knowledge on biomass processing, providing value to industry and enabling commercialization of technologies for the conversion of biomass to biofuels and bioproducts.



COMMENTS

- The work is largely complete; however, no timeline was provided. The implementation strategy and risks were lacking. Any real and measurable impact of this work is unclear. New analytical tools are noted, but who is going to be using them, and how will they obtain them? Given what was learned, how can this benefit the process? Where are the cost savings and/or increased efficiencies?

- The team has used a robust approach to developing a variety of interesting analytical methods, but the real-world use and impact of these methods is not given adequate attention. Previous reviewers have also commented on this point. The analytical methods may indeed be very relevant industrially, and surely some more than others, but this research comes across as a random exploration of potential ways to characterize biomass. In my opinion, it probably doesn't make sense for these researchers to be responsible for developing their own techno-economic models, but their efforts might still be informed by the TEA of others. It would be useful to know which industrially relevant problems these analytical methods are aimed at solving, how big those problems are, and how much improvement they might expect.

- The project seemed to spend more time on physical processing of the feedstock and less on developing models to better predict and process feedstock to desired conditions. The project implies that it would develop technologies, but that does not seem to be the case, especially as explained in the live presentation. Extensive analyses were conducted, but there does not seem to be a cohesive overarching strategy to integrate the various analyses to reveal broader and practical findings. There is strong communication of results to the research community. The entire Montana State University and INL team (>12 people) appears to have 100% gender homogeneity.

- The objective of investigating fractionation methods was accomplished in a thorough manner. Estimating the power required (per kilogram or tonne) to accomplish this separation (power draw by fans at various speeds for biomass throughput) would have been informative. The overall use of multiple biomass analysis/characterization techniques on classified anatomic fractions helped in developing improved biomass handling and conversions of these fractions. I found the low-field NMR and fiber image analysis particularly informative. One of the primary goals is to develop analytical techniques that can distinguish the various anatomical fractions in a mixed sample. The fiber image analysis seemed to accomplish this very well. The low-field NMR data and usage seemed very promising, and how that might be converted to an online technique is worthy of exploration. I would have liked to see a PCA of the near-infrared (NIR) spectra data with loadings plots to determine the weighting factors to predicted values. Some of the prediction plots showed higher variation in prediction than one might expect. For example, in the stalk/pith weight fraction graph on Slide 22, at zero measured weight fraction, there are a great number of data points that skew widely from the predicted values from >−0.1 to 0.2. The cluster of data points around 0.18 and 0.33 measured weight fractions show similar behavior. A good PCA analysis with a vector loading plot could help narrow this. Finally, although outside of the scope of the project, how fractionation can help capture value in the conversion of biomass to products is difficult to imagine. I don't feel that fractionation results in "streamlining" the process.

- The project has demonstrated the ability to effectively fractionate corn stover using multiple stages of air classification and sieving. The project has applied multiple analytical methods to characterize corn stover fractions and predict the performance in preprocessing and enzymatic hydrolysis. Most of the tasks discussed are shown as complete, although the presentation does not discuss the number of milestones outstanding. I assume that the project is on track to be completed by September 30, 2023. It is not clear that the analytical techniques can effectively predict performance in preprocessing or handling processes. The presentation cited some laboratory work by the team but did not present any verification demonstrating commercialization potential. The presentation mentioned that the new technologies could replace current methods but did not identify the performance or cost advantages for replacing the current technologies.
- The overall approach of the project was a bit hard to follow. The team explained that they would develop/adapt technologies for corn stover fractionation and tools for characterizing the stover, but it was hard to see how all of the tasks and their results fit together. Clear evaluation criteria were provided for each milestone, but it would have been helpful if the context for the evaluation criteria were provided. TEA was suggested by previous reviews but was not implemented. Although a full TEA or LCA is not required, some evaluation of impact (e.g., referencing a publication showing that achievement of 75% yield and purity of stems would decrease costs or improve pretreatment severity by X%) would be helpful to include in the approach. In terms of progress, the team has consistently met all milestones and deliverables. They have developed reference materials from the fractions, which can be used to develop standards for measurement. The team provided many examples of data and innovative and interesting measurement methods. In terms of impact, the team has published three papers and has three that are in development or have been submitted. They have also presented results at 10 national conferences. The overall impact of the work was difficult to determine, and although this may be due to its fundamental nature, some assessment of the significance of any of the results would be helpful. Understanding and communicating the potential impact of this work is critical so that it does not appear to be disconnected experiments rather than a well-thought-out project with the potential for improving biomass handling and conversion.

PI RESPONSE TO REVIEWER COMMENTS

- Comment: The team has used a robust approach to developing a variety of interesting analytical methods, but the real-world use and impact of these methods is not given adequate attention. Previous reviewers have also commented on this point. The analytical methods may indeed be very relevant industrially, and surely some more than others, but this research comes across as a random exploration of potential ways to characterize biomass. In my opinion, it probably doesn't make sense for these researchers to be responsible for developing their own techno-economic models, but their efforts might still be informed by the TEA of others. It would be useful to know which industrially relevant problems these analytical methods are aimed at solving, how big those problems are, and how much improvement they might expect.

- Response: We are planning on working with the analysis team at INL to perform TEA on select fractionation scenarios during the remainder of the project.
- Comment: The project seemed to spend more time on physical processing of the feedstock and less on developing models to better predict and process feedstock to desired conditions. The project implies that it would develop technologies, but that does not seem to be the case, especially as explained in the live presentation.
- Response: Due to the limitations of the BETO Peer Review presentation format, we could not present in detail all the work performed for this project. The presentation focused on demonstrating how we achieved project milestones, but the current and pending publications provide significantly more detail on both the models developed and the fractionation performance at the pilot scale.
- Comment: The objective of investigating fractionation methods was accomplished in a thorough manner. Estimating the power required (per kilogram or tonne) to accomplish this separation (power draw by fans at various speeds for biomass throughput) would have been informative. The overall use of multiple biomass analysis/characterization techniques on classified anatomic fractions helped in developing improved biomass handling and conversions of these fractions. I found the low-field NMR and fiber image analysis particularly informative. One of the primary goals is to develop analytical techniques that can distinguish the various anatomical fractions in a mixed sample. The fiber image analysis seemed to accomplish this very well. The low-field NMR data and usage seemed very promising, and how that might be converted to an online technique is worthy of exploration. I would have liked to see a PCA of the NIR spectra data with loadings plots to determine the weighting factors to predicted values.
- Response: Due to the space and time constraints of the Peer Review format, we did not present the loading plots for the PCA work. These are in our publication: https://doi.org/10.3389/fenrg.2022.836690.
- Comment: The overall approach of the project was a bit hard to follow. The team explained that they would develop/adapt technologies for corn stover fractionation and tools for characterizing the stover, but it was hard to see how all of the tasks and their results fit together. Clear evaluation criteria were provided for each milestone, but it would have been helpful if the context for the evaluation criteria were provided. TEA was suggested by previous reviews but was not implemented. Although a full TEA or LCA is not required, some evaluation of impact (e.g., referencing a publication showing that achievement of 75% yield and purity of stems would decrease costs or improve pretreatment severity by X%) would be helpful to include in the approach. In terms of progress, the team has consistently met all milestones and deliverables. They have developed reference materials from the fractions, which can be used to develop standards for measurement. The team provided many examples of data and innovative and interesting measurement methods. In terms of impact, the team has published three papers and has three that are in development or have been submitted. They have also presented results at 10 national conferences.
- Response: All the previous DOE BETO projects I've been involved with have had an LCA and/or TEA component. However, this was not required for this FOA and, consequently, we did not budget personnel time to do this work. During the no-cost extension for this project, we will commit to performing a TEA comparison of several fractionation approaches performed in this work.
- Comment: The overall impact of the work was difficult to determine, and although this may be due to its fundamental nature, some assessment of the significance of any of the results would be helpful. Understanding and communicating the potential impact of this work is critical so that it does not appear to be disconnected experiments rather than a well-thought-out project with the potential for improving biomass handling and conversion.

- Response: The major contributions were (1) development of new characterization tools to predict anatomical fraction abundance (NIR and image analysis models) and physics-based air classification performance validated with experimental data, and (2) identification of fractionation strategies to yield target separations for ash removal, cob separation, stem separation, and pith/rind separation.

SWIFT: SINGLE-PASS, WEATHER INDEPENDENT FRACTIONATION TECHNOLOGY FOR IMPROVED PROPERTY CONTROL OF CORN STOVER FEEDSTOCK

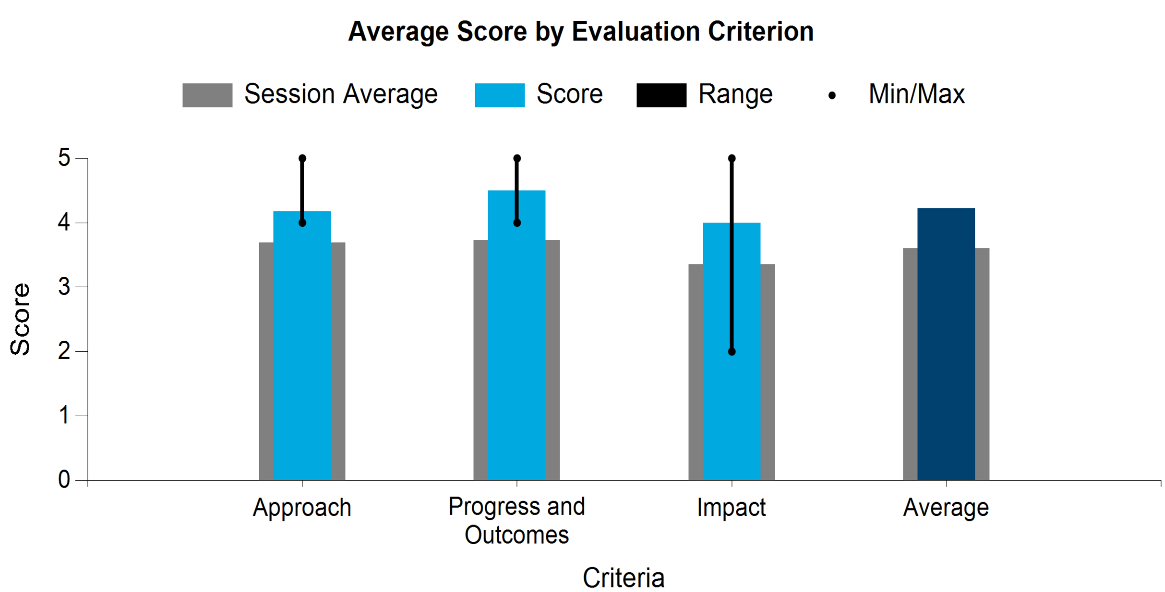
University Of Wisconsin

PROJECT DESCRIPTION

WBS:	1.2.2.101
Presenter(s):	Kevin Shinners
Project Start Date:	10/01/2019
Planned Project End Date:	06/30/2023
Total Funding:	$1,565,400.00

Corn stover is an abundant source of biomass that can be utilized for bioenergy production. It represents 70% of the available crop residues in the United States. However, recent projections estimate that over 60% of corn stover will be collected at moisture levels that exceed 20%. This is incompatible with conventional baled logistics systems due to unwanted microbial degradation. For the 40% of the stover that could be utilized with current technology, multiple other technical challenges exist. The result is a persistent inability to produce a reliable feedstock. Consequently, there are no real existing markets into which this potentially valuable cellulosic material can enter.

To solve this biomass challenge, we propose a paradigm-shifting technology: Single-Pass, Weather Independent Fractionation Technology (SWIFT). SWIFT streamlines collection by eliminating multiple time-consuming, costly, non-value-added, field- and weather-dependent steps that comprise the current technology in corn stover harvest. The novel approach employs four basic operations: whole-plant harvest, distributed anaerobic storage, cotransport of grain and stover, and fractionation at the biorefinery. SWIFT allows unprecedented control of the physical and chemical characteristics of corn stover biomass, enabling a reliable commodity market for corn stover.



COMMENTS

- The harvesting piece of this project is the most valuable and appears to provide a cost benefit. The TEA was provided but stopped at the feedstock collection. The TEA should be expanded to cover the other aspects of the project to provide real insights into any benefits to storage techniques and pretreatment costs (e.g., if washing is needed due to lactic acid buildup over time, this is likely not economical and also not ideal from an LCA standpoint). More work needs to be done from this aspect. Additionally, if the mechanical fractionation process is necessary to separate husks and stalks, this is an additional process cost. The management plan and risk identification were not included in the presentation. The work is mostly complete, but no timeline was provided.

- The researchers clearly identified and articulated challenges associated with the present state of corn stover harvest and storage systems. In developing SWIFT, they leveraged both scientific methodology and practical field experience/experimentation. They also published a strong paper examining the economics of the SWIFT process relative to the state of the art. The presentation could have spent more time on the TEA, however. The published paper has many interesting and important graphs showing the impact of process parameters on cost. A good sequence for the presentation (and R&D in general) might be: (1) start with a TEA of the current state of the art, (2) examine graphs of how various process parameters affect costs, (3) explain why and how particular process parameters were targeted for R&D, and (4) show how R&D efforts have improved those parameters and the impact on cost. Separately, the team's current TEA does not take into consideration the downstream impact of SWIFT-processed corn being slightly fermented. To provide a more equivalent comparison to the current SOT, they should add this to the TEA.

- This is an excellent real-world project that also addresses three significant feedstock challenges—transportation, handling, and cost. The principal lead has strong industry connections that offer future synergistic opportunities for the project. The project had the excellent outcome of achieving a better cost benefit than the current SOT by using a single pass rather than the current bale system. Unlike most of the other projects, this project is dealing with in-the-field applications and tiering the project focus to a total feedstock cost. Adjustments of different harvesting/processing equipment, especially when harvesting the grain and stover together without soil contamination, is highly beneficial to industry. The presentation mentions students trained, but no other DEI efforts. However, striving to reduce costs is an equalizing factor for farmers.

- The modified silage-style collection, transport, and storage of corn stover, cobs, and kernels developed and demonstrated here shows an alternative approach to the typical collection of corn kernels and stover in a separate manner. It has the potential to reduce the collection/transportation and storage costs, and the mechanics have been well demonstrated. I don't need to be convinced that the storage of stover in bales is at the very least problematic—large fires at all of the pioneer cellulosic ethanol plant storage yards as well as bale degradation demonstrate this. However, given that no current facility takes both the stover and the kernels, I wonder if this is a viable business approach. The fractionation methods and developed device show it is viable (facile?) to separate the kernels and the various anatomic fractions of the stover. However, the kernel gains moisture during storage. This may affect the value of the kernel, which is the primary economic driver for the farmer. The presenter stated that combining the leaves and stalk reduces severity, and that processing separately reduces pretreatment severity by 30% on 40% of the biomass. As one can't possibly afford to reject 60% of the biomass, it is hard to imagine how savings could be realized from this approach. Processing different fractions in separate campaigns is complicated and costly. Multiple processing trains would require a great deal of capital expenditure (CapEx). Finally, managing multiple streams in a plant is logistically very difficult. The SWIFT approach would be very valuable if combined kernel/stover processing could be envisioned, but I am not aware of such a plant. Past studies have shown that a certain percentage of stover must be left on the field from year to year. If the fractionation method used in SWIFT (which looks portable) could be used to collect/transport and store only the more valuable fractions and leave the most recalcitrant fractions in the field, this method would be a real success.

- The project has modified a combine harvester to harvest the grain and stover simultaneously and store it under anaerobic conditions. The project has demonstrated more consistent control of the physical properties of the stover and improved TEA compared to conventional harvest methods. The team has made excellent progress but did not include a milestone table or a Gantt chart, so it is not possible to determine whether the accomplishments were achieved on schedule. To verify the commercialization potential, the team needs an industrial partner committed to manufacturing the modified harvester. Industry partners should be engaged to verify the reduction in pretreatment costs and ash material in a biorefinery.

- The approach is well thought out and attempts to address the issues of minimizing feedstock variability and improving the cost-effectiveness of harvesting by developing single-pass harvest technologies with anaerobic digestion and simple processing at industry-relevant scales. The approach developed for the harvesting technology was especially intriguing. Implementation of the approach appears to be on schedule and achieving the expected results. It is not clear whether or how the measurement of physical properties will be used to improve any of the stages of the technology and/or downstream processing. This effort seemed to be disconnected from the rest of the project, even though it appears that this is a central tenet of the FOA (Area of Interest 2A: Relating Biomass Physical and Chemical Characteristics to Feedstock Performance in Handling and Conversion Operations). Collaboration with industry was not addressed in the presentation. The team has made great progress and has met the BETO goals of developing a feedstock technology with a cost of <$70 per dry ton (2016 dollars).

PI RESPONSE TO REVIEWER COMMENTS

- The reviewers recognized SWIFT's potential to improve the cost efficiency and practicality of corn stover biomass harvesting and storage. Appreciating its real-world applicability, they noted that the technology simplifies the process by allowing the simultaneous harvest of grain and stover, mitigating transportation, handling, and cost challenges. They also highlighted the SWIFT project's unique approach to storage and its potential to reduce feedstock loss and risk of fire. The reviewers found promise in the use of fractionation methods to separate kernels and stover anatomical fractions while expressing concerns about logistical feasibility. They recognized the SWIFT process' weather-independent nature and utility for reducing ash contamination for their potential to significantly impact commercial viability. Lastly, the reviewers saw the TEA demonstrated by the project as indicative of possible reductions in pretreatment costs in a biorefinery setting. However, the reviewers also identified areas for improvement, including the need for more comprehensive TEA, stronger DEI efforts, verification of results and commercialization potential, and exploration of the downstream impacts of SWIFT-processed corn fermentation. We agree about the need to expand the TEA beyond the feedstock collection phase to provide more insight into the potential benefits from SWIFT. We are working on a more comprehensive TEA for our final project report (Task 10). This analysis will be expanded to cover additional processes, such as fractionation, washing, pretreatment, and hydrolysis of the feedstock. The primary reason for this staged approach was to first determine the extent of the reduction in pretreatment severity that could be attained by adopting a fractional approach through Task 3 that would offset those costs. Regarding the team's DEI efforts, the reviewer's comment on our work's potential equalizing effect for farmers by striving to reduce costs is well taken. We see this as a critical aspect of our mission and will continue to focus on it in our ongoing and future projects. Additionally, we want to highlight that a female graduate student has been trained on this project. Given the underrepresentation of women in the machinery systems specialization of biological systems engineering, we believe this is significant. Moreover, the current student on the project is a first-generation college student. We will continue to foster a diverse and inclusive environment in our future work, as we understand its crucial role in fostering innovation and ensuring the broad applicability of our research. The concern about the viability of a business approach where no current facility accepts stover and kernels is valid. This project demonstrates a potential shift in industry practice, which is warranted given the current SOT limitations and the benefits demonstrated in our field to biorefinery gate TEA. We understand that the logistics of managing multiple streams and the associated costs are significant considerations. With this in mind, our final TEA (Task 10) will compare two scenarios: one where the two stover fractions (cob and leaf, stalk, and husk) are run in separate campaigns through the same processing equipment, and another where they are processed in parallel. This comparative analysis will clarify our approach's potential cost savings and practicality. Concerning commercialization, industry engagement, and third-party verification: We are working with John Deere as an industry partner on the machinery aspects of the project. John Deere has contributed significantly to the cost share in this project, donating capital equipment and engineering support. The Deere team has attended regular meetings and has visited the field site to optimize the equipment. Given our anatomical groupings and pretreatment severity, we also planned to work with POET on hydrolysis yields. However, due to a change in their company's focus during our project, we had to seek alternate external validation for our pretreatment and hydrolysis yields elsewhere. To that end, we have engaged with the Sustainable Bioprocessing and Bioproducts Lab at the State University of New York College of Environmental Science and Forestry. Finally, regarding the grain feedstock, we have presented data in our quarterly reports that will also be part of our final technical summary demonstrating the grain's utility for fermentation to ethanol. Further, there is a significant body of knowledge on using fermented grain, commonly called high-moisture corn, for livestock feed. We recognize that this limits the marketability of the grain fraction, but there are documented benefits in starch availability in ruminant nutrition. Additionally, we have a manuscript in preparation that documents reduced grinding energy of fermented corn kernels. However, after washing the former, our ethanol yields were similar between fermented and unfermented grain. Additionally, our team just published a paper on the physical properties of the grain fraction that will be useful for those handling and processing grain derived from the SWIFT process. We thank the review panel for their time and thoughtful review of our project and the SWIFT process. We hope our responses address your concerns and reassure you of our commitment to delivering a comprehensive and impactful project.

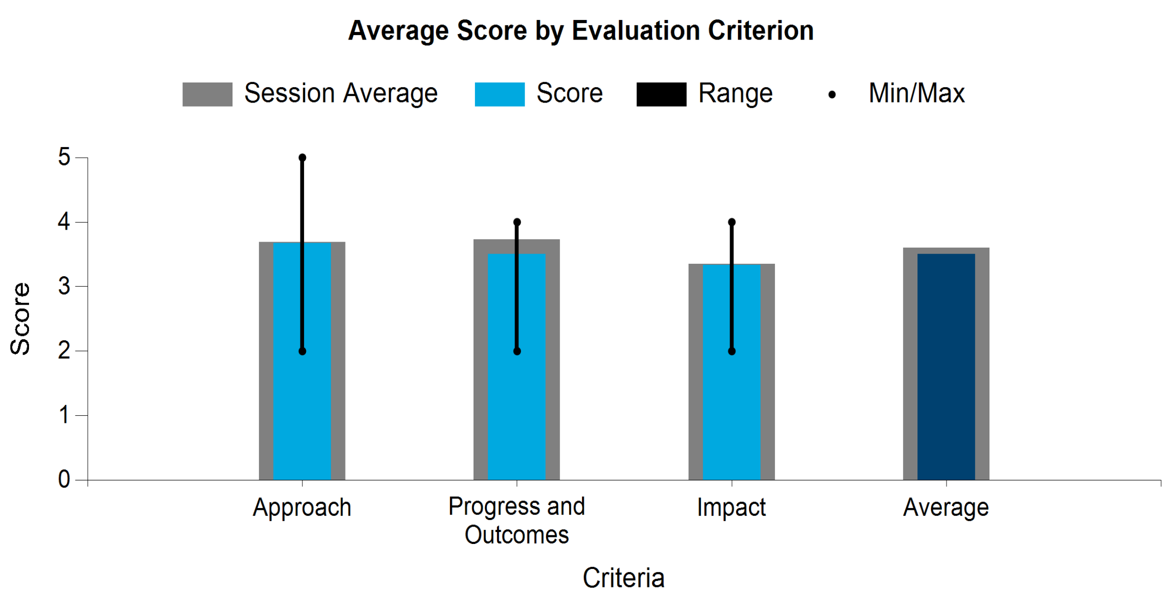
SULFUR PROFILING IN PINE RESIDUES AND ITS IMPACT ON THERMOCHEMICAL CONVERSION

University of Kentucky

WBS:	1.2.2.102
Presenter(s):	Jian Shi
Project Start Date:	10/01/2019
Planned Project End Date:	01/31/2025
Total Funding:	$2,056,352.00

PROJECT DESCRIPTION

Sulfur content varies widely depending on the biomass type, growth conditions (e.g., soil, weather, and age), and harvesting practices. It represents an important concern to thermochemical conversion platforms due to its effects of catalyst deactivation (e.g., in the Fischer-Tropsch reaction), equipment wear, and air pollution. Results from surveying 18 pine residue samples (including 87 fractions) suggest that precommercial thinning and logging residues collected near the coastal regions appear to have higher sulfur-containing fractions than samples from piedmont and sandhill regions. Air classification and bioleaching were shown to be effective in removing sulfur-/ash-rich fractions and producing a cleaner and more consistent feedstock for thermochemical conversions such as fast pyrolysis and gasification. Preliminary TEAs suggest a 5%–10% reduction of the MFSP with the implementation of low-cost sulfur mitigation/preprocessing strategies such as air classification in a biorefinery. An LCA was also performed to evaluate the global warming potential of the conversion processes. This study provides a better understanding of sulfur variability and the form and fate of sulfur during thermochemical conversion, facilitating the development of effective feedstock preprocessing and sulfur mitigation strategies.



COMMENTS

- The timeline provided was extremely high level. No risks or mitigations were provided. There appeared to be several partners on the project, but how they worked together was not addressed. It's unclear why the PI chose to exclude the leaching data, as this would have been valuable information to present. Other areas of the presentation could/should have been reduced to allow for inclusion of this information. The assumptions made in the TEA for this piece were also unclear. It was nice to see even a high-level TEA and LCA.

- The researchers have taken a methodical approach to developing technology and data around sulfur profiling and have effectively made a case for its industrial relevance through TEA. It is excellent that they are leveraging tools like tornado diagrams and sensitivity analyses to understand the key factors. In this case, it seems that the TEA is actually independent of the R&D work. As such, it could have been performed prior to the R&D work, and then used to evaluate the potential impact of the work and to direct research efforts to target the highest-impact parameters. As mentioned above, the researchers made good choices for the sensitivity analyses. Tornado diagrams, however, are far more valuable if actual best/expected/worst case scenarios are used, rather than simple percentage deviations. Also, it would have been useful to see more process parameters in the tornado diagram, like the sulfur content of biomass. It is unclear how the tornado diagram, as shown, would be used to inform decision-making in this R&D effort.

- Comprehensive analyses, testing, and diverse subtasks are used to assess sulfur content and the impact on conversion to biofuel. One of the market benefits is the cost/benefit analysis of the sulfur reduced feedstock versus the status quo, especially on the projected fuel cost. The capital cost analysis and minimum fuel selling baseline on Slide 19 are very informative and daylight a comprehensive assessment of the costs of various processes associated with sulfur reduction. Strong collaboration with industry, which delivered the feedstock samples, and diverse partnering are attractive attributes of this project. The project funded several underrepresented graduate students, which demonstrates an effort toward DEI.

- The work that was done (18 pine residue samples/87 anatomical fractions) is extensive and thorough. However, as the authors point out, the impact of the sulfur and the various forms of sulfur on the downstream catalysts "is not well understood." As this appears to be the driving force for the work, it would seem that this aspect (the effect of sulfur species on the catalyst) could be studied by just doping various sulfur species into the pyrolysis stream and measuring the effect so that the levels and species to avoid/eliminate could readily be focused on. From the work that has been done, it appears that the needle fraction is relatively small on a mass basis, and it seems that one would be better off rejecting this fraction. Finally, the driving force of this work is somewhat muted, as the catalyst industry has well-developed methods of handling sulfur in an economic manner.

- The project has identified the source of sulfur in several pine samples from different locations in the Southeast United States. They have examined two methods for reducing the sulfur content of the feedstock prior to entering the thermoconversion process: bioleaching and air classification. Higher sulfur fractions from air classification can then be discarded or sent to a bleaching step. Needle-rich fractions had the highest sulfur concentration. They are showing a 5% reduction in MFSP from a 30% reduction in sulfur. Slide 20 demonstrates the potential sources of sulfur impact but does not clearly discuss how this will be accomplished. For example, does this model include the increased cost of biomass from bioleaching or discarding a fraction(s) for the biomass? The project has not determined how sulfur is released during the thermochemical processes (Objective 3) or the impact of sulfur on the Fischer-Tropsch catalyst of choice. Without a milestone table or a Gantt chart, it is difficult to determine if the project is on schedule for meeting its project goal or end-of-project milestones.

- The team outlined an approach that outlined the issues with sulfur in biomass and identified a systematic series of interconnected tasks that addressed each. The team has several partners, and the approach does a good job of integrating each. The team did an excellent job of framing the problem they are addressing. The team clearly identified the methods to obtain representative and homogenous samples, which is critical to ensure a basis for comparison. DEI was adequately addressed in the presentation, and the project has included Red Rock Biofuels as a project partner as well as other industry advisors. In terms of progress, the team provided results and trends from their experiments in sulfur composition by anatomical fraction and correlation with other components, as well as the results of air classification to concentrate or remove the sulfur. It was difficult to determine whether the project was on target, as the results were not tied to specific milestones. In terms of impact, the team outlined the framework for TEA/LCA analyses and conducted preliminary analyses. The team did a nice job identifying which steps had the highest impact for global warming potential (GWP) and economics and providing boundaries for expected improvements. The tornado sensitivity study varied important factors by ±20% from baseline, including operating hours from a baseline of 8,000 hours. An increase of 20% in the operating hours would mean that the plant would operate for 9,600 hours, which is more than 8,760 hours per year. This is not possible unless the equipment can be pushed past its rated capacity. Because this was identified as the most important factor in reducing costs, it should be noted that not only do operating hours need to increase, but the equipment capacity would also need to increase. The economic sensitivity shows that the amine solution demand goes down with an increase in sulfur reduction. This is not intuitive and should have been explained; the presenter could not explain this. Assessing the impact would be strengthened by including some assessments of which technologies/pathways are currently hampered by high sulfur contents and how solving this would have an impact in the overall commercialization of biofuels. This is not critical, but it would help provide context. The team has made several presentations and an ArcGIS story map, and one manuscript has been submitted.

PI RESPONSE TO REVIEWER COMMENTS

- The project is currently in Budget Period 3. During the Peer Review meeting, we presented the progress from Budget Period 2 (12 months into the project). The Budget Period 2 go/no-go decision points are to (1) collect 15–20 pine residue samples and statistically analyze their sulfur content and anatomical fractions for significant differences using ANOVA; and (2) complete baseline TEA and demonstrate a 5% reduction of the minimum selling price of biofuels assuming an interim sulfur removal goal (30%) and associated ash removal goal are achieved. Both criteria have been met. Due to time constraints, we did not present data from the bioleaching test. However, we screened three candidate microorganisms and demonstrated Aspergillus niger NRRL 2001 as the most effective sulfur and metal element remover, with a maximum sulfur removal of 30% from certain pine residue samples. We have presented the research outcomes at professional conferences and recently published them in a reputable peer-reviewed journal. We have developed a vigorous risk management plan that allows continuous identification and logging of risks, development of mitigation strategies, and monitoring of risk resolution. The specific risks that we identified in Budget Period 2 include (1) lab safety issues associated with sulfurous gases; (2) not enough (or representative) pine residue samples collected from proposed suppliers; and (3) the uncertainty of techno-economic factors associated with the sulfur removal technologies being developed. We have taken actions to mitigate those potential risks. We have implemented standard operation protocols and lab safety measures for sulfur gases. The team identified four pine residue suppliers/sources and collected 18 pine residue samples and 87 anatomical fractions in total. The collected samples cover various ages, locations, harvesting practices, species/genetics, and anatomical fraction factors. As a major change to the initial statement of project objectives (SOPO), we added Task 3 into Budget Period 2 to build a baseline TEA model on biomass preprocessing and syngas sulfur removal operations. This allows us to identify uncertainty and risks associated with system integration and cost factors early on during the project. Regarding the reviewers' comments on TEA, we conducted initial sensitivity analysis during Budget Period 2 to help guide project efforts. Prior to the experimental data becoming available, it was not clear what the best- and worst-case scenarios would be for all parameters. For some parameters, best- and worst-case values can only be determined from an actual commercial project. Thus, we followed common TEA practices to select parameters based on literature values or assumptions to identify the most important factors. These parameters and parameter ranges will be updated to reflect an improved understanding gathered from the project. The model includes additional capital and operating costs associated with bioleaching and discarding fractions of biomass. Bioleaching and its associated equipment add $5.9 million in pretreatment capital costs and an increase in operating costs. However, an increase in the fraction sent to bioleaching slightly decreases biofuel costs. This indicates that the costs of reducing the sulfur content are less than the additional revenue generated. Increasing the fraction of biomass sent to the boiler increases the MFSP. Because bioleaching can increase the biomass fraction lost to the boiler, there is a trade-off to consider in this approach. The initial sensitivity analysis employs ±20% ranges to provide guidance on which parameters to focus on during the project. The ranges will be updated based on project findings with more realistic values. The amine solution demand is proportional to the hydrogen sulfide concentration in syngas. Increasing sulfur reduction decreases the hydrogen sulfide syngas concentration and amine solution demand. Sulfur is a well-known contaminant for Fischer-Tropsch synthesis (FTS) catalysts, so this technology has the potential to improve the reliability of biofuel production from sulfur-containing feedstock. Regarding the reviewers' comments on sulfur poisoning on FTS catalysis, during Budget Period 1, we showed, from pyrolysis-gas chromatography analysis of pine residues, that hydrogen sulfide and carbonyl sulfide are the dominant sulfur species present in the effluent. However, their impact on cobalt catalysts for syngas conversion during FTS must be tested individually to assess catalyst stability with respect to those sulfur species. Our preliminary investigation of carbonyl sulfide poisoning (500 parts per billion) on a manganese-modified cobalt Fischer-Tropsch catalyst suggests that adding manganese to the cobalt catalyst not only helps control the production of methane, but also improves both olefin and C5+ selectivity compared to an unmodified cobalt catalyst. The beneficial effect of manganese on catalyst tolerance toward carbonyl sulfide needs further investigation, given that the manganese-modified catalyst undergoes slower deactivation than the unmodified cobalt catalyst at low temperature (220°), while at higher temperature (230°), both catalysts exhibit similar deactivation rates. Finally, the project is engaged in ongoing pyrolysis-gas chromatography analysis of preprocessed pine residues, the results of which will guide us regarding exactly what types and concentrations of sulfur species should be tested in syngas conversion to determine catalyst activity, stability, and selectivity toward various FTS products.

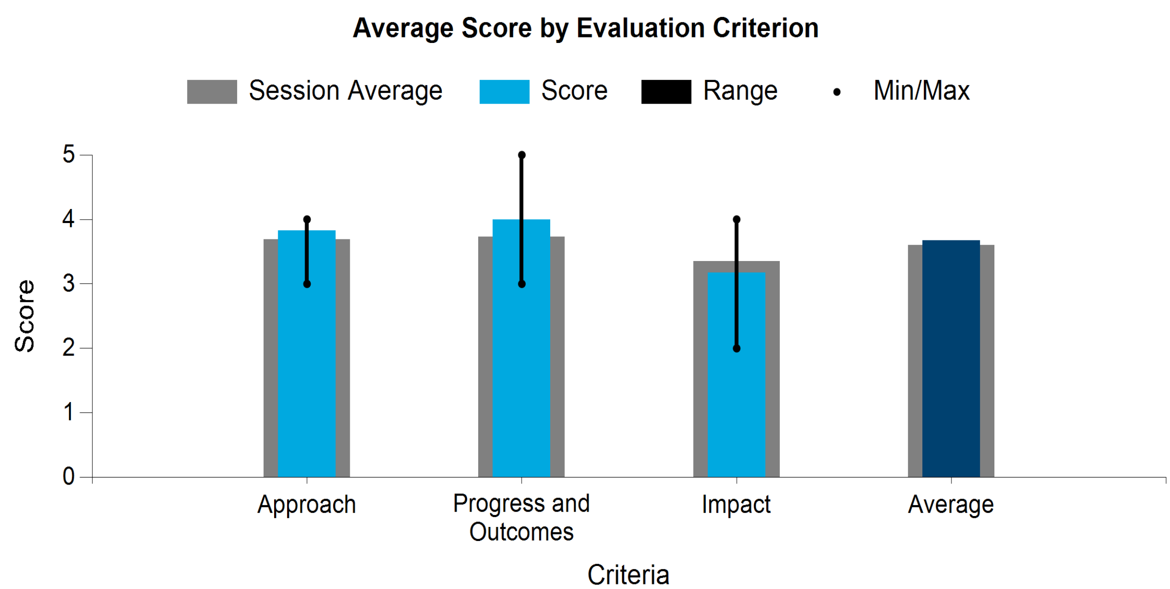
MODELING FEEDSTOCK PERFORMANCE AND CONVERSION OPERATIONS

Purdue University

PROJECT DESCRIPTION

WBS:	1.2.2.103
Presenter(s):	Michael Ladisch
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2023
Total Funding:	$1,724,750.00

Significant progress has been made in developing combined enzyme hydrolysis and fermentation technologies for transforming lignocellulosic feedstocks into ethanol and other bioproducts. Various routes described in the literature show that low-carbon-footprint processes efficiently convert the cellulose and hemicellulose fractions of pretreated corn stover, wood chips, and sugarcane bagasse to sugars and to ethanol. Combinations of different pretreatments at high or low pH or in liquid hot water, followed by enzyme hydrolysis and fermentation or direct conversion of cellulose to ethanol (i.e., by consolidated bioprocessing), have been demonstrated. These successes have brought the need to prepare the feedstock—before it enters the biorefinery—into focus. This report addresses developments in liquefying corn stover before pretreatment so that slurries with yield stresses below 200 pascals are obtained and a "pumpable" corn stover slurry is obtained for initial solids loadings of 200–300 g/L. Results to date address modeling of conditions and the experimental determination and validation of parameters that lead to formation of aqueous slurries at high solids loadings, and corn stover that has been fractionated by air classification.



COMMENTS

- The overall approach is sound and well laid out, though it was missing risks. Understanding the overall impact of the preprocessing on the economics, particularly the hydrolysis step, will be important in assessing the industrial viability of the process.

- The researchers made progress toward characterizing and improving the properties of biomass feedstock slurries. While they are probably correct that corn stover will be easier to handle as a slurry than as a solid, they did not quantify the potential benefit as well as they could have. The researchers are using TEA retrospectively to see “how well they did.” It would have been better if they had built a techno-economic model at the beginning. Then, they would have been able to use it to understand the key factors driving the economics of their envisioned process and focus their R&D to address them. The researchers might also consider using Microsoft Excel instead of Aspen for modeling this process. The accessibility, transparency, and flexibility of Excel tend to make it a better option for modeling early-stage technologies that do not require the advanced capabilities of process simulation.

- Producing a slurry is a strong opportunity to facilitate feedstock compatibility for higher-value end products. This project adequately assesses the feedstock characteristics associated with generating a slurry, but fails to forecast the next steps needed to generate practical opportunities for industry in real-world applications. The project implied that costs were to be explored, but it ultimately did not quantify real-world costs. The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model analysis seems out of scope in relative importance but might have been required. The project leads conducted stakeholder meetings despite the pandemic to communicate results. Based on the written presentation, the project appears to be delayed in meeting some objectives on the designated timeline.

- This project has made good progress in investigating the separation of four anatomical components of corn stover (cob/stalk/husk/leaf) by air fractionation. It is of particular note that the comminution energy of the various fractions was measured and recorded, with cob apparently having the highest specific energy. Note that the final ground size was very small (2 millimeters), which appears to be smaller than needed for commercial applications. It was implied that pelletization was done on the separated anatomic fractions, but no data were presented on the pelletization process of the various fractions. The authors are in the process of performing an LCA/TEA on the method of preprocessing a corn stover stream from pelletized materials for introduction into a pretreatment section. It is noted that water absorption of feedstock is a “key indicator” for ready slurry formation—further elaboration on this observation is desired. A TEA/LCA on pelletization is desirable, and it is unclear if this is part of the planned LCA/TEA. The authors claim that using enzyme-treated slurries can avoid the solid handling challenges experienced in pioneer biorefineries. These challenges were encountered when trying to add materials into processes at elevated pressures. The presentation didn’t mention the pressures they were attempting to pump against and thus didn’t clearly demonstrate overcoming this hurdle. Finally, there is currently no supply chain laid out in which pelletization of corn stover would/could be broadly accomplished. This limits the clear commercialization potential of the discoveries presented.

- This project focuses on creating an aqueous slurry with a high loading of corn stover fractions that can be pumped into a biorefinery instead of conveying solid, dry material to the pretreatment step of the biorefinery. The team has been able to demonstrate high solids loading using pellets created using different corn stover fractions. They have created rheological models of a highly solids-loaded slurry and verified the models experimentally. They have completed a preliminary TEA/LCA. The project is on schedule, as demonstrated by the Table of Tasks from the SOPO as well as the timeline/Gantt chart. They have involved partners from national labs and industry. The presentation indicates that corn stover must be pelletized in order to create a high-solids slurry. The pelletizing process should be included in both the TEA and LCA calculations. The benefits of pumping a high-solids slurry versus solids conveyance should be verified in a pilot or demonstration biorefinery. Without this experimental comparison, it will not be possible to determine commercialization potential or verify the TEA. The team should identify a partner with a pilot or demonstration-scale biorefinery.

- In terms of approach, the team did a good job of framing the magnitude of the biomass solids handling issue and how their approach for tackling it would look. The team developed a nice approach to assessing biomass and feedstock characteristics and the impacts of bioprocessing. The diagrams showing the processing steps as well as how they integrate with laboratory project partners was especially helpful. The integration of the industrial partners, Forest Concepts and AdvanceBio Systems LLC, was not clear, and I could not determine how they were providing input. The team has made excellent progress in meeting project milestones, and the presentation outlined this well. As far as impact, the team has published numerous articles on their work and has included their data in the Materials Property Database. The validated shear stress model will be extremely helpful for the bioprocessing industries. The summary of the overall impact of the project could have been stronger if the team had provided preliminary estimates of the GWP, cost reductions from the impact of slurry formation, or other achievements, and/or framed this in terms of the wider biofuels processing industry.

PI RESPONSE TO REVIEWER COMMENTS

- Comment: They did not quantify the potential benefit as well as they could have.
- Response: The reviewer is correct that the potential (and actual) benefits need to be further defined, although the major effect shown in Slide 4 (of the Peer Review presentation) clearly shows the impact (increase in productivity by a factor of >3). We plan to continue this work to address these and other questions, although they are not part of the approved SOPO and the budget allotted.
- Comment: The researchers might also consider using Microsoft Excel instead of Aspen for modeling this process.
- Response: Indeed, we are considering Microsoft Excel as well as Aspen. Excel tracks material balance, and the material type or behavior is irrelevant. Excel does not depend on software versions for use and is more user friendly. Aspen dynamically updates and propagates changes downstream and is designed to handle processes at scale. Costs are tracked and updated as changes are made. However, Aspen is not easily updated as software versions change, and does not easily handle biomass (cellulosic materials). Forecasting of next steps was not part of this project's SOPO. It is important, and will be pursued.
- Comment: This project fails to forecast the next steps needed to generate practical opportunities for industry in real-world applications.
- Response: This is a work in progress. A key is also to test concepts at pilot scale in an operating biorefinery or a test facility, based on selected corn stover fractions, fermentation of the resulting slurries, and estimates of the costs and potential cost benefits.
- Comment: It is noted that water absorption of feedstock is a "key indicator" for ready slurry formation—further elaboration on this observation is desired.
- Response: We agree and will continue to work on this.
- Comment: The presentation didn't mention the pressures they were attempting to pump against and thus didn't clearly demonstrate overcoming this hurdle.
- Response: This is addressed by yield stress criteria. This project measured and developed predictive models, validated with data, of the slurry rheology, which in turn define "pumpability" or the ability to mix slurry in terms of shear stress as a function of shear rate, as well as yield stress (determines energy needed to initiate mixing). The overall impacts were presented in Slide 21, although the yield stress curve was not discussed in detail. We agree that the benefits of pumping should be vetted, and this will likely be part of future proposals if the FOA addresses this topic. The current scope of work (and resources) does not include pumping tests.

- Comment: The pelletizing process should be included in both the TEA and LCA calculations. The benefits of pumping a high-solids slurry versus solids conveyance should be verified in a pilot or demonstration biorefinery.
- Response: The TEA for the pelleting process was determined previously and is not part of the scope of this work. This is available from INL and was addressed at Argonne National Laboratory, with results being reported by INL. The effect of pelleting on overall LCA is small.
- Comment: The integration of the industrial partners, Forest Concepts and AdvanceBio Systems LLC, was not clear, and I could not determine how they were providing input.
- Response: The roles of Forest Concepts (feedstock acquisition and crumbling) and AdvanceBio (reactor design for introducing feed into process) were addressed in graphics in Slides 7, 14, and 19.
- Comment: The summary of the overall impact of the project could have been stronger if the team had provided preliminary estimates of the GWP, cost reductions from the impact of slurry formation, or other achievements, and/or framed this in terms of the wider biofuels processing industry.
- Response: The reviewer is correct. Nonetheless, the SOPO/resources did not extend to the overall biorefinery, although impact is given in Slides 4 and 19. We thank the reviewer for an excellent suggestion for future work.

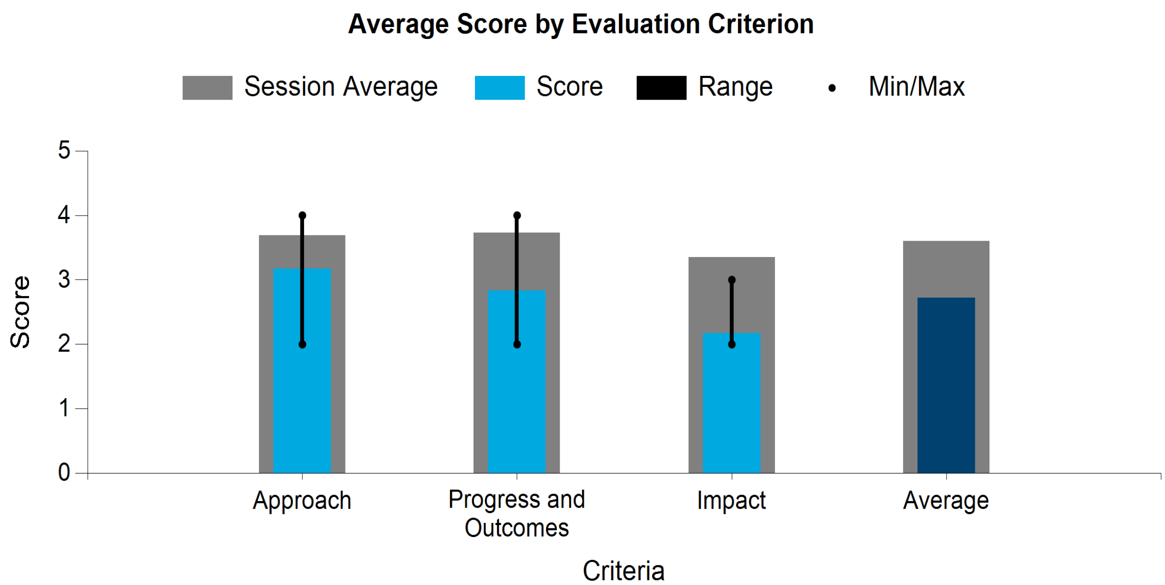
MACHINE LEARNING BASED MODELING FRAMEWORK TO RELATE BIOMASS TISSUE PROPERTIES WITH HANDLING AND CONVERSION PERFORMANCES

University of Georgia Research Foundation Inc.

PROJECT DESCRIPTION

WBS:	1.2.2.104
Presenter(s):	Sudhagar Mani
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2024
Total Funding:	$1,814,678.00

The project is aimed at developing a robust ML modeling framework to relate biomass tissue properties to feedstock handling and conversion performance using ML techniques such as artificial neural networks. Two biomass types—corn stover and southern pine forest residues—were selected and sourced to capture biomass variations. About 60 samples of corn stover bales collected from three different harvest methods and two different locations and years (2018 and 2020) were manually separated into four tissue fractions (cob, husk, leaves, and stalk) along with bulk fractions to determine chemical and physical properties and to develop an NIR-based hyperspectral imaging (HSI) instrument. Then, the tissue fractions were treated with the enzymatic hydrolysis method to determine hydrolysis performance. Similarly, five different samples of southern pine forest residues were sourced, collected, and manually sorted into four tissue fractions (juvenile wood, branch wood, bark, and needles) and were scanned using NIR-based HSI models to predict physical and chemical properties. The forest residue tissue fractions were used to carry out the fast pyrolysis performances using pyro-gas chromatography with a mass spectrometer (pyro-gas chromatography–mass spectrometry instrument. The ongoing research includes studying the grinding and bulk handling performances of both biomass samples and developing predictive models using ML tools. Preliminary ML modeling activities are carried out with existing data from the literature, and the developed framework will be adapted to the project results to evaluate prediction performance metrics ($R^2 > 0.8$). The developed ML models will guide selective preprocessing operations to produce highly flowable and conversion-specific feedstock for the smooth operation of a biorefinery. They can also be used to design modern biomass depots aimed at manufacturing uniform and standardized feedstock for a specific conversion while developing optimal strategies to monitor, manage, and control powder flowability during handling and storage and thus improve the operational reliability of a biorefinery. The successful completion of the project will not only meet BETO's feedstock-conversion interface goals, but will also deliver science-based strategies to preprocess biomass at the tissue level to unlock the feedstock-conversion interface challenges and flowability issues for a biorefinery.



COMMENTS

- An interesting approach is provided, but the long-term significant impact is not well defined. This appears to be largely academic work. It is unclear whether the models are actually being made publicly available. The cost and potential cost benefit of this work are not described. This was not a FOA requirement, but it would have been a measurable metric for this project. No other real measurable impacts were defined; all were qualitative. A metric will need to be defined just to determine when the models would be considered reliable.

- This work may have important implications for industrial feedstock handling, but it was difficult to discern from the presentation. I would have liked to see more content on how these software tools would be used in industry and what benefit they might have. It is also critical for the researchers to understand these factors so that they have the necessary context for decision-making.

- The ML aspect of the project appears to be largely based on literature review and not on more rigorous ML software or analyses that can analyze the feedstock characteristics that correlate with bio-pyrolysis. The project fails to accomplish a primary objective to achieve a novel ML tool. This project would benefit from forestry and biofuel industry partnerships. Extensive forestry feedstock analyses have been done, yet this project implies that much is unknown. However, the live presenter pointed out that it is the particle-level characteristics that are widely unknown. The presenter said that the ML tools can be used to help prioritize feedstock from biomass depots, but in doing so, failed to recognize that forest biomass depots do not segregate feedstock to an ultra-refined level for that to apply. The weakness of this project is the lack of industry engagement and strong connections to market or industry needs.

- This is an ambitious study in which NIR HSI will be used to correlate with the processability of both (1) corn stover lignocellulosic conversion using dilute acid pretreatment/enzymatic hydrolysis/fermentation to ethanol and (2) pine component conversion with pyrolytic conversion. Tackling one of these areas would be ambitious, and I don't know the benefit of tackling both objectives when only the analytical method is common. As a result, the effort seemed unfocused. Currently, the corn stover method wet conversion appears to be based on a meta study of previous acid pretreatment and enzymatic hydrolysis, dividing the samples into "seven features." However, as none of the actual samples analyzed were converted, there appears to be a disconnect between the imaging/modeling and analysis (unchecked assumptions). This may be more misleading in criteria selection than beneficial to related criteria selection. The predictive abilities of the NIR models for handleability are "underway" and are unable to be evaluated. The pyrolysis prediction model seems more advanced than the corn stover predictions, although there is still some of the meta-analysis disconnect that the corn stover model appears to suffer from. The relationship of pyro/gas chromatography/mass spectrometry to commercial pyrolytic conversion remains to be proven in relationship to commercial unit operations—it is indicative, but gaps exist.

- The project has developed a rapid analysis technique for using NIR with HSI to determine the chemical composition of the anatomical fractions of both corn stover and pine forest residue. Using ML technology, the team is training the software to predict conversion in both enzymatic hydrolysis and fast pyrolysis. If successful, the application will advance the state of the art for predicting the yield of feedstocks in the conversion processes. In parallel, the team is evaluating physical properties and utilizing ML to predict grinding performance and flowability in the biorefinery processes. Based on the project schedule for Budget Period 2, the team has a strong likelihood of achieving Budget Period 2 goals. The presentation does not describe the tasks intended for Budget Period 3, which would help in determining the probability of achieving the end-of-project goal. The project is designed to demonstrate the potential for significant impact in both a low-temperature and a high-temperature environment using lab and pilot equipment. Engaging partners to evaluate the effectiveness of the NIR/HSI technology in both high- and low-temperature pilot conversion as well as preprocessing equipment are needed to verify the technology and increase the probability of commercialization.
- In terms of approach, the team outlined the issue of feedstock variability and the need for being able to predict the composition well. The outlined approach was difficult to understand; the roles of the various partners and a list of tasks, milestones, and goals were not provided. It is not clear how the team will solve this issue. It does not look like the team has any industrial partners, coalitions, etc. to provide feedback. In terms of progress, the team provided results, but it was unclear how the results will be used, and the ranking of the most important features seemed trivial, as most would be apparent. No discussion was provided on whether the project was on target, other than the fact that a task was completed. That is, no information on the attainment of specific milestones was provided. Also, some tasks are complete for the fourth quarter, but others are not. Is this because the project is ahead, behind, or on target? In terms of impacts, the team has published and/or presented five publications on this work. An ML model would be of great benefit to the biomass processing industry. However, it was unclear how predictive the model is and where the project goes from here. There was no assessment of the economic, GWP, or other impacts.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for the feedback and comments on this project. The project team agrees that the project is very ambitious. The project is intended to understand the variability of biomass at the tissue component level while evaluating its impact on conversion and handling properties. This is the first fundamental study that is focused on the heterogeneity of biomass physical and chemical properties impacting conversion performance. In addition, we will develop physical and chemical property prediction models based on the HSI spectra method, a nondestructive approach to rapidly determine biomass properties. Unlike other R&D projects evaluated during this Peer Review, this project is not intended to develop new technologies or provide a cost estimation; instead, we are building an ML modeling framework to relate biomass tissue properties to conversion and handling performance. The ML modeling approach will be of great benefit to the biomass industry, as confirmed by our project advisory board, which represents the biomass processing industry. ML models can advance agricultural and industrial practices and predict biofuel yields, leading to significant improvements in prediction and process control of conversion technologies. In addition to determining the conversion potential of various tissue fractions (e.g., pyro-GCMS technique), we are also collecting conversion data in the published literature to augment biomass variability and its relation to conversion performances to develop robust ML models. Access to ML models is typically given by providing the code and models upon request or through repositories like GitHub or public web servers. The feature ranking methodology will evaluate the influence of each feature on the model's final prediction by implementing a game theory approach. This leads to the identification of the key factors involved in the conversion of biomass into biofuels, providing invaluable insights for future R&D in this field. For example, if the biomass industry is willing to share its biomass input properties and its basic conversion process conditions, the ML model can instantly predict the conversion yields during commercial operations.

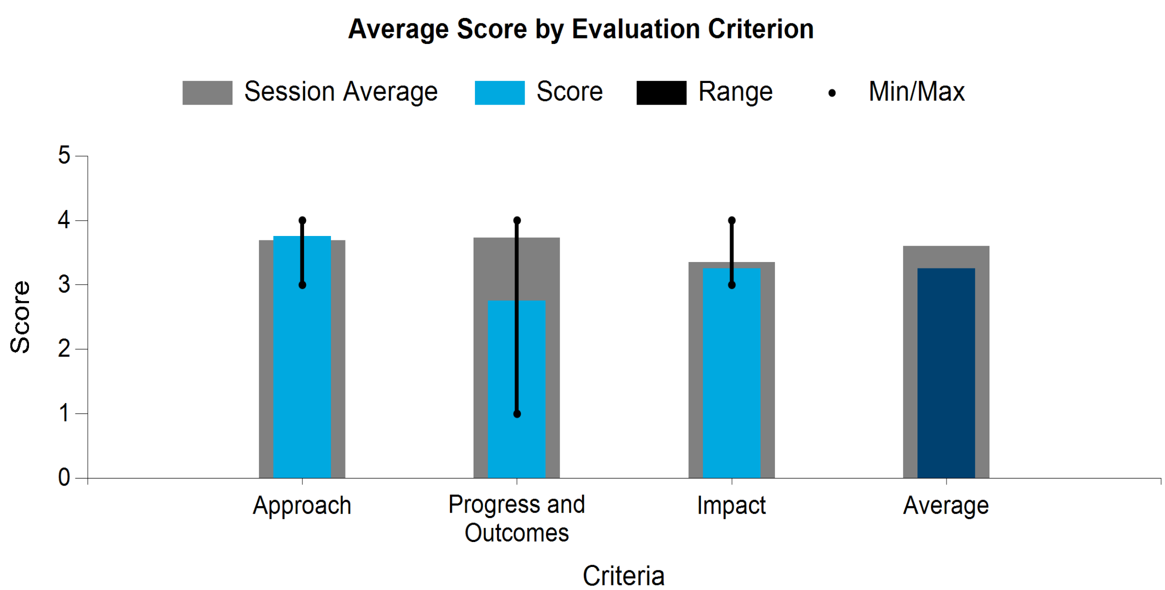
ARTIFICIAL NEURAL NETWORK FOR MSW CHARACTERIZATION

AMP Robotics

WBS:	1.2.2.105
Presenter(s):	Carson Potter
Project Start Date:	10/01/2020
Planned Project End Date:	03/31/2024
Total Funding:	$2,538,653.00

PROJECT DESCRIPTION

AMP Robotics' project "Artificial Neural Network for MSW Characterization" is an effort to model out a cost-benefit analysis of different sensor packages for characterization of MSW. By modeling sensor performance across a range of multimodal inputs, and utilizing deep learning techniques to fuse the sensor data, AMP hopes to produce a state-of-the-art tool for MSW characterization. The work includes profiling which sensors are the most impactful and economically viable for long-term characterization and chemical control of MSW for the production of low-carbon fuels and feedstocks, and will enable future research on efficient separation of critical fractions such as pyrolysis and bioenergy feedstocks.



COMMENTS

- The project is about 75% behind schedule (Slide 11) due to vendor issues, and UV/X-ray fluorescent (XRF) will not be carried out as planned. Question: What is the impact of these on the overall fidelity of the proposed approach and expected outcomes? The TRL was expected to go from TRL 3 to 5 after the completion of the project. Is that still the case with the mentioned issues/compromises? It would be useful to hear about the team's experience and track record in carrying out a project of such complexity and variability in a closely related application. It would also be good to have industrial partners.

- This is a good project with some details on the approach being used. More explanation is needed to address the strategies for mitigating the project's risks. In terms of P&O, although the project has had delays due to third-party sensor array procurement, it is making progress. The project needs to address the inconsistency of the AI training data from different sources. As far as impact, the cost/benefit of this robotic sorting system compared to a mechanical/manual system is not clear. A commercialization plan with clearly defined customers is needed.

- Land use change and competition with food production are often cited as concerns for lignocellulosic feedstock production. Development of NMSW as a feedstock is warranted because it does not compete with agriculture for food production, and because the use of NMSW will offset the flow of waste into landfills and mitigate landfill methane emissions. Conversion of wastes into useful products and services is a basic aspect of circular economies. BETO has made significant investments into NMSW research, including the projects reviewed in this report. Some of the challenges of developing NMSW as an economic resource include (1) the extreme heterogeneity of NMSW, and (2) the presence of toxic and undesirable constituents. Therefore, BETO has made significant investments into NMSW characterization, sorting, blending, and milling to overcome these challenges. The objective of this project is to develop an AI system to characterize NMSW using NIR reflectance data and Red-Blue-Green imagery. The investigator mentioned that the project is about 9 months behind schedule and noted some significant challenges due to the difficult environment of working with NMSW and material heterogeneity. Nevertheless, this project warrants continuation. I will note that on-board NIR analysis has been developed for grain harvest combines, which are also a difficult environment, albeit the material is more consistent than NMSW.

- In terms of approach, it was an excellent idea to include the first chart, which shows “short forms.” This was especially helpful, and thought should be given to including this in all presentations. Including roles of the project team would be very helpful. There are realistic challenges that may be very difficult to overcome for successful implementation of this technology. This is a novel and interesting approach for classifying MSW. As far as P&O, the project has gotten slightly off track with sensor delays. However, other work is proceeding well. The team can always look at the two missing sensors if time/funds allow at the end of the study and the PIs feel that they would contribute to better classification. In terms of impact, the project has the potential to be impactful if it is successful in characterizing feedstocks. A collaborator on the gasification end would be helpful to the team, as would a collaborator in the waste management industry.

PI RESPONSE TO REVIEWER COMMENTS

- In response to the first comment: I believe there are some misunderstandings from the presentation material. The project is not 75% behind schedule; we are 75% of the way through the second budget period, which was a total of 9 months behind schedule. That 9-month delay was driven by a third-party vendor chosen by INL to construct a sensor array at the BFNUF for use in this project and others. The delay was in no way driven by AMP’s participation in this project. AMP is our industrial partner, and has extensive partnership with Waste Connections, Casella, and many other leading industry processors. On top of that, AMP has over 300 robotics and AI systems deployed across 14 countries, making it the leading industrial provider of waste AI and robotics. The TRL will still progress from 3 to 5, just with the exclusion of some initial modalities from which we were hoping to gather additional data on chemical control. For the key performance parameters of this grant, we do not anticipate needing XRF or UV to fulfill the accuracy desired by BETO.

- In response to the second comment: It would help to clarify the nature of the inconsistencies the reviewer is concerned about. Bias in training sets is consistently a problem when developing large-scale AI models, and for the BETO grant in particular, we are definitely concerned about overfitting to the sample material provided. However, that material was sourced from landfills across the western United States, and should be fairly representative within the U.S. waste stream. Any production-ready version of this technology that AMP deploys will likely benefit from a mix of training data across more than 100 U.S. sites, with an emphasis on regional MSW recorded from robots deployed in our fleet. This is a common practice for us to ensure the robustness of the data and, ultimately, the performance of the model.

- Regarding points 3 and 4, we agree! We will produce a cost/benefit analysis of this use of a sensor; however, this project is not tied to a specific sorting mechanism, so it could be paired with almost any common mechanical approach. Wherever that sorting mechanism or energy conversion process will benefit from a better understanding of composition and an ability to track specific items as they move across the conveyance of the process (for the purposes of chemical control), this sensor will certainly provide a unique and cost-justified advantage.
- Regarding the fourth comment: Agreed! We have leveraged BETO's extensive network to have conversations with Gas Technology Institute (GTI) and a few other gasifiers, and we are exploring partnership with Fulcrum for future infrastructure funding opportunities through DOE. If we took a future iteration of this project to the stage where we were designing full-fledged sorting systems, it would be invaluable to partner with a gasifier and a waste processor (such as Waste Connections or Waste Management) for process flow optimization. AMP has experience and partnerships here, but nothing expressly directed at the ultimate realization of this specific award's focus, in a production environment, for gasification preprocessing of MSW.

DECONTAMINATION OF NON-RECYCLABLE MSW AND PREPROCESSING FOR CONVERSION TO JET FUEL

Gas Technology Institute

PROJECT DESCRIPTION

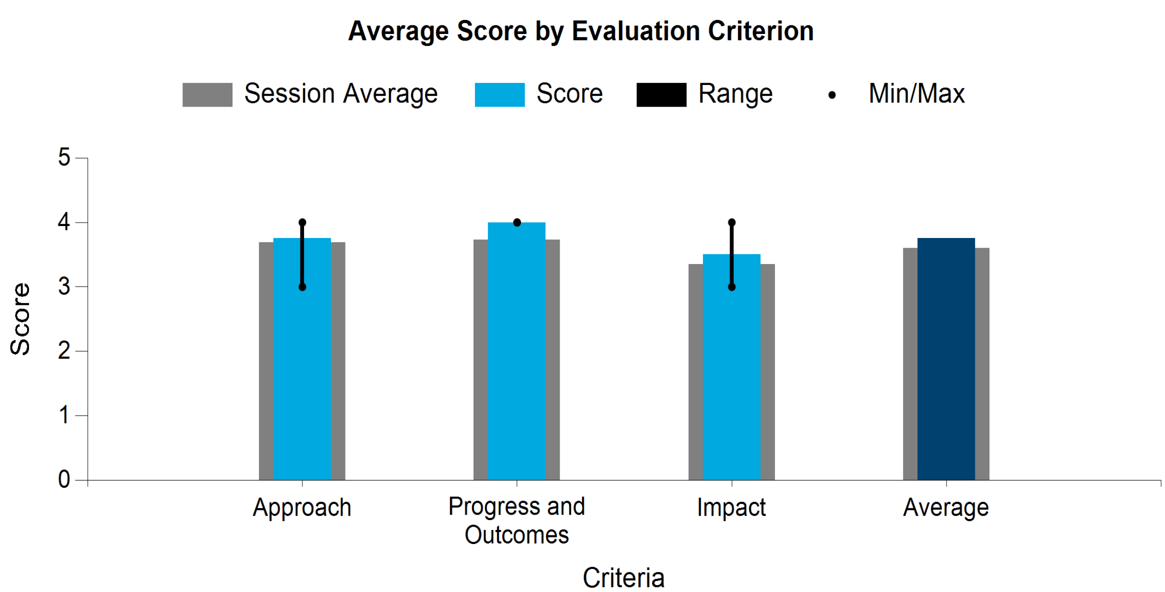
WBS:	1.2.2.106
Presenter(s):	Timothy Saunders
Project Start Date:	10/01/2020
Planned Project End Date:	05/31/2024
Total Funding:	$3,128,383.00

The project goal is to create a new path for NMSW to produce jet fuel, capture secondary value streams, and minimize landfill.

GTI has demonstrated U-GAS, a single-stage fluidized bed gasifier applicable for converting biofuels and NMSW, which has been selected as an applicable baseline technology for converting NMSW to jet fuel. The project will develop a novel AI sorting algorithm to produce high-purity feedstock from NMSW and will enhance physical methods for fractionation of NMSW. The AI algorithm will be tested on a commercial-scale sorter machine. The commercial conversion process will utilize a novel solids pump that injects the processed NMSW directly into gasification pressure for conversion.

Specifically, the project will:

1. Develop a novel AI sorting algorithm for increasing the purity and efficiency of fractionation and decontamination of NMSW.
2. Undertake physical and chemical characterization of NMSW.
3. Develop fundamental numerical models to predict plug formation of NMSW fractions and blends and validate in an adapted solids pump.
4. Test an adapted semi-scale solids pump for homogenous feedstock injection at pressure.
5. Undertake a commercial TEA and LCA showing viability and impact of integrated process from NMSW receipt through conversion to jet fuel.



COMMENTS

- This is a well-balanced team with the necessary expertise in waste collection, sorting, separation, characterization, and AI-based data analysis and informatics. Active participation from Waste Management is a plus. The project seems to be on track and has met key metrics and go/no-go decision stages. Slide 8 clearly details the risks and their mitigation steps. It is not quite clear how the project would be transitioned into a field trail. Slides 5 and 7 detail the proposed approach. It looks like it mostly addresses the solid components of the waste stream. What about chemical contaminants, such as forever chemicals?

- This is a sound project with some details on the approach being used. More explanations could be used to further address the strategies for mitigating the project's risks. In terms of P&O, substantial progress is needed to address the association of decontamination with the yield of jet fuel relative to specific conversion pathways. It is not clear how AI can help remove the contaminants. Will AI detect other contaminants besides chlorine? As far as impact, there are no touchable impacts reported at this phase of the project.

- Land use change and competition with food production are often cited as concerns for lignocellulosic feedstock production. The development of NMSW as a feedstock is warranted because it does not compete with agriculture for food production, and because the use of NMSW will offset the flow of wastes into landfills and mitigate landfill methane emissions. Conversion of wastes into useful products and services is a basic aspect of circular economies. BETO has made significant investments into NMSW research, including the projects reviewed in this report. Some of the challenges of developing NMSW as an economic resource include (1) the extreme heterogeneity of NMSW, and (2) the presence of toxic and undesirable constituents. Therefore, BETO has made significant investments into NMSW characterization, sorting, blending, and milling to overcome these challenges. This project is developing NMSW as a feedstock for SAF through Fischer-Tropsch/gasification. The team's approach is to remove harmful constituents, such as polyvinyl chloride (PVC), from the feedstock by developing AI-based characterization. They are also developing a continuous-feed dry solids pump to feed decontaminated NMSW into the gasifier. This project appears to be on track, and the team is gaining basic experience with the safety and physical risks encountered with NMSW.

- In terms of approach, using black instead of grey font would be helpful. Slide 3 was good; it attempted to show the involvement of the collaborators. I appreciated the definition of the TEA and LCA on page 6. Regarding the <$30/ton add-on cost for processing above the $86/ton delivered cost: How does that apply to this project, where the anticipated cost of NMSW would be lower than better feedstocks at $86/ton? Some of the slides in this presentation were impossible to see and also contained far too much information to comprehend in a short amount of time, i.e., Slide 8. The 15 key performance parameters are an excellent way to track the project. This system could be utilized by a number of projects to make the success criteria clear and tracking more direct. (I only wish I could read the slide.) P&O seems to be on target and progressing well. In terms of impact, the commercialization potential is not very clear. The TEA and LCA will determine commercial feasibility. The next steps to commercialization were not mentioned—i.e., who would be the customer for this application, and has the group been in communication with the intended SAF manufacturer to understand feed systems and feedstock requirements?

PI RESPONSE TO REVIEWER COMMENTS

- GTI is currently considering a commercialization plan that incorporates testing of the feed system to be developed. Initial testing will most likely be at a gasifier test site at a GTI facility where the feed system will be used to inject NMSW into an operating U-GAS gasifier. Field testing of the NMSW preparation process will be undertaken in conjunction with INL and suppliers of the process equipment. We envision asking Waste Management to support on-site testing of such processing equipment for validation at actual materials recovery facilities.

- GTI is confident that the project risks can be managed by the team, as the key deliverable is a feed system able to deliver into 150 psi—a pressure that the team has successfully achieved with other materials. The process equipment for the NMSW preparation being used by INL is all commercially available except the AI system; consequently, risks related to performance are very low. The AI system will need training, but the narrow focus for the material target simplifies the process objective.
- The AI system to be developed for the project will target a single contaminant: chlorine compounds, primarily PVC. The number of specific targets in the as-received NMSW containing PVC are relatively small, and so far, they appear easily identifiable by the sensor suite employed, offering a high confidence of successful performance. The project will use AI for PVC targeting only, and there are no plans to expand this requirement.
- The program commercialization steps are in development by GTI, as mentioned in the response above. The TEA and LCA will define the cost parameters for both the processes being developed in the project and the larger plant-scale economics. Once these are defined, the best approach for commercialization can be developed. Having the nation's largest waste handler as a partner opens many opportunities for process applications, operations, and locations. The team will expand contact with municipal operators as the project develops and expects to have additional interested parties joining the evaluation process as a first step to identifying test targets. Included in this process will be manufacturing companies for process equipment development and future sales to interested markets. It should be noted that the feed system will have many applications in addition to NMSW—biomass, for example—so there will be parallel commercial opportunities to take advantage of upon success in meting operating targets.

ADVANCED SENSING FOR CHARACTERIZATION AND SORTING OF NON-RECYCLABLE PLASTICS USING SENSOR FUSION WITH ARTIFICIAL INTELLIGENCE

UHV Technologies

WBS:	1.2.2.107
Presenter(s):	Nalin Kumar
Project Start Date:	10/01/2020
Planned Project End Date:	03/31/2025
Total Funding:	$3,125,000.00

PROJECT DESCRIPTION

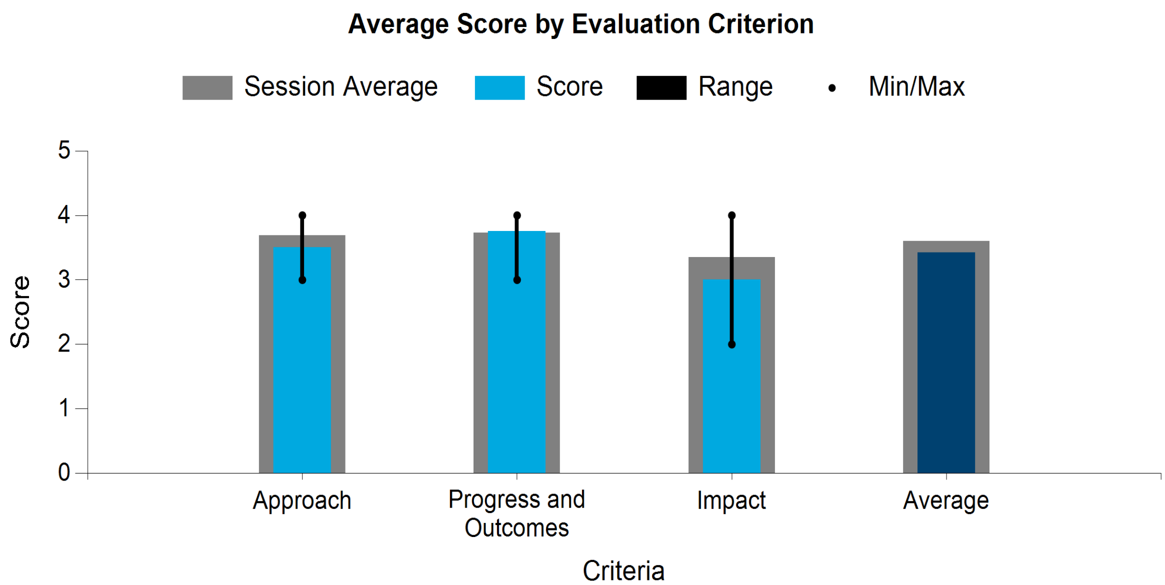
Objectives: The first objective is to develop an instrument that can quantify individual pieces of plastic with multiple sensors and assign a unique fingerprint, containing organic and inorganic data, to each piece. The second objective is to create a novel classification system for polymer and multilayer polymers in this stream with deep learning and AI algorithms. The third objective is to develop three different products with catalytic pyrolysis to determine which of the novel sorted fractions are most viable for the creation of products. The fourth objective is to perform end-to-end TEA and LCA to ensure economic viability of the sorting technology.

Description: The project goal is to advance state-of-the-art plastic sorting capabilities by employing cutting-edge technologies such as sensor fusion and AI-based deep learning algorithms. The proposed technology will develop advanced and techno-economically viable sorting and preprocessing methods tailored to MSW. To this end, an existing stream of nonrecyclable MSW plastics such as #3–#7, which is currently produced at an existing material recovery facility from NIR sorters, will be investigated to divert from disposal for conversion to fuels and products.

Methods: Deep learning neural networks will be developed to perform chemical-based classification of components found in the nonrecyclable plastic waste stream. An experimental apparatus will be developed that uses air nozzle jets to perform sorting, fractionation, and decontamination of this waste stream. Pyrolysis testing will be used to evaluate the viability of the novel fractions to produce new products.

Potential Impact: Novel fractions from this waste stream have the potential to become a valuable feedstock for the production of gases and fuels. These 1,200-pound bales created from this plastic waste stream sell for $6–$10 in current open-market conditions. This sorting technology potentially enables a new low-cost feedstock for the creation of new products.

Major Participants: UHV Technologies Inc., INL, the University of Illinois Urbana-Champaign, Penn State University, and Palm Beach Solid Waste Authority.



COMMENTS

- This is a well-articulated project with clear objectives, approaches, necessary tools/capabilities, and go/no-go metrics. The team has the necessary skill sets and capabilities to carry out the tasks outlined in the project. Are there any concerns about additives such plasticizers and perfluoro compounds in the plastic waste stream? How will they be handled? It would be helpful to have an industrial partner on the team. Slide 7 shows 70% conversion. What is the other 30%? How is that handled? On Slide 11, is the initial weight given dry weight? In the run with the catalyst, dry conversion is shown as 64.41% and liquid is shown as 31.96%. I do not quite follow this. Slide 13 claims a plant cost (CapEx?) of $12 million–$15 million for a 60,000ton/year facility. Is the product bio-oil or a further upgraded one?

- This is a sound project with some details on the approach being used. In terms of P&O, the project is making progress. A baseline was created in Budget Period 1. It is not clear whether decontamination is considered. The calculation of the MSW cost of $20–30 per ton needs to be further refined and clarified to achieve the target of $3/GGE. For example, how is the logistical cost or transportation cost considered in the process? As far as impact, there are no touchable impacts reported at this phase of the project. In the coming years, dissemination of the project findings and commercialization will help generate substantial project impacts. The TEA and LCA also need to be further improved, especially through clarification of data sources (lab work, existing literature).

- Land use change and competition with food production are often cited as concerns for lignocellulosic feedstock production. Development of NMSW as a feedstock is warranted because it does not compete with agriculture for food production, and because the use of NMSW will offset the flow of wastes into landfills and mitigate landfill methane emissions. Conversion of wastes into useful products and services is a basic aspect of circular economies. BETO has made significant investments into NMSW research, including the projects reviewed in this report. Some of the challenges of developing NMSW as an economic resource include (1) the extreme heterogeneity of NMSW, and (2) the presence of toxic and undesirable constituents. Therefore, BETO has made significant investments into NMSW characterization, sorting, blending, and milling to overcome these challenges. This project aims to develop systems to characterize NMSW constituents and sort out undesired constituents. The team is developing a complicated system of Visible, NIR, XRF, and Mid Infrared Range sensors to drive AI-enabled characterization and sorting. Their current goal is to obtain one million images to train the system. Obtaining and characterizing this number of images is daunting; however, the results will lead to a robust calibration set for the system. This work is on track and will have a significant impact on NMSW processing irrespective of the biofuel conversion system.

- In terms of approach, more specificity on the project goal and specific aims (Slide 2) would help situate the project within the BETO portfolio. I don't see an alignment with the BETO objectives. Collaborators are listed on page 3, but there are no details on how each is involved in the project. It is unclear whether a value of inorganic/organic content is generated by the sensors, or how this information will be used. The project will take the sensor footprints and relate them to a camera image, but the classification of the material is not clear to me. In terms of P&O, for the proof of concept through the lab-scale pyrolysis system: What type of fuel is it, and where can it be used? I don't understand the costs on Slide 7. On Slide 11, highlighting the meaning of the important results in this table would be helpful. It would be helpful to have both the plastic type and the classification number on the same slide (Slide 8). How much of 4, 5, and 6 are available in the marketplace? As far as impact, it is not clear how this fits with the BETO objectives. Details on the revenue slide (Slide 12) would be helpful. I'm not sure what this slide is showing. My thoughts are that this system would need to ensure that markets already exist for the #1, #2, and aluminum in an area. Otherwise, this would significantly affect project feasibility. A comparison with the use of this material in a waste-to-energy conversion plant should be considered. It seems like a high cost for processing a low-value material that may not have a high value-added application as a liquid fuel of some sort. What is the application of the fuel? Does the cost target of $30/tonne for sorting include all handling, waste disposal, etc.? Is it the entire plant cost?

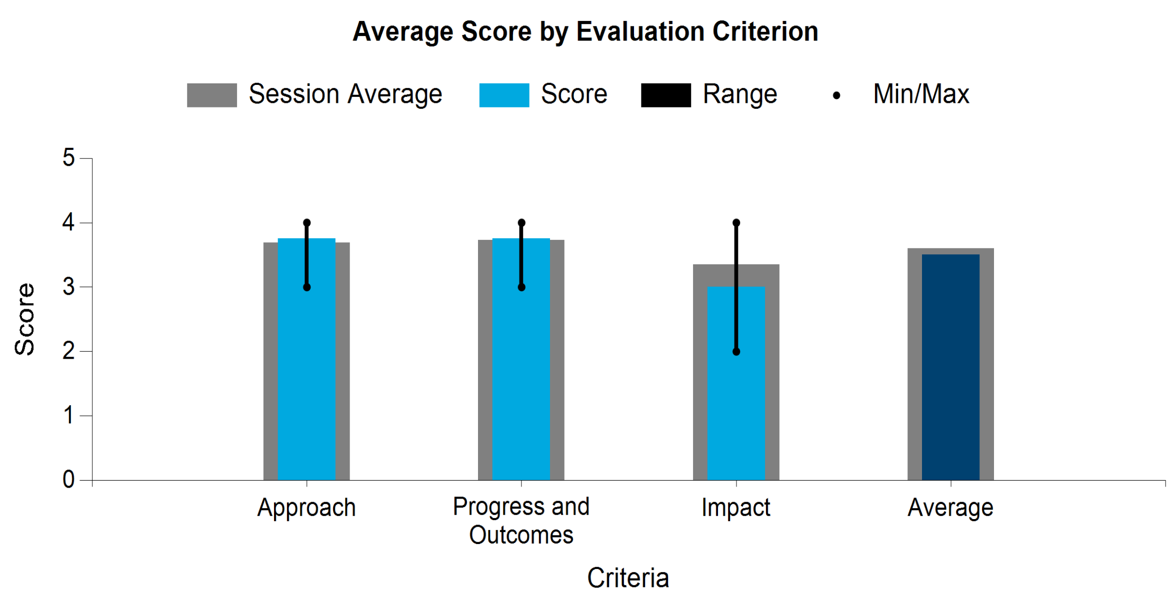
HIGH PRECISION SORTING, FRACTIONATION, AND FORMULATION OF MUNICIPAL SOLID WASTE FOR BIOCHEMICAL CONVERSION

University of Cincinnati

WBS:	1.2.2.108
Presenter(s):	Maobing Tu
Project Start Date:	10/01/2020
Planned Project End Date:	03/31/2025
Total Funding:	$2,651,991.00

PROJECT DESCRIPTION

MSW represents a valuable source of low-cost feedstock for the production of biofuels, biochemicals, and bioenergy. However, most MSW is generally destined for landfills. The heterogeneity and variability of MSW due to the presence of plastics, metals, and other impurities are the major bottlenecks for biochemical conversion, and only the organic fraction can be used. Significant gaps exist in understanding the heterogeneity of MSW and effective mitigation strategies for managing MSW to improve its cost-effective utilization and maximize valorization. Moreover, the initial baseline evaluation of the traditional screening and sorting processes, i.e., vibratory and trommel screening with nonrecyclable MSW, resulted in an organic fraction with a limited purity of only 50%–70% in this project. Therefore, the main goal of this project is to develop advanced sorting and fractionation technology to separate the organic fraction from the MSW and blend and formulate the organic waste (>95% purity) with lignocellulosic biomass for biochemical conversion. This project will employ the integration of dynamic disc screening, mechanical milling, and ballistic screening as an innovative approach to address MSW heterogeneity and facilitate effective separation of the organic fraction. Subsequently, blending and formulation of the sorted organic fraction with lignocellulosic biomass will be carried out to reduce feedstock variability. Finally, the TEA and LCA will be performed to evaluate the technical and economic feasibility of the proposed novel MSW sorting, fractionation, and blending pathways. The successful implementation of the current project will result in producing conversion-ready feedstock in support of the BETO cost target of $73/dry ton and will have a great impact on MSW management and waste-to-energy industries by developing a new sorting and milling technology.



COMMENTS

- This is a well-detailed project with objectives, an approach, relevant tasks, and milestones. The team is well rounded and has the necessary skill sets and capabilities. The project has met the milestone goals and is on track. In terms of impact, the project has the potential to be significant and to meet BETO goals.

- Who is the ultimate customer for the finished product—equipment/process, etc.? Slide 13 shows an efficiency in the 85%–90% range. What are the components—metals and others that are not removed? Could they have a negative impact on downstream conversion processes such as catalyst poisoning? Are there any concerns about residual hazardous chemicals such as forever chemicals?

- In terms of approach, on Slide 5, two challenges were discussed: shredder breaking glasses and disc screening issues. It is not clear how the team has handled or will handle and mitigate these risks. Regarding challenges for TEA and LCA, rather than boundary or scope, I like to say that data consistency and accuracy would be a major challenge to TEA and LCA. In terms of P&O, the project is making good progress. Regarding target performance metrics, for operating cost, the project needs more data support to address where it will achieve this target of <$30/ton for MSWs. As far as impact, it needs to be specific, especially on industry collaboration and engagement, and scale-up of the system. The decontamination work is not clear in the project, which needs to be a part of the total cost. It is not clear if contaminants of MSWs were removed before they were considered to be blended with biomass.

- Land use change and competition with food production are often cited as concerns for lignocellulosic feedstock production. Development of NMSW as a feedstock is warranted because it does not compete with agriculture for food production, and because the use of NMSW will offset the flow of wastes into landfills and mitigate landfill methane emissions. The conversion of wastes into useful products and services is a basic aspect of circular economies. BETO has made significant investments into NMSW research, including the projects reviewed in this report. Some of the challenges of developing NMSW as an economic resource include (1) the extreme heterogeneity of NMSW, and (2) the presence of toxic and undesirable constituents. Therefore, BETO has made significant investments into NMSW characterization, sorting, blending, and milling to overcome these challenges. Rather than employing AI-enabled characterization and sorting systems for NMSW, this project is developing milling as a means of improving the homogeneity of NMSW feedstocks and as an approach to blending NMSW with lignocellulosic feedstocks. The team has made good progress by procuring a disc mill, and installation of a test bed is currently underway. They are also collaborating with the Tuskegee Institute to elevate DEI as an objective in this project. This project will establish important capabilities at the University of Cincinnati, and the collaboration with INL reinforces the impact of the national lab.

- In terms of approach, the use of the term "organic fraction" is very confusing, as plastic (hydrocarbons) are organic molecules. Is the project referencing the separation of the bio-based organic fraction? If the end use of the material is to direct combustion/gasification, then it may not be desirable to remove the plastics. The prescreening stage (removing ferrous metals) must be commercially established already. How is this being designed in this project? The concept of grinding and then separating is a novel approach. This seems to be a high preprocessing cost for such a low-value feedstock. The team should mention the industrial collaborators by name in the presentation. It would be helpful to know what industries they are associated with. I appreciate the detailed investigation of equipment for new applications. In terms of P&O, what will be the start and end of the process for the LCA? How will the TEA show the benefit of this technology? It isn't clear how the technology will integrate with a biorefinery process in the LCA and TEA. As far as impact, no industrial partners are mentioned in the quad chart. This may make commercialization more difficult. What is the intended conversion pathway? Sugar conversion may not be the most favorable use. The material may be too contaminated for biochemical conversion pathways, and prove too costly to process. The team should maybe consider a gasification pathway.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their encouragement and constructive comments. We appreciate the positive feedback regarding our progress and outcomes, team skill sets and capacities, and milestone goals. We will address key questions raised by the reviewers below.
- Comment: Who is the ultimate customer for the finished product—equipment/process, etc.?
- Response: The goal of this project is to develop advanced sorting and fractionation processes that can separate the bio-based organic fraction from MSW to achieve a high-purity byproduct for blending with lignocellulosic biomass in a biochemical conversion process. The ultimate customer will be MSW handling companies and feedstock production companies.
- Comment: Slide 13 shows an efficiency in the 85%–90% range. What are the components—metals and others that are not removed? Could they have a negative impact on downstream conversion processes such as catalyst poisoning?
- Response: Depending on their size, some of the metal, glass, textile, and plastic will not be removed in the screening process and will end up in the organic matter fraction. These contaminants might have a negative impact on the downstream biochemical conversion process, but their impact is expected to be minimal. This potential impact will be evaluated in Budget Periods 2 and 3.
- Comment: Are there any concerns about residual hazardous chemicals such as forever chemicals?
- Response: We do have some concerns about forever chemicals such as perfluorooctane sulfonate and perfluorooctanoic acid in the bio-based organic fraction due to their presence in plastics and textiles. However, these materials will mostly be removed from the bio-organic fraction, and their contamination is expected to be minimal.
- Comment: In terms of approach, on Slide 5, two challenges were discussed: shredder breaking glasses and disc screening issues. It is not clear how the team has handled or will handle and mitigate these risks.
- Response: The shredder breaking glass could potentially be an issue. We plan to mitigate this risk by developing a presorting process without shredding and comparing the decontamination efficiency to the process with shredding.
- Comment: Regarding challenges for TEA and LCA, rather than boundary or scope, I like to say that data consistency and accuracy would be a major challenge to TEA and LCA.
- Response: We agree that data consistency and accuracy could be a key challenge to TEA and LCA. We will increase the sample size and the number of replicates to improve the data accuracy and consistency.
- Comment: In terms of P&O, the project is making good progress. Regarding target performance metrics, for operating cost, the project needs more data support to address where it will achieve this target of <$30/ton for MSWs.
- Response: We agree that more data support is needed to address the final target performance metrics; this will be addressed in Budget Periods 2 and 3.
- Comment: The impact needs to be specific, especially on industry collaboration and engagement and scale-up of the system.
- Response: Industrial collaboration and engagement and scale-up of the system will be specified in Budget Periods 2 and 3.

- Comment: The decontamination work is not clear in the project, but it needs to be a part of the total cost. It is not clear whether MSW contaminants were removed before they were considered to be blended with biomass.
- Response: Decontamination of the bio-organic fraction is defined as the removal of metal, glass, textile, and plastic in this project. Thus, the goal is to remove these contaminants as much as possible before blending the bio-organic fraction with biomass.
- Comment: In terms of approach, the use of the term "organic fraction" is very confusing, as plastic (hydrocarbons) are organic molecules. Is the project referencing the separation of the bio-based organic fraction?
- Response: We will use the term bio-organic fraction in future project reports. Yes, it is referencing the separation of bio-based organic fraction.
- Comment: If the end use of the material is to direct combustion/gasification, then it may not be desirable to remove the plastics.
- Response: The end use of bio-organic fraction is biochemical conversion, so plastic removal is desirable.
- Comment: The prescreening stage (removing ferrous metals) must be commercially established already. How is this being designed in this project?
- Response: The removal of ferrous metals will take place in the prescreening stage using a magnetic apparatus, as has been established by industry.
- Comment: The concept of grinding and then separating is a novel approach. This seems to be a high preprocessing cost for such a low-value feedstock.
- Response: The cost of preprocessing will be evaluated by TEA, which will assess if the process is cost-effective in producing conversion-ready feedstock.
- Comment: The team should mention the industrial collaborators by name in the presentation. It would be helpful to know what industries they are associated with.
- Response: The industrial collaborators include TORXX Kinetic Pulverizer and GoForward Solutions. Their associated industries may be found on their websites.
- Comment: I appreciate the detailed investigation of equipment for new applications.
- Response: We thank the reviewer for the positive comment.
- Comment: In terms of P&O, what will be the start and end of the process for the LCA?
- Response: The LCA will start from MSW preprocessing and will end with biofuels production and usage, composting, and refuse-derived fuel utilization.
- Comment: How will the TEA show the benefit of this technology? It isn't clear how the technology will integrate with a biorefinery process in the LCA and TEA.
- Response: The TEA will help optimize the prescreening, fine-tune the screening/sorting processes, and identify which products/processes are more valuable for MSW utilization.
- Comment: As far as impact, no industrial partners are mentioned in the quad chart. This may make commercialization more difficult.

- Response: The industrial collaborators are TORXX Kinetic Pulverizer and GoForward Solutions. They will be mentioned in future reports.
- Comment: What is the intended conversion pathway? Sugar conversion may not be the most favorable use. The material may be too contaminated for biochemical conversion pathways, and prove too costly to process. The team should maybe consider a gasification pathway.
- Response: The intended conversion pathway will be biochemical conversion to useful end products. We believe that if the contaminants can be removed, the sorted bio-organic MSW fraction will be suitable for biochemical conversion. The recovered plastics could be used for refuse-derived fuel and potentially for gasification as well if such facilities are near the MSW sorting process.

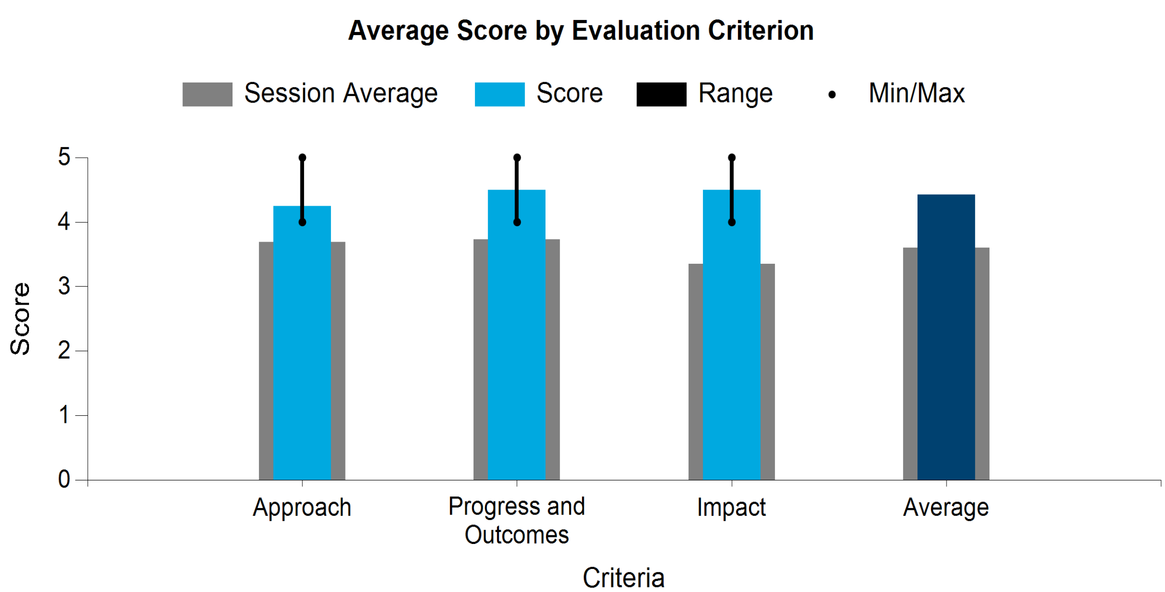
BIOENERGY FEEDSTOCK LIBRARY

Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.2.2
Presenter(s):	Rachel Emerson
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$750,000.00

Variability in bioenergy feedstock properties continues to be a primary challenge to integrated biorefineries achieving continuous operation and meeting the yield requirements necessary for commercial-scale production of biofuels and chemicals. The BFL is an important resource for understanding biomass variability; it provides a centralized location that is readily and easily accessible and understandable to bioenergy researchers and industry stakeholders. The objectives of this project include using the existing functionality already developed for the BFL to: (1) archive samples, metadata, and analytical data as necessary in a standardized way for BETO's FOAs and other BETO-funded projects; (2) develop sample and data management plans to provide policies for physical sample archival and disposal, data sharing, and pathways for eventual public release; (3) facilitate easy access to data and sample sets; and (4) maintain the BFL database through necessary software updates to ensure consistent access to samples, data, and results by bioenergy stakeholders. These objectives will be met through two tasks. Task 1 ensures that the samples and data generated through BETO's FOA projects are archived. Task 2 provides management and maintenance of the BFL samples, data, and database overall.



COMMENTS

- This is a very important initiative to collect, organize, and disseminate relevant feedstock information to meet BETO's overall goals. It looks like most of the users of the data/website are academics/national labs, with about 20% of users from industry. How can we get more industry participation? On Slide 11, are some of the tasks behind schedule?

- This is a good and useful project for a variety of audiences nationwide. DOE should continue to support this effort, which will benefit the national strategy on biomass for energy. The approach is good. In terms of P&O, the collaboration with the Bioeconomy Development Opportunity Zone Initiative was discussed. It is not clear how exactly the team associated the feedstock characteristics and quality variation with the Bioeconomy Development Opportunity Zone's regional, spatial, and temporal variability. As far as impact, this is a great project. More outreach may be needed to promote and disseminate the use of BFL.

- Computational modeling is important for conducting foundational analysis and forecasting the costs, availability, and characteristics of biomass feedstocks. The feedstocks are also expected to complement existing crop and livestock production systems. Projections need to support production goals for sustainable climate-smart systems. Modeling systems are necessary to predict feedstock variability, illuminate management options for risk mitigation, and understand feedstock fractionation, separation, sorting, and blending. This project is providing outstanding service to the biomass industry and is an essential resource for the pending circular bioeconomy. They have archived more than 60,000 biomass feedstock samples, of which over 30,000 have associated constituent data available for public use. This work has been well executed by INL and will have a significant impact for many years ahead.

- This is a very worthwhile and impactful project. The size of the data bank and its accessibility are to be commended. There is lots of important information on biomass variability that can help address questions about various aspects of biomass quality. The regionality aspect of the data is also very useful. The database has strong potential for use by academics/scientists. It is a good example of the impact of data synthesis to answer questions. The project has an extensive list of collaborators. In my opinion, the sample storage, while nice to have, is not as important as the characterization and database. Because samples are stored dry and may be kept for prolonged periods of time, they do not represent the biomass that a biorefinery would receive. Ideally, the greatest benefit of the samples would be for use in testing/designing for a biorefinery. Rachel did mention that the samples can provide a bridge for scientists from disciplines outside forestry to access biomass. This is an important use of the samples. As far as concerns, the characterization work may consider using the same procedures for at least a subset of the testing so that it is highly comparable. In the presentation, the pasted charts were very difficult to read, and there was too much information on each slide. This may not be the fault of the presenters, as they have a lot of information to present in a short time. Some thought should be given to the presentation format—maybe it could be more focused around the questions that reviewers are asked to evaluate.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' unanimous support of the BFL as a publicly available resource for bioenergy feedstock data and information. We agree with the reviewer's thoughts on the physical samples that are stored in the BFL. Many of the dried samples stored for prolonged periods in the BFL do not exactly represent the fresh or stored biomass a biorefinery might see; however, these samples can represent other types of chemical and physical variability that are useful to understand. The BFL has supported hundreds of requests for these physical samples. We will work on making the value of these physical samples clearer and better incorporating the additional data that is generated from meeting the requests for physical samples in the future. The reviewers noted that this project needs to continue focusing on outreach and dissemination strategies to engage with industry and build industry participation. We completely agree with this assessment. This project has a multifaceted dissemination strategy that we will continue to modify as necessary to increase the impact. Currently, this project publishes an end-of-year summary report highlighting the availability of samples, data, tools, and knowledge; has a yearly presence at industry-relevant conferences as part of INL's BFNUF; and is planning to have at least one webinar as part of the end-of-project milestone in FY24. The opportunity to present at events like BETO's Project Peer Review has also led to a noticeable increase in industry membership in the BFL. Additionally, the reviewers identified the need for modeling and projections using the BFL database resource. Although this project does not currently have the scope to develop these models, it does support other BETO projects, both at INL and other institutions, focusing on this type of work by providing relevant curated data sets. In FY23, projects including INL's Feedstock Supply Chain Analysis project (1.1.1.2) and ORNL's Supply Scenario Analysis project (1.1.1.3), which are responsible for the research supporting the *Billion-Ton Report*, were given large data sets representing variability in biomass characteristics to support various feedstock models. The continuous communication between modeling projects and the BFL team since the conception of the BFL has been important in generating and reinforcing the development of comparable data sets.

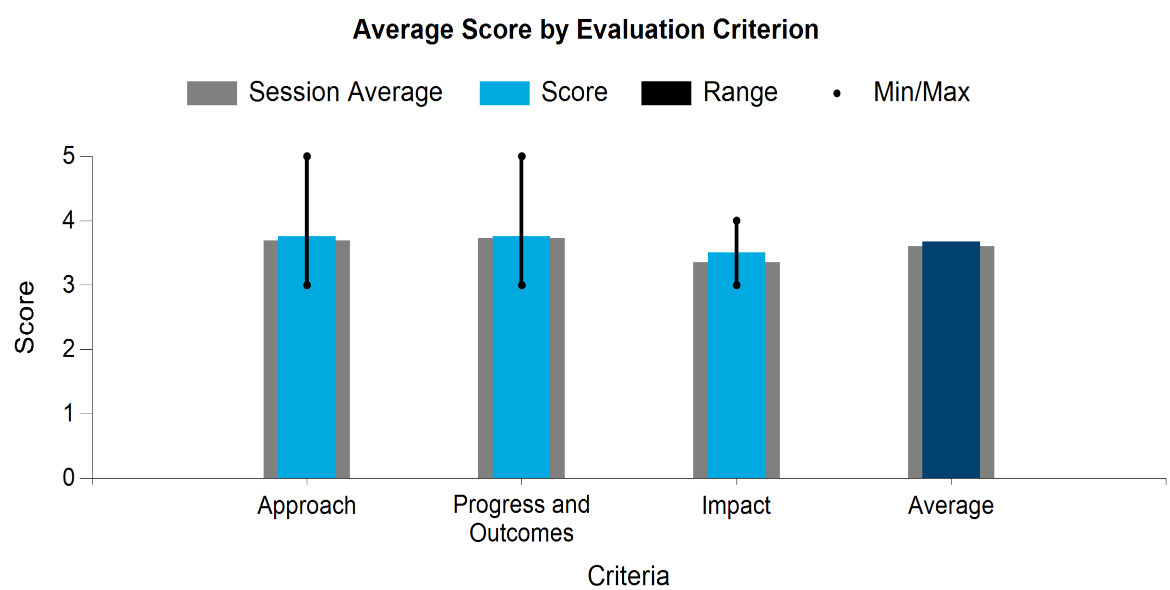
AI-ENABLED HYPERSPECTRAL IMAGING AUGMENTED WITH MULTI-SENSORY INFORMATION FOR RAPID/REAL-TIME ANALYSIS OF NON-RECYCLABLE HETEROGENOUS MSW FOR CONVERSION TO ENERGY

North Carolina State University

PROJECT DESCRIPTION

WBS:	1.2.2.203
Presenter(s):	Lokendra Pal
Project Start Date:	10/01/2021
Planned Project End Date:	12/31/2024
Total Funding:	$3,557,339.00

MSW is a potential low-cost abundant feedstock that can be used to produce fuels and products, but its heterogeneous nature causes significant hurdles that must be addressed for efficient valorization to fuel and products. We have proposed the use of AI-driven real-time characterization to enhance separation and preprocessing at different MSW facilities to enable efficient and economic valorization of MSW. Our project aims to tackle this valorization of MSW by building (1) an ML visual imaging model to conduct front-end discrimination of a broader classification of the materials based on shape and color, and (2) an ML hyperspectral imaging model to identify materials through being trained on specific material spectral signatures to obtain intelligently labeled hyperspectral images, augmented by multisensory information. We will present recent progress made in this project by demonstrating MSW identification and characterization, data gathering for hyperspectral imaging, visible camera ML models, and development of cloud-based data repository systems.



COMMENTS

- This is a good, solid project to better quantify the “quality” of a complex mixture in a typical municipal waste stream by using known analytical tools and metadata analysis with AI and imaging. The team is well qualified and has the required skill set and capabilities. The project seems to be on track, with about 25% completed. Would the proposed approach detect hazardous chemicals such as perfluoro compounds? There are other projects in the BETO portfolio addressing closely related areas. It isn’t clear if this effort is coordinated with those projects. Who is the ultimate customer? Would your approach lead to a certification-type outcome for a given downstream end use? What is the industry participation?

- This is a good project with sound approaches being used to achieve the project goals. In terms of approach, I agree that the preexisting availability of relevant data is a key challenge. What about the consistency of AI training data from different sources? Some loops need to be defined in the AI pipeline to improve the AI modeling process. As far as P&O, the project is making good progress with results. In terms of impact, I am curious how this project will be used in a real-world application. The future plan needs to be specific, especially on industry collaboration and engagement and scale-up of the system. LCA and TEA scope should be clearly defined with essential cost components.

- Land use change and competition with food production are often cited as concerns for lignocellulosic feedstock production. Development of NMSW as a feedstock is warranted because it does not compete with agriculture for food production, and because the use of NMSW will offset the flow of wastes into landfills and mitigate landfill methane emissions. Conversion of wastes into useful products and services is a basic aspect of circular economies. BETO has made significant investments into NMSW research, including the projects reviewed in this report. Some of the challenges of developing NMSW as an economic resource include (1) the extreme heterogeneity of NMSW, and (2) the presence of toxic and undesirable constituents. Therefore, BETO has made significant investments into NMSW characterization, sorting, blending, and milling to overcome these challenges. This project is using hyperspectral image analysis to develop an AI-enabled system for NMSW characterization. The team is composed of experts from North Carolina State University, the National Renewable Energy Laboratory (NREL), INL, IBM, and the town of Cary, North Carolina. Their primary progress has been on establishing data input, storage, and training for real-time analysis while materials are in motion on the conveyor. They have also had significant outreach accomplishments through a workshop, meeting presentations, publications, and a provisional patent disclosure.

- In terms of approach, there is a good focus on the characterization of NMSW. Effort is not wasted on material that can already be sorted and recycled. There is some emphasis on sharing the data set and models through the web platform. Not being in this field, I'm wondering who would want to use this data set. Is there a large demand for this type of data? On Slide 13, what about multilayer packaging—how is that optically different than some other paper grades (i.e., how will you detect that visually)? What about additives in the paper, i.e., chlorine or fluorine chemicals? Will it be possible to identify them? In terms of P&O, there has been much progress with this project. Over 80,000 images of waste have been collected. On Slide 10, what type of composition analysis will be done? The characterization should be aligned with the potential conversion process. I'm not sure what end use is intended in this case. As far as impact, for TEA and LCA, where will the start and end of the process go, and how will this work account for changes to an LCA for biofuel conversion? It's not clear how the results of this project can be incorporated. I would like to see more explanation about who the collaborators are and who the end user of the technology would be. Has a commercialization plan been developed that would take place after the pilot facility is successful?

PI RESPONSE TO REVIEWER COMMENTS

- Dear BETO and Peer Review panel members: Thank you very much for your time and effort in providing valuable comments from the Peer Review meeting for this project. We have carefully reviewed the comments and have added our responses below for major comments. We don't anticipate any impact on scope, schedule, or budget due to these comments.

- Comments: This is a good, solid project to better quantify the "quality" of a complex mixture in a typical municipal waste stream by using known analytical tools and metadata analysis with AI and imaging. The team is well qualified and has the required skill set and capabilities. The project seems to be on track, with about 25% completed. Would the proposed approach detect hazardous chemicals such as perfluoro compounds? There are other projects in the BETO portfolio addressing closely related areas. It isn't clear if this effort is coordinated with those projects. Who is the ultimate customer? Would your approach lead to a certification-type outcome for a given downstream end use? What is the industry participation?

- Response: Thank you for your comments. We agree with the reviewers that our project team has made significant progress toward meeting/exceeding the SOPO goals. HSI is a very adaptable technology that can detect hazardous chemicals, as documented in the literature. This feature played a significant role in the decision to utilize HSI for NMSW characterization, given its ability to detect a wide range of chemicals. However, perfluoro compound detection is not currently within the scope of this project. Our SOPO goals include a demonstration of the viability of identifying and characterizing major fractions of NMSW (i.e., paper and paperboard, plastics, food waste, textiles) with at least 50% accuracy at varying conveyor speeds. However, our system is scalable; we can incorporate additional data into our model to predict polyfluoroalkyl substances and other hazardous contamination. In addition, we are closely working with the DOE-BETO team to leverage other projects that are also focusing on NMSW spatial/temporal data collection, including polyfluoroalkyl substances and other hazardous contaminant issues, which could be combined with our system to tackle grand challenges of deeply characterizing the NMSW. Our ultimate customers are municipalities, waste management companies, dirty materials recycling facilities, materials recycling facilities, waste management companies, recyclers, biorefineries, equipment suppliers, technology developers, researchers, educators, etc. We envision these partners would be the primary users of this technology with the following immediate use cases:
    - Use case 1: Raw and labeled data sets available for research use
    - Use case 2: Raw and labeled data sets available for commercial use via licensing
    - Use case 3: Materials recycling facilities (MRFs) for improved detection and sorting
    - Use case 4: Conversion-ready feedstocks from nonrecyclable MSW for various industry segments.

  We plan to design various protocols, including new characterization techniques, homogenization/blending techniques, a raw and labeled data repository, ML models, and an end-to-end data and AI pipeline for system deployment. For example, we have developed a robust method for NMSW sampling, manual sorting, and imaging that could be leveraged as a standard across the waste industry. Our patent application focuses explicitly on the effective homogenization, densification, shipping, and storage of heterogeneous NMSW for accurate analysis of relevant chemical, compositional, and thermal characterization, and conversion to appropriate biofuels and bioproducts. This approach could allow for certification, as suggested by the reviewers. We have many industry partners, including one of the largest recycling facilities, which is a 15-minute drive from our North Carolina State campus. They have expressed a strong interest in our technology, as they would like to further automate their operations and enhance the quality of their final outputs. We are sampling their residual materials that are destined for landfill. Further, we are working directly with a municipality that continues to provide us NMSW samples. Finally, we have identified strategic partners for each waste stream, each of whom plan to evaluate the feasibility of the application of our technology. We will continue to engage them and others to promote our technology, and we can see a path to potential implementation. Our team will disseminate technology advancements through publications in peer-reviewed journals, conference presentations, and publications within the open-source environment. Public release of IP will only occur after the property is appropriately protected. Along with the IP from the deep learning portion of this project, the optimized wavelength for characterizing the MSW will be supplied to a hyperspectral camera manufactured in addition to the AI system.

- Comments: This is a good project with sound approaches being used to achieve the project goals. In terms of approach, I agree that the preexisting availability of relevant data is a key challenge. What about the consistency of AI training data from different sources? Some loops need to be defined in the AI pipeline to improve the AI modeling process. As far as P&O, the project is making good progress with results. In terms of impact, I am curious how this project will be used in a real-world application. The future plan needs to be specific, especially on industry collaboration and engagement and scale-up of the system. LCA and TEA scope should be clearly defined with essential cost components.

  Response: We agree with the review panel that data consistency is an important consideration when using AI for meaningful data interpretation, especially when training data is obtained from different sources. During the presentation, we mentioned that data sets are available for visual recognition of clean MSW, which can serve as training data for ML models in MSW object characterization. These images can be utilized alongside the data being collected as a part of our project. Basic object labeling is adequate for training ML models; however, the principal challenge lies in accurately labeling the data with relevant metadata, such as physical characteristics, process parameters, and radiometric information. Given the novelty of this research area, there is currently no universally established data labeling protocol. Therefore, part of our work aims to establish a comprehensive labeling protocol. This is crucial because the characteristics of NMSW are specific to each region, and for potential global deployment of this work, the existing ML models will need to be expanded and enhanced. Similar issues exist with existing HSI data sets; for example, there are companies working on HSI ML models for specific material within the MSW, but they are not consistent in their metadata. Therefore, we are developing a universal labeling protocol for HSI, visible color imagery, and other sensory data, which will be of universal value and appeal. This is an ancillary benefit from the execution of the current effort. Further, as discussed during the Peer Review meeting, our ML models will be updated with a primary focus on continuous improvement in a loop as we expand our database for scaling to industry standards. Our AI and data pipeline approach includes these circular steps: (1) data connections, (2) data preparation, (3) algorithm selection, (4) training infrastructure, (5) model deployment, and (6) continuous improvement. We envision the four immediate use cases listed above. As stated earlier, we have a robust plan for industry collaboration and engagement, with the implicit end goal being the final scale-up of the system. We have also clearly defined the LCA and TEA scope with essential cost components as we develop various use cases for this technology. For TEA/LCA, our baseline process includes the current practice of hauling the nonrecyclable (residual) MSW (NMSW) to landfill sites by trucks. The purpose of the TEA/LCA modeling is to clearly understand the valorization pathways of waste in the bioenergy relative to landfilling the waste in order to guide our research and process optimization. Biomass sources that need waste management, such as NMSW, have the highest potential for economic profitability and CO_2e emission reductions.

- Comments: In terms of approach, there is a good focus on the characterization of NMSW. Effort is not wasted on material that can already be sorted and recycled. There is some emphasis on sharing the data set and models through the web platform. Not being in this field, I'm wondering who would want to use this data set. Is there a large demand for this type of data? On Slide 13, what about multilayer packaging—how is that optically different than some other paper grades (i.e., how will you detect that visually)? What about additives in the paper, i.e., chlorine or fluorine chemicals? Will it be possible to identify them? In terms of P&O, there has been much progress with this project. Over 80,000 images of waste have been collected. On Slide 10, what type of composition analysis will be done? The characterization should be aligned with the potential conversion process. I'm not sure what end use is intended in this case. As far as impact, for TEA and LCA, where will the start and end of the process go, and how will this work account for changes to an LCA for biofuel conversion? It's not clear how the results of this project can be incorporated. I would like to see more explanation about who the collaborators are and who the end user of the technology would be. Has a commercialization plan been developed that would take place after the pilot facility is successful?

- Response: To tackle the grand challenge of valorization of NMSW, the development of a raw, labeled, and cleaned data set is critical for ML models to meet specific use cases, as described earlier. Further scalability of the data repository is important to continue in order to account for major input changes in materials composition, as NMSW is extremely heterogeneous. This is especially true as new product development continues. There is thus a real and significant demand for this type of data from municipalities, waste management companies, industry, equipment manufacturers, and many other stakeholders we have contacted. The HSI system does not have a deep penetrating depth and would have difficulty providing such detection if the object were multilayer packaging. Because of the limited ability to penetrate deeply into an object, we have coupled the system with an optical system that will have the ability to distinguish between multilayer packaging and other paper grades. As previously mentioned, HSI can detect hazardous chemicals, as has already been demonstrated in many publications. This feature played a significant role in the decision to utilize HSI for NMSW characterization, given its ability to detect an extensive range of chemicals. Based on our progress to date and the SOPO goals, we are now conducting the following analyses: (1) physical (proximate) analysis—moisture, density, total solids, ash content, chloride content, particle size distribution, etc.; (2) chemical (ultimate) analysis—elemental analysis (C, H, O, N, S, C/N ratio), Fourier-transform infrared spectroscopy; (3) compositional analysis—cellulose, hemicellulose, lignin, extractives, etc.; and 4) calorimetry—energy content/calorific values. We are targeting paper and board fractions/subclasses using existing conversion pathways such as mild mechanical/alkali pretreatments and enzymatic hydrolysis/catalytic upgrading to biofuels such as SAF, guided by TEA/LCA. Our simulation results will provide detailed process economics, material requirements (chemicals, water, etc.), and energy balances for a complete process under optimal conditions. Sensitivity analysis will be performed by varying the amount of usable major fractions, providing an estimate of potential benefits from residual MSW recovery. The TEA/LCA results will be used primarily to prioritize the characterization of specific materials based on their intrinsic economic benefits. For example, within paper and paperboard, how does fractionating corrugated only versus other paper products affect the global economics? The primary LCA input parameters that will be investigated will be characterization and separation efficiency, because these are critical measures of the success of our system. Additional exogenous input parameters will also be investigated to explore how they affect the potential performance of the system (e.g., waste composition, moisture content, carbon content, landfill, and anaerobic digestion operating parameters). Additional parametric sensitivity analyses will be performed on the most important input parameters to get a better evaluation of the direct relationship between the input and outputs. We have a diverse team of collaborators from academia (North Carolina State University), a national lab (NREL), industry (IBM), and a municipal corporation (the town of Cary) working hand-in-hand to develop this technology. Further, we have many potential commercialization partners, including one of the largest recycling facilities, which is a 15-minute drive from our North Carolina State campus. They have expressed a strong interest in our technology, as they would like to further automate their operations and enhance the quality of their final outputs. Additionally, we have identified strategic partners for each waste stream (paper, plastics, and food) to evaluate our technology. We will continue to engage them and other potential commercialization partners to promote it while ensuring compliance with the overall scope of our project.

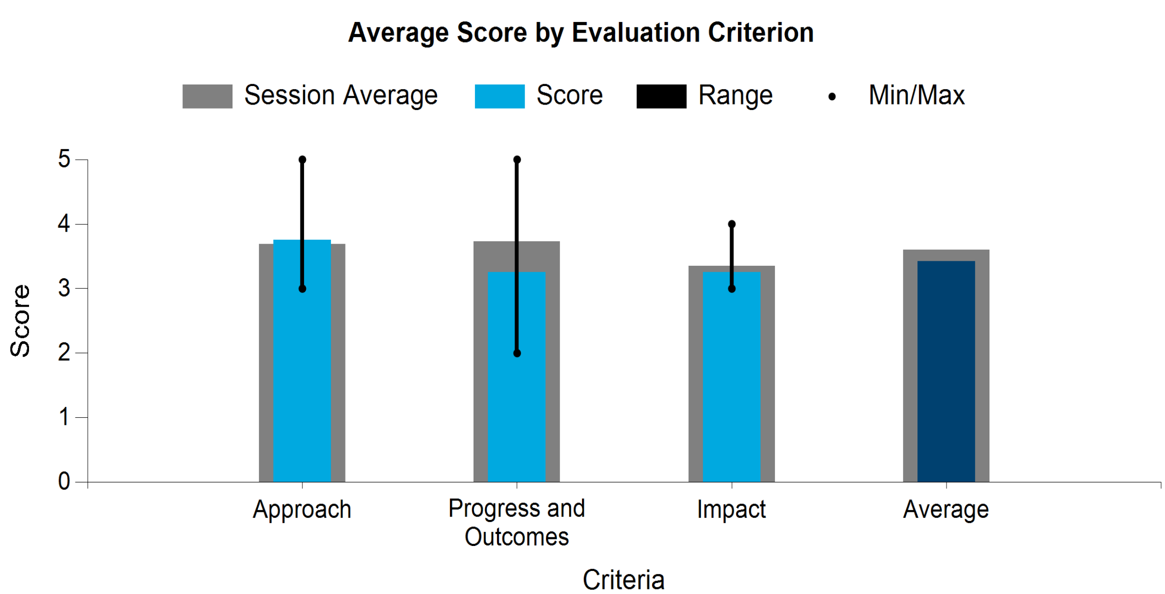
INTEGRATED LIBS-RAMAN-AI SYSTEM FOR REAL-TIME, IN-SITU CHEMICAL ANALYSIS OF MSW STREAMS

Lehigh University

PROJECT DESCRIPTION

WBS:	1.2.2.204
Presenter(s):	Zheng Yao
Project Start Date:	10/01/2021
Planned Project End Date:	01/31/2025
Total Funding:	$3,513,104.00

The overall goal of this project is to demonstrate a leap in developing measurement technology for application in MSW operation, particularly in the characterization of feedstock entering a biofuel reactor that would otherwise be going to a landfill. The end-of-project goal is to improve the throughput of the characterization technology, with a minimum target of 25% improvement over the baseline characterization technology. The proposed technology will allow rapid, in situ characterization of feedstock, providing critical characterization data in minutes for continuous confirmation of feedstock specifications and potential feed-forward process control of downstream biofuel production processes. This represents a hundredfold improvement over current methods of grab sampling, compositing, and costly laboratory analyses that, at a minimum, take several hours to obtain results at a cost of more than a thousand dollars per sampling event. This project targets overcoming challenges associated with packaging laser-induced breakdown spectroscopy (LIBS) and Raman spectroscopy together with AI/ML algorithms into a functional prototype for deployment and demonstration at a gasification process development unit. The project has been able to gather actual refuse-derived fuel, and it is in the process of conducting laboratory testing of material samples under static conditions, while meeting targets for measurement accuracy and precision.



COMMENTS

- The project objectives and approaches are sound and have many similarities to other BETO-funded projects in this area. It is not clear how well and closely these are coordinated. The team is very strong and has the needed skill sets, capabilities, and track record. The project has industrial participation. The project is in the second year of funding. It is not clear what has been accomplished against the milestones and the forward path for Year 3. It would be useful to have a slide showing this information clearly. Slide 7 has details and is not clearly explained. One of the deliverables is an improvement in the overall reliability of waste quality by >25% from the baseline. It isn't quite clear what this means from a practical implementation perspective. It would be better to have a minimum quality needed for gasification at TRL and judge the progress against this metric. Who is the customer for the product from the project at the end of Year 3? What is the expected TRL?

- In terms of approach, the perceived risks and associated mitigation strategies could be further improved. In terms of P&O, the project is making good progress. The development of new algorithms needs to be specific to compare and evaluate them. As far as impact, the presenter said that the project is close to downstream gasification, with TRL 2 to TRL 6. Therefore, its commercialization potential and details on the work plan with Energy Research Company need to be discussed and provided in the upcoming review.

- Land use change and competition with food production are often cited as concerns for lignocellulosic feedstock production. Development of NMSW as a feedstock is warranted because it does not compete with agriculture for food production, and because the use of NMSW will offset the flow of wastes into landfills and mitigate landfill methane emissions. Conversion of wastes into useful products and services is a basic aspect of circular economies. BETO has made significant investments into NMSW research, including the projects reviewed in this report. Some of the challenges of developing NMSW as an economic resource include (1) the extreme heterogeneity of NMSW, and (2) the presence of toxic and undesirable constituents. Therefore, BETO has made significant investments into NMSW characterization, sorting, blending, and milling to overcome these challenges. The other NMSW projects are focused on characterization and sorting at early stages of feedstock preprocessing. This project is developing an AI-enabled system for feedstock characterization immediately before entrainment into the gasifier. The team is using LIBS and Raman spectroscopy, both of which are appropriate for this work. This approach will conduct a chemical constituent analysis rather than looking at NMSW constituent types. The work is on track and is expected to be impactful. They expect a CapEx of $300,000–$500,000 for the system, which seems to be affordable.

- The approach is novel compared to other sensor technologies in that the sensors are positioned downstream, near the gasifier. The real-time data is intended for use in feed-forward process control and has the potential to significantly impact process efficiency. I appreciate the inclusion of the personnel and their roles in the project on page 5. In terms of P&O, good progress has been made. The combination of Raman spectroscopy and LIBS is very useful for characterizing some of the more fundamental chemical properties of the MSW. Comprehensive characterization is proposed, which will cover many applications. The AI model will allow for the identification of important chemical characteristics of variable materials. The aim is to eliminate the cost of sampling/compositing and lab analysis. However, I would expect that sensors would need calibration/verification on a continuing basis. In terms of impact, the team provided a clear evaluation of the value of this technology through operational and maintenance cost reductions yielding a 1-year payback on the instrument cost. The partnership with Covanta is excellent for making sure this will work and make sense in an industrial setting with MSW. This also provides a great opportunity for commercialization. Also, the partnership with ThermoChem Recovery International (TRI) is very helpful for understanding gasification requirements. Both organizations have widespread expertise in their fields.

PI RESPONSE TO REVIEWER COMMENTS

- Response to Comment 1: A slide with an updated report on the milestones has been included in a PowerPoint file uploaded in response to the Project Review comments. Slide 7 has been expanded to clarify it, as well as to explain the 25% improvement deliverable. Slide 7 is included in the uploaded PowerPoint file. TRI participates in the project as the customer for its process development unit. Potential customers of the technology include gasifier designers and operators, waste-to-energy plant operators, and operators of coal refuse circulating fluidized bed boilers. The expected TRL at the end of the project will be 6–7.
- Response to Comment 2: An updated list of risks and mitigation strategies has been included in the uploaded PowerPoint file. Progress on new algorithms is being reported with more detail in quarterly reports. Energy Research Company's LIBS instrument has an advanced TRL of at least 6. It has been used in multiple industrial applications. The commercialization potential for its use, coupled with Lehigh's AI and the National Energy Technology Laboratory's Raman instrument, is quite high, as it will have a payback of well under one year. This is based on its ability to optimize the gasification process. Specifically, it will reduce the oxygen use to its minimum value and increase the hydrogen or syngas production and its heating value.
- Response to Comment 3: No responses were required.
- Response to Comment 4: Concerning the calibration/verification on a continuing basis: That is correct. The instrument will first need to be calibrated, or, in terms of AI, will need to be trained. This is a requirement shared by all instruments if accurate quantitative results are required. The approach is straightforward. Samples of the MSW, in the form used by the customer, will be sent to a lab for analysis. The instrument will provide spectral data from these samples, which will then be processed by the AI models, along with the lab results, for its training. It is important that as wide a range of MSW properties as possible be provided in the customer's MSW feedstock. After the initial training, the instrument will need to be periodically drift corrected. This is still being considered by the team, and will likely entail periodically taking MSW samples, sending them to a lab, and then modifying the AI models.

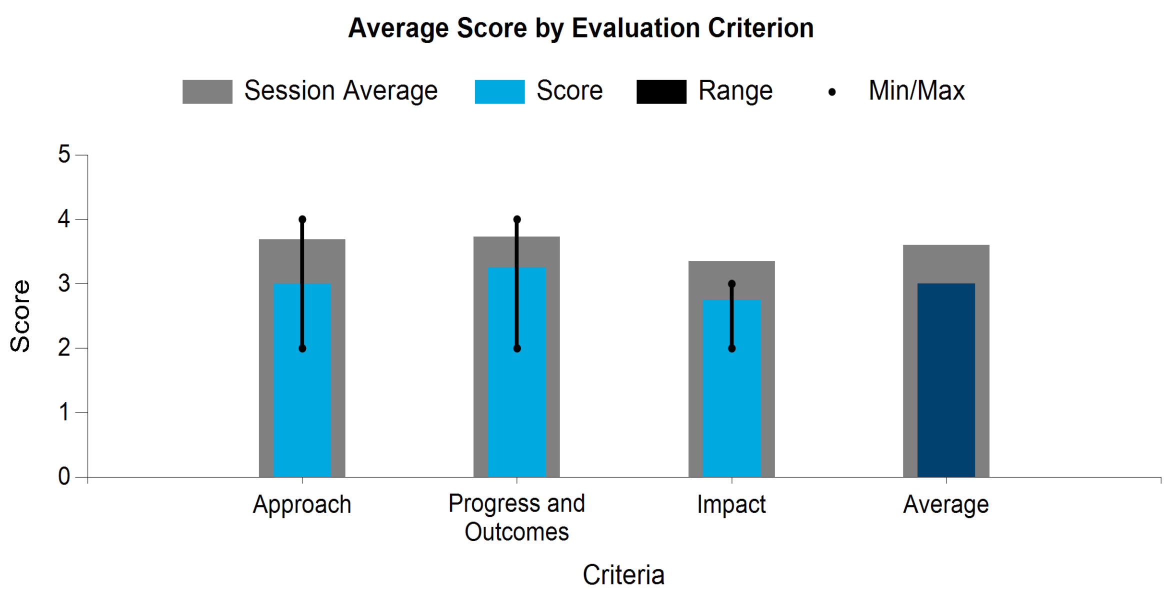
ADVANCING FOREST BIOREFINERIES TOWARDS COMMERCIAL APPLICATIONS THROUGH FRACTIONATION OF BIOMASS WASTES

Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.2.3
Presenter(s):	Luke Williams
Project Start Date:	01/04/2022
Planned Project End Date:	12/31/2024
Total Funding:	$3,000,000.00

Currently, a significant number of pulp and paper mills in Maine are idle or underutilized, and these brownfield facilities could contribute to SAF production. Researchers from the Forest Bioproducts Research Institute at the University of Maine (UMaine) have been working to develop technologies to use these underutilized infrastructures, leading to the development of the thermal deoxygenation (TDO) pathway/technology to convert the cellulose fraction of woody feedstocks to fuels and chemicals. Technical R&D has progressed from market pulp as an ideal feedstock in the Biomass to Bioproducts Pilot Plant to more difficult feedstocks like sawmill residues (sawdust) and forest residues. These new woody feedstocks are presenting challenges due to the physical and compositional material attributes of these waste biomass sources. This project aims to identify the feedstock CMAs for the operational and yield performance of the TDO process and to quantify acceptable limits. Preprocessing strategies will be developed to meet these feedstock CMAs, utilizing the wide range of preprocessing equipment available in the BFNUF at INL. This project will determine the physical and compositional CMAs for the TDO process while also helping define optimal pilot plant operational parameters for improved reliability.



COMMENTS

- The project is primarily focused on improving flow, handling, and processing of woody biomass feedstock for conversion into fuel and chemicals in a TDO unit at UMaine. The approach outlined focuses on particle size, moisture, and grinding of woody biomass to produce a more uniform feedstock for subsequent treatment in a TDO unit. The experimental work is supported by modeling and data analytics. To date, the project has shown some encouraging results and seems to have met the interim milestone. The team is experienced in the technical aspects of the project tasks. The level of potential commercial partner engagement is not clear. What is the current TRL, and what is the projected TRL at the end of the project? Risks and their mitigations are discussed on Slides 10–12. It looks like there are some significant issues related to access of proprietary design data needed for planned activities that may lead to dropping (?) this task. I'm not sure what the impact of such a change would be on the overall outcome of the project. Also, there seem to be some staffing issues. The impact of this is not clear. It would be helpful to have a clear chart showing the expected outcomes, status, etc. in light of these issues. The project needs to have a credible partner and commercialization path. It appears that interaction with potential partners is limited. I recommend that this be given a high priority. The team should work closely with potential customer(s) of the product resulting from the project. Levulinic acid is one of the products targeted in the project. It isn't clear what the market justification for this is. To date, various attempts to commercialize levulinic acid have not been successful. It would be helpful to share some of the successful outcomes of the TDO technology in the field.

- This is a good project. It is not clear if it is an integrated pilot project of INL's pilot and UMaine's pilot plants. I am curious if this integration is the best for future commercialization. In terms of P&O, for char produced from the Biomass to Bioproducts Pilot Plant as a coproduct, it will be good to consider its potential application for future analysis. As far as impact, the pilots are the focus at this point. How far is it for this project to be commercialized with an industry partner?

- BETO investments in feedstock pretreatment are important for optimization of the use of off-spec materials, stabilization during storage, and preparation for conversion processes toward specific products such as SAFs, composite materials, or high-value chemicals. Maine has a successful history in wood product manufacturing and the pulp and paper sector. With the decline of the pulp and paper sector, however, many businesses have ceased operations. The state hosts many underutilized assets in this sector, driving interest in converting these plants for chemical production instead of paper production. This project team includes experts from UMaine, NREL, and the INL BFNUF. They are working to better characterize available feedstocks, reduce C5 sugars, improve the pathway, and reduce char formation. This project is in early stages of implementation and seems to be on track.

- In terms of approach, although this is a nice, detailed study of specific equipment for a specific purpose, it lacks broad application for biorefinery. I am not confident that the information developed within this project will get widespread use in the industry. The aim of uniform delivery of woody wastes is a huge problem and should be looked at, but I don't feel this project has the scope to solve the problem. When defining the contributors on Slide 6, it would be beneficial to identify their roles in the project. I don't see any industrial partners/equipment manufacturers on the collaborator list. Being limited by the IP rights of manufacturers really limits the project's ability to provide meaningful information on specific equipment. In terms of P&O, the progress of the project as designed seems to be on time and appropriate. I'm not sure about the applicability of the particles selected for the screw feeder. Are they a size commonly used by industry now? As far as impact, the project has limited impact for industrial applicability (see approach). The specific customer who could use the project outcomes should be clearly specified.

PI RESPONSE TO REVIEWER COMMENTS

- The overarching goal of this project is to define and meet the physical and chemical CMAs (particle size distribution, aspect ratio, and chemical composition) for biochemical conversion of waste woody biomass to levulinic acid. Biofine Developments Northeast is our commercial partner, and they are planning to build a commercial facility in Lincoln, Maine, to produce levulinic acid and ethyl levulinate from waste woody biomass. We expect that the ongoing project will address processing at the commercial scale with the conversion of waste woody biomass to levulinic acid at the commercial scale by successfully establishing physical and chemical CMAs for the waste woody biomass. As far as limitations/risks, the risks mentioned in the slides around equipment information and personnel have already been overcome by switching the flow system that is being addressed with fundamental models from the progressive cavity pump at Maine that was proprietary to the compression screw feeder at INL. Staff acquisition occurred on time, in part due to the offset start date for the project, and was also accomplished in a way that drastically increased the diversity on the project. Additionally, the limitation of obtaining proprietary information about the pumps will be addressed in the future by (1) experimentally measuring the flow patterns at the pilot scale, (2) exploring a relationship with another pump manufacturer, and (3) investigating smaller-scale pumps designated for research purposes. In terms of broader impacts, the current project findings are also applicable to any biorefinery pretreatment process that employs low-viscosity organic solvents and requires a woody biomass particle size of less than 10 millimeters. The following future work proposed in the new AOP will further broaden the application for biorefineries: (1) establish the physical and chemical CMAs for corn stover, switchgrass, and the biogenic fraction of MSWs; (2) determine the synergistic effects of blending various biomass feedstocks (e.g., corn stover and forest residues) on the performance of biochemical conversion; and (3) upgrade preprocessing rejects from different biomass feedstocks to biocomposites. Additionally, the pilot plants at INL and UMaine are not fully integrated, which leads to added steps around material handoff between the two facilities. This is being addressed with cold flow tests on identical feedstocks. In future research, we intend to look at feedstocks beyond woody material from the Northeast to broaden the applicability of feed handling knowledge to multiple geographic locations.

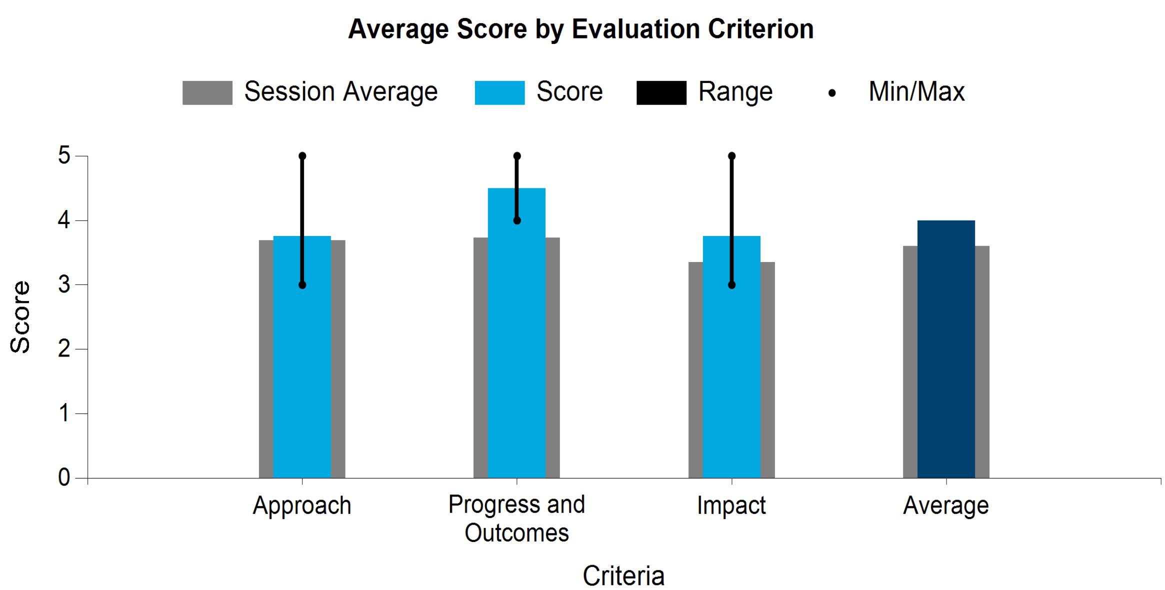
ROADS TO REMOVAL

Lawrence Livermore National Laboratory

PROJECT DESCRIPTION

WBS:	1.2.2.302
Presenter(s):	Roger Aines
Project Start Date:	09/01/2021
Planned Project End Date:	09/01/2023
Total Funding:	$1,000,000.00

Our team is conducting the first economy-wide technical evaluation of CO_2 removal options for achieving net zero by 2050. We are evaluating feasibility, performance, and costs with county level resolution in the United States, considering all well-developed removal methods. We have identified methodology and system boundaries for: forest sequestration, soil sequestration, direct air capture and storage, and biomass carbon removal and storage (BiCRS), and are also evaluating geologic storage, resource availability, and environmental justice. Our initial findings show: (1) improved forest management practices like reducing stocking densities in high fire risk areas and lengthening rotations can increase forest C stocks and decrease forest C emissions. (2) Soil C storage can be increased most effectively by increasing the amount of year-round plant cover and root inputs. Converting low productivity corn/soy cropland to C-crops could lead to soil C increases on the order of 10-20 Mt CO_2 y-1. (3) Much of the United States has geologic storage availability, however some areas will require transport to adjacent areas. (4) We have developed in-depth TEA for 16 unique BiCRS pathways with TRL>8 and integrated these into a model for facility spatial optimization. Our analysis suggests BiCRS has capacity for 0.5 Gt CO_2/yr removals using multiple conversion technologies. (5) Priority regions for direct air capture must have both geologic storage and land for renewable energy.



COMMENTS

- This is a very strong team that has a well-laid-out approach with milestones. The metrics for deployment are not clear. It also isn't clear how much interaction has occurred with end users/commercial entities. On Slide 9, various approaches for mitigation are shown, the highest being converting to electricity followed by H_2 production. It would be helpful to estimate/project the probability for each outcome given the current state of technologies/deployment/TEA, etc.

- In terms of approach, "bioenergy carbon capture and storage" is a commonly used term. The project uses "biomass with carbon removal and storage" (BiCRS). The team needs to describe the difference between these two terms. We also need more details on the improved forest management used in the project, such as management plans and outcomes, especially on plantation, pulpwood, and mass timber production. In terms of P&O, the project needs to provide a little in-depth discussion on progress and outcomes in the next review. As far as impact, we need more details on economic assessments of the five pathways for carbon capture with sensitivity analysis. CO_2 reutilization should be considered. Logging residue for BiCRS in the Northeast should be further discussed.

- Lignocellulosic feedstocks are gaining greater interest as a mechanism to fix atmospheric CO_2 to drive carbon sequestration in natural systems. The decades of bioenergy feedstock production research are foundational to catalyzing current research on atmospheric CO_2 removal, especially if lignocellulosic resources are to serve multiple purposes. This project is very extensive and includes a comparative analysis of five CO_2 removal systems: forests, agricultural soils, BiCRS, direct air capture, and geologic storage. The team is developing a geospatial model, and publication of results is forthcoming, with the intended primary use being a policy development resource. This project has a strong environmental justice component; however, the project is encouraged to also consider transition periods in their timelines.

- This is a very comprehensive high-level project (WOW). It provides important national and regional information on CO_2 removal capacity and costs. This is an important project to better understand the potential of the various mechanisms for CO_2 removal. In terms of approach, the project has a diverse group of collaborators representing the whole nation. Even though the project dealt with five very different CO_2 removal strategies, it appeared that the team had a solid grasp of each. Implications for climate change and other future predictions were not mentioned. These might be significant, as the time frame for CO_2 removal is 2050. As far as P&O, the project end date is quickly approaching, and it appears that the project is on track for successful completion. A lot was accomplished in a short time. The project provided efficient and meaningful information. In terms of impact, the presentation noted that "each region has a story and opportunity"—practical information may be ascertained from this study! The county-by-county assessment brought high-level thinking to the level where it can impact the planning and implementation of some of the relevant strategies.

PI RESPONSE TO REVIEWER COMMENTS

- Comment 1: We appreciate the positive and constructive comments provided by our BETO peer reviewers. With regards to our engagement with "end users," our stated goal for our national carbon dioxide removal assessment was to remain entirely neutral and only engage with industry within limits. The technologies we are assessing are only those where there are "no miracles required"—meaning sufficient evidence of efficacy and broad-scale applicability was available to us as of March 2022. That said, the cost curves we are generating are real and reflect the investment we estimate will be needed in new approaches and technologies. We expect that there will always be unforeseen hurdles to carbon dioxide removal implementation, but we are looking at close-to-commercialization approaches.

- Comment 2: Our group coined (and published) the term "BiCRS" a couple of years ago with our *Getting to Neutral* report, and we feel it is more comprehensive than "bioenergy carbon capture and storage." For BiCRS, the biomass feedstock need not be purpose grown—indeed, in many cases it is literally garbage. Regarding improved forest management, we are certainly assessing specific silvicultural practices and appropriate practices for each of our regional case studies. We do not think that CO_2 reutilization (to fuel) is a type of true removal, and thus we consider it out of scope. If processes can lead to syngas, we would count the financial benefit. However, most CO_2 utilization avenues are not going to result in true CO_2 removals.

- Comment 3: We agree that transition periods are an important element of our national road to removing CO_2 from the atmosphere at scale. However, although timing is certainly important, assessing it was not part of our original mandate, and we feel that an analysis for transition timing would be out of scope. For example, although we are assessing impacts on jobs, we are not forecasting job losses and gains that would involve ramp-up for hiring.
- Comment 4: Regarding how we are considering implications for climate change, we are basing our projections on crop yields in light of climate change. Direct air capture also includes climate shifts, although it is a relatively small factor. For forestry, we are not including CO_2 fertilization effects in our assessment. However, many things that affect forests are projected to get worse (drought, fire, insects), so, while these are not forecastable in a meaningful way, we are assessing the management practices that are needed to deal with them. For soils, our team is including an uncertainty analysis from five different climate projections, because climate change is likely to change projected crop yields, which affects costs. We also have an analysis of transition periods (e.g., 2025 versus 2045).

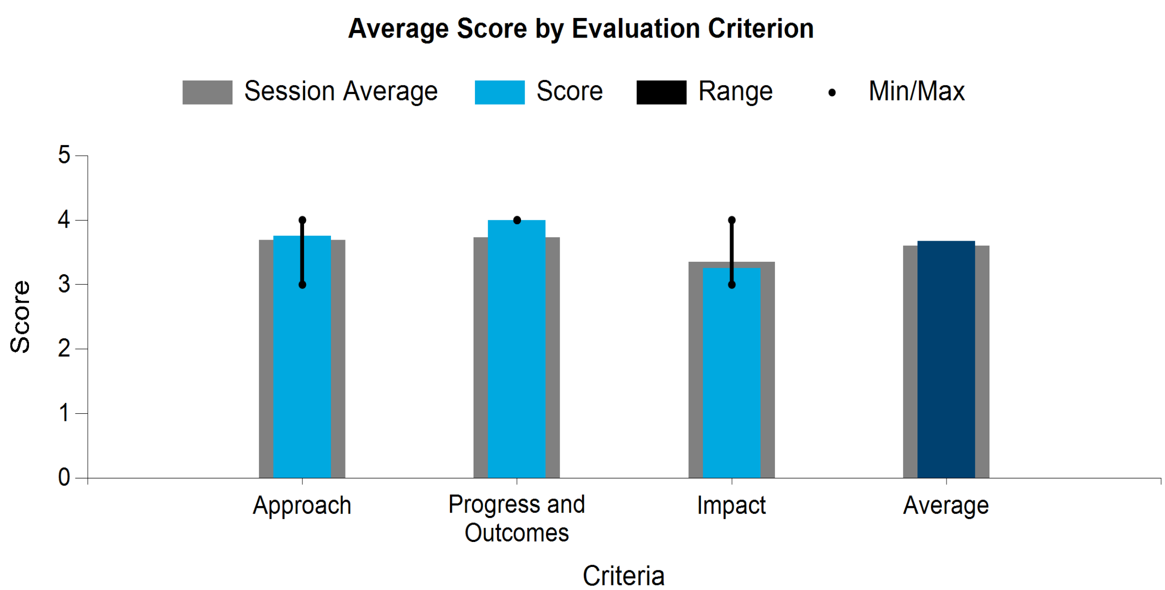
POLYMER PRODUCTS FROM LIGNIN THROUGH DE-AROMATIZATION AND COOH FUNCTIONALIZATION

University of South Carolina

PROJECT DESCRIPTION

WBS:	1.2.3.109
Presenter(s):	Michael Kent
Project Start Date:	10/01/2019
Planned Project End Date:	08/31/2024
Total Funding:	$1,129,722.00

The project focuses on a new method to convert lignin into valuable products. Currently, in the biofuels industry, lignin is burned for heating and therefore has a low economic value. We use a room-temperature oxidative process to open the aromatic rings within the lignin structure and generate a polymeric polyacid material that functions as a commercial agricultural dispersant, micronutrient complexation agent, or water-absorbent material. This project is a collaboration between Ingevity Corporation, the University of South Carolina, and Sandia National Laboratories.



COMMENTS

- This is a very challenging and potentially impactful project to valorize the ubiquitous low-cost supply of lignin. The proposed chemical modification schemes are fairly well known and are practiced to some degree in the industry. Working with an industry partner—Ingevity—to get product performance and cost requirements is a plus. The team has the needed chemical synthesis and characterization/formulation skills to carry out the proposed tasks and deliverables. The project seems to be on track. Some questions: Modified lignin-based formulations that have met the performance requirements seem to have the required cost limit. Does this estimate include the final, fully loaded manufactured cost for the product? Are there any details on the manufacturing process/CapEx/OpEx, etc.? For the hydrogel applications, it looks like the lignin-based carboxy compounds are blended with standard polyacrylic acid (PAA) and polyacrylamide (PAM) hydrogels. What is the swelling ratio of the pure polyacrylic acid (PAA/PAM) hydrogels, and what is it with various levels of the lignin compounds? What is the glass transition temperature (Tg) of the lignin compounds that have shown good swelling? Typically, higher-Tg polymers show lower swelling. Has there been any feedback from Ingevity?

- In terms of approach, more details are needed to explain how related tasks can be implemented. Who will do the field trials for hydrogels? Will it be at lab scale? In terms of P&O, the project is making progress. However, more explanations on the P&O will be needed for the coming year's reporting. Soil type should be considered if hydrogels are applied for soil amendment. The unit cost of hydrogels and the potential mix ratios with biochar need to be clearly addressed with cost/benefit analysis. In terms of impact, some kind of commercialization plan with industry should be addressed.
- BETO investments in feedstock pretreatment are important for optimization of the use of off-spec materials, stabilization during storage, and preparation for conversion processes toward specific products such as SAFs, composite materials, or high-value chemicals. This project focusses on the conversion of lignin to polymers that can be used for chemical dispersants, water purification, hydrogels, and delivery of nutrients in cropping systems. The team evaluated several approaches to cleaving aromatic rings and achieving stabilization via carboxylation. They have conducted informative TEAs on the various approaches and have chosen to emphasize further development of hydrogels for delivery of biochar onto agricultural soils. Field trials will begin in 2023. They have an industry partner to help further develop the products. Two papers have been published thus far.
- A more holistic approach taken by BETO is to be commended. The utilization of byproducts from energy utilization of biomass is important for the economic viability of all biorefinery processes. Lignin, as many know, has a lot of potential and may one day be readily available in the marketplace. Currently, it comes from pulp mills, but it could potentially be generated at a bioethanol refinery. In terms of approach, the team is small but seems to be highly focused. Intimate involvement with Ingevity has its pluses and minuses. They will be focused on current market demand (which is positive) but may miss important opportunities that have longer-term benefits. It may be a concern that Ingevity performs TEA for all samples—there may be some bias. In terms of P&O, lignin use for these applications shows promise. The TEA is not very clear. It produces the metric of $1.5/pound. I would like to see more detail on what is contributing to the TEA. Is this at lab scale, pilot scale, or full scale? As far as impact, this is a product development project that has clear market viability. Product development at the lab scale is demonstrated, but I found details of the TEA lacking and therefore not clear in terms of the viability. The project's success will depend solely on Ingevity commercializing the products, which are high risk. The IP will most likely belong to Ingevity, which limits its accessibility.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the review panel for their constructive feedback and positive comments on the Polymer Products From Lignin project. The TEA was performed by Ingevity to generate the dollars/pound values and included the final fully loaded manufactured cost for the product. The estimates are based on an OpEx model using existing facilities. The lignin hydrogels were generated by reacting oxidized lignins with PAM (not PAA), and the reaction scheme is reported in a publication and also included in one of the supporting slides. We appreciate the panel's question about the swelling ratio of the pure PAM hydrogels compared with that of the lignin-based hydrogels. That is one of the milestones for Budget Period 3. Regarding the Tg for the lignin compounds that have shown good swelling in water, we have not measured the Tg, but we expect it to be low. We note that the lignin is heavily oxidized prior to cross-linking. Although lignins have a range of Tg, it is not considered a performance metric for lignin derivatives used for dispersant applications. Regarding field trials for hydrogels, we apologize if this was not clear in the presentation, but field trials with hydrogels are beyond the scope of the current project. The current project will include measurement of the hydraulic properties of soils mixed with hydrogels as well as the biodegradability of the lignin-derived hydrogels. A follow-on proposal has been submitted to the "Reducing Agricultural Carbon Intensity and Protecting Algal Crops" FOA to perform field trials with lignin-derived hydrogels mixed with biochars. That proposal addresses soil types common in the

Southwest United States, includes a commercialization plan, and involves the agriculture department at New Mexico State University and BioChar Solutions Inc. Regarding the TEA, Ingevity uses the same model for all the samples in this project. Thus, the results can be used for benchmarking with existing product controls. Regarding the review panel's request for more information on the TEA, this is proprietary information that must be protected. We note that the work done within this project was performed at lab scale. Regarding IP, the process for oxidizing lignin and the method for cross-linking oxidized lignin were covered under IP filed prior to this project. Any IP related to formulations developed by Ingevity that include oxidized lignins will be owned by Ingevity.

PERFORMANCE-ADVANTAGED BIOPRODUCTS, BIOPROCESSING SEPARATIONS, AND PLASTICS

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Plastics and Performance-Advantaged Bioproducts Technology Area is one of 12 technology areas reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 48 presentations were reviewed in the Plastics and Performance-Advantaged Bioproducts session by 8 external experts from industry, academia, and other government agencies. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks (www.energy.gov/eere/bioenergy/2023-project-peer-review).

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $68.3 million, which represents approximately 12% of the BETO portfolio reviewed during the 2023 Project Peer Review. During the Project Peer Review meeting, the presenter for each project was given 20–30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Coralie Backlund as the Performance-Advantaged Bioproducts Technology Area review lead, with contractor support from Jessica Phillips of Boston Government Services. In this capacity, Coralie Backlund was responsible for all aspects of review planning and implementation.

PERFORMANCE-ADVANTAGED BIOPRODUCTS REVIEW PANEL

Name	Affiliation
Michael Mang*	Danimer Scientific
Vera Schroeder	Safar Partners Venture Capital
Alper Kiziltas	Amazon
Debbie Mielewski	Dione Solutions

* Lead Reviewer

PLASTICS DECONSTRUCTION AND REDESIGN REVIEW PANEL

Name	Affiliation
Sharon Haynie*	Independent Consultant
Vera Schroeder	Safar Partners Venture Capital
Michelle Seitz	American Association for the Advancement of Science Fellow
Margaret McCauley	U.S. Environmental Protection Agency
Wei Gao	Dow

* Lead Reviewer

PERFORMANCE-ADVANTAGED BIOPRODUCTS AND PLASTICS REVIEW PANEL SUMMARY REPORT

Prepared by the Performance-Advantaged Bioproducts and Plastics Deconstruction and Redesign Review Panels

INTRODUCTION

The review panel members brought a range of experience in different technology areas, from basic science to application development and finance, which provided an excellent cross section of perspectives to the assessments. The panelists' disciplines include biocatalysis, chemical synthesis, chemical engineering, environmental engineering, and materials science. The review panel's research and work experiences cover the sustainable synthesis of monomers and polymers, venture capital funding, environmental assessment, metabolic engineering, polymer processing, and polymer characterization.

The review process was well coordinated, and the panel was able to review a large number of programs and projects quite efficiently. The tools available for the review process worked well. The presentation template used facilitated the flow of each project, making it particularly easy to assess the projects' objectives and progress. The presentations incorporated previous suggestions about including technology readiness levels (TRLs) and process diagrams, making them more effective. The in-person format allowed for good question and response periods, and good discussion was had throughout.

In a relatively short time, the technology manager actively engaged with the projects and exerted the requisite technical knowledge and managerial skills to oversee the work in this relatively large and complex portfolio. The 3-day Project Peer Review session was coordinated well. Each project team was provided with a presentation slide deck to ensure the presence of some key unifying elements among the presentations—specifically, the quad chart, strategy, approach, progress, and impact slides. The in-person meeting allowed adequate time for the review panel (and the general public) to engage in a Q&A with the presenters.

The projects presented to the review panel showed impressive breadth and depth across a broad range of technology areas, demonstrating effective implementation of the program strategy and good scientific and technological progress across the effort. The portfolio has been shaped by a road map formulated from roundtables and then refined with input from many stakeholders from various sectors (advocacy, academia, government, and industry). The value chain of industry partners includes producers, suppliers, waste collectors, and processors. The project themes follow the recommendations that emerged from the roundtable, and projects fall into the categories of deconstruction, upcycling, recycling by design, and scaling and deployment.

STRATEGY

The Performance-Advantaged Bioproducts and Bioprocessing Separations strategy has been to define and develop new fuels and chemicals that provide a genuine environmental benefit over incumbent petroleum-based products, such as an improved carbon footprint. By considering an integrated approach from feedstock to application, the program is able to develop technologies that have a higher likelihood of industrial success and that will meet the strategic goals of the program. The specific targets as they relate to bio-based aviation fuels, new chemical products, and plastics are clearly articulated and relevant to current technological problems. The structure of the Separations Consortium is an excellent example of a focused technology area that exhibits how the strategy is intended to be deployed.

The program design considers input from stakeholders from national laboratories, academia, and industry to design the program strategy and direct the management of the program to the greatest effect. A greater level of broad industry and academic input at the beginning of projects—with the aim of improving the target selection for industrially practical topics—would be valuable, especially in the bioproducts area. In the current program, once the topics are established, there are overall good interactions with industry partners, which helps maintain a focus on commercial acceptance and implementation. There is a good portfolio approach to the program with projects at various stages of development as well as technical risk. The use of techno-economic analysis (TEA) and life cycle analysis (LCA) is valuable, but some effort to standardize how those analyses are carried out will improve their utility in future project designs and assessments. The program is using appropriate funding mechanisms for the various projects with combinations of lab calls (as part of the annual operating plan) and funding opportunity announcements (FOAs).

This technology area has a clear and focused strategy with its own specific goals and technical targets. The strategy is well developed with input from all key stakeholders (industry, advocacy, academic, and government). Since 2021, the plastics technology area has expanded its objectives and sharpened its metrics. First, a specific objective around greenhouse gas (GHG) emissions has been added: designing recycling strategies that mitigate ≥50% of GHG emissions relative to virgin resin or plastic intermediates. Second, addressing the end-of-life fate now has a quantitative target metric and will address end-of-life fate for ≥90% of all plastics (replacing "most").

This technology area funds a mix of early-, mid-, and later-stage programs; the split between the FOA and annual operating plan funding mechanisms seems appropriate. A casual analysis of project descriptions suggests that there is a reasonable number and diversity of projects in the key goals outlined for the strategy for plastics innovation: deconstruction, upcycling, recycling by design, and scaling and deployment; however, one reviewer recommends that the managing agencies (DOE/BETO) take an additional step and map the current portfolio by keyword metrics. For example, for project focus, that could include new material development or deconstruction and upcycling process development, type of polymer, application, and waste stream. Scrutiny of the projects in this manner may reveal whether there are funding gaps and whether the appropriate mix of activities is being pursued by BETO. Moreover, if this analysis included other DOE technology areas that fund plastic circularity activities (e.g., Advanced Materials and Manufacturing Technologies Office [AMMTO]), BETO could seek and monitor mutual activities (communications, collaborations) across these technology areas that may be beneficial.

STRATEGY IMPLEMENTATION AND PROGRESS

The technology area is funding a strong cross section of projects that strongly ties to the strategic goals of the program. There are three primary technology objectives outlined for the program in aviation biofuels, new chemical products, and polymers. The funded projects effectively address some aspects of each objective. The adsorptive denitrogenation project was rated highly by the review panel and has an excellent approach with excellent alignment with the aviation biofuel objectives. The effort to broadly include TEA and LCA is particularly valuable. Any advances made in the broad area of bioproducts require three elements: technical performance, economic viability, and environmental benefit. Including the TEA and LCA helps ensure that the technical work does not proceed too far without proper consideration of the economic and environmental performance. Further integration of those methods will help ensure that future work is being done to most effectively further the strategic goals of the technology area. Artificial intelligence (AI) and machine learning (ML) may be technologies that are too immature to provide value to current efforts.

The Separations Consortium is well structured to advance the strategic objectives of the technology area, with an excellent collaborative nature and very good interactions with industry partners. The impact of the industry advisory board's (IAB's) input is apparent, with good alignment of projects toward industrially relevant technology objectives. The biobutanol project is a particularly good example of this, showing how the integration of separation technologies with front-end biological manufacturing can demonstrate considerable technical value along with reduced costs and lower emissions.

The projects funded by the technology area represent a broad portfolio of project maturities, from early stage to the small pilot scale. The portfolio approach helps mitigate the technical risk associated with the early-stage projects. The work across projects can be described as leading edge and is consistent with high-quality technical efforts throughout. One good example is the volatile products recovery project, which scored highly on both approach and impact.

The projects individually showed good progress. Some early-stage projects had only a few months of effort, but progress was apparent, and the later-stage projects (some of which were essentially completed) showed that the individual project objectives had been met. Because of the design of the portfolio and the way risk mitigation strategies have been employed across the program, progress against strategic objectives has a good probability of success in both the short term and the medium term. The longer-term industrial acceptance of many of these products and technologies is still uncertain, but the perspective carried forward with the integration of TEA and LCA with input from industry partners will increase the likelihood of success.

The projects are also well managed both individually and at the program level to provide beneficial outcomes for the performer and the government. The overall program approach to project management is very active, with regular review, industry and academic partner input, and good use of go/no-go points as checks against progress keeping the projects on track toward completion. There is better industry engagement with the Separations Consortium than with the Performance-Advantaged Bioproducts (PABP).

The projects are well aligned with the strategic objectives of the technology portfolio. Only a single project (Highly Recyclable Thermosets for Lightweight Composites) was flagged as one that may better fit with another technology office. The reviewers were impressed with most projects. The scores and the individual comments supported project ratings where strengths exceeded (or far exceeded) project weaknesses. In general, the range in panel review scores aligned with comments on a particular project, and the panel comments were more complementary than divergent. Most projects in the plastics portfolio with scores trending below the Project Peer Review session average were early-stage projects. Although the diversity, equity, and inclusion (DEI) activities across projects in this portfolio were not uniform in their depth and breadth, most project teams did an adequate job of addressing and describing DEI activities.

The portfolio is examining the deconstruction of a diverse array of plastic waste compositions (e.g., polyester [polyethylene terephthalate, or PET], polyurethanes [PUs], and polyolefins [polyethylene, or PE, and polypropylene, or PP]). The material forms were also diverse: multilayer films, single-material plastic, composites, waste flake, and fabric (post-consumer waste and industrial waste). The reviewers commend the addition of PET fabrics to the waste stream, as this was an important target gap that was highlighted in the 2021 Plastics Project Peer Review. The deconstruction strategy featured projects with diverse technologies, including thermal, pyrolysis, chemical, and biological options—a multipronged strategy that allows greater leeway to choose the most promising and efficient path. Within the plastics portfolio, there are early-stage and novel technologies represented with an opportunity to demonstrate proof of concept. The Bio-Optimized Technologies to Keep Thermoplastics out of Landfills and the Environment (BOTTLE™) Consortium is a crown jewel in the BETO portfolio, and the panel was aligned in assigning high scores for each area (management, approach and implementation, and impact) for nearly every BOTTLE Consortium presentation. The review panel applauds the quick sunsetting of the technologies that did not fulfill expectations (e.g., the photochemical and electrochemical deconstruction approaches described in BOTTLE 3).

LCA/TEA and industry engagement were key focal points in this Project Peer Review. The strong consensus among the reviewers is that the integration of LCA and TEA early on in a program increases the probability of better project outcomes. Better engagement of industry members (through IABs) was a recommendation from the 2021 Project Peer Review panel. This recommendation is validated because this 2023 Project Peer Review panel sees a correlation between impact and a potential path to commercialization when there is early, active engagement by an industry partner.

This Project Peer Review panel feels that the current portfolio of projects is likely to meet most of the stated near-term and medium-term goals in the four goal areas under the plastics strategy. The detailed project commentaries support this overall view of the progress in this portfolio. In this high-level summary, we offer five projects that are representative of the spectrum of progress toward the goals. The review panel was enthusiastic about the progress made in the Lubricating Oils From Upcycled Plastics (LOUPs) project, which converts single-use polyolefins into higher-valued lubricating oils. The LOUPs team was noted for performing parallel LCA/TEA, and the team's early success has yielded a spinoff company. Additionally, the LOUPs project team had a clear vision and addressed nearly all the elements in the value chain (additives, processing considerations, and end applications). For the goal of recyclability by design, the panel recognizes the new chemistry achievements of the Responsible Innovation for Highly Recyclable Plastics (ResIn) project. The project team addressed the concerns raised in the 2021 Plastics Project Peer Review and is on track to deliver bio-based PU derivatives that are moving toward the portfolio target metrics. In addition, the tunable PU derivatives bring functional value to engaged industry partners. Another recyclable-by-design project that is on the leading edge of science discovery work is supported in the BOTTLE redesign and modeling work—in particular, the redesign by Eugene Chen and colleagues to create chemically circular melt-processable polyhydroxyalkanoates with physical properties similar to those of other polymer classes. This project has related BETO-funded work that was recently featured in *Science* (https://doi.org/10.1126/science.adg4520) and rebroadcast in other technical trade journals. The IBM-led project to upcycle PET via the volatile catalyst (VolCat) process is a higher-TRL development project with a clear commercial goal. Its target product, bis(2-hydroxyethyl terephthalate) (BHET), can plug into existing infrastructure. This program has tested real PET industrial waste streams (flake and fabric) and is focused on the right elements to pilot the process within the next year. For a project targeting a long-term deconstruction goal, the panel was intrigued by the novelty and potential of AMO.01—which deploys microbial spores that were evolved to survive higher temperatures and to grow on a thermoplastic polyurethane (TPU). Although the presence of the evolved spore strains has not shown any significant impact on TPU degradation rates, the team has demonstrated considerable progress in their biological work. The progress to date is consistent with the expectation that advancing biological systems for deconstruction is a long-term goal (up to 10 years).

These final three comments around strategy implementation cut across the portfolio:

- The review panel suggests two additions to the presentation content. The reviewers noted that there were gaps or a lack of clarity around how the industry partners were engaged in many projects. The panel felt that it would benefit the review process if BETO were to establish a rubric for categorizing industry participation (e.g., advisory, collaboration, funding, material or prototype suppliers). This industry engagement descriptor could be placed on the quad chart. Second, the reviewers urge that all project teams (a) supply a Gantt chart with tasks, milestones, go/no-go decision points, and project quarters; and (b) include an absolute timescale on the chart (e.g., overlay with the program years).

- An alternative view was offered on the cooperative research and development agreement (CRADA) template for industry engagement with the BOTTLE Consortium. Specifically, the reviewer stressed that exclusive licenses are a barrier to pushing technologies out for broad deployment and could compromise the achievement of objectives. It was suggested that BETO should explore alternative licensing models and not offer exclusive licenses to single companies if the work is partly government-funded.

- A reviewer raised a concern that polymer processing considerations in early projects within the portfolio were largely absent. Chemistry-push projects should be integrated with expert guidance on polymer processing, as it is important to consider whether the new materials can feed into existing infrastructure or if new infrastructure will be required.

RECOMMENDATIONS

Recommendation 1: Independent assignment of TRL.

We recommend that an entity outside the team—e.g., the technology manager—assess/assign the TRL for each project in the portfolio. There was general skepticism among the reviewers about the accuracy of the self-assessed TRLs. The panel disagreed with some individually assessed TRLs for projects and felt that the review would have been more effective if those TRLs were assigned by an external party or parties. The TRL assignments did not align with the reviewers' sense of the project's technology status. We recommend that the person with this role offer a concrete example as a benchmark. We recognize that there will be some subjectivity in the assessment, but a single assessor would generate more consistent assignments across the entire portfolio. Engaging the principal investigator (PI)/research team in a dialogue to reconcile the TRL would also be a healthy educational opportunity. This could be part of the regular management and review process and would allow progress to be assessed on a consensus basis.

Recommendation 2: Encourage project teams to perform LCA and TEA early in the project.

We suggest further developing a consistent framework for TEA and LCA during the life cycle of a project. There should be a standard applied to early-stage projects that becomes increasingly detailed and more probable as a project matures. The framework should be broadly communicated so that it is clear what calculations have been applied and how likely they are to be correct for each project. The reviewers strongly encourage integrating this from the beginning to steer choices; it should be used in the individual go/no-go decisions, as it will become adopted by teams if it is institutionalized. If BETO encourages cross-project sharing of LCA/TEA boundaries and assumptions, this will enhance consistency and the ability of reviewers and the technology manager to compare across projects. It may be useful to connect this framework to the TRL.

Recommendation 3: Encourage engagement of teams across the portfolio.

We recommend aiming to build bridges (communication, collaboration) between projects that appear to have natural synergies or interests. A hypothetical example is the all-PET multilayer film project engaging with other PET recycling projects to understand key end-of-life issues. Consistent use of industry and subject matter experts with more involvement from IABs from the onset of projects and throughout will substantially improve the relevance of the programs. There is considerable variability in the application of external reviews, with excellent involvement in the Separations Consortium but less in some of the other project areas. A more formal approach to industry engagement and cross-project collaboration may be helpful here.

PLASTIC DECONSTRUCTION AND REDESIGN PROGRAMMATIC RESPONSE

INTRODUCTION

The program thanks the reviewers for their dedication and thoughtful review of this diverse portfolio. BETO greatly appreciates the reviewers' efforts and expert recommendations, which will significantly contribute to the success and effectiveness of our initiatives. The program agrees with the reviewers' assessment that the plastics portfolio continues to benefit from industry engagement, though inconsistency with reporting this could be streamlined to facilitate the review process. Future development of industry engagement could be strategically used to shape new material design via expert guidance on polymer processing. Specific recommendations and feedback will be discussed and considered when working on future project selection and program design, as future appropriations allow. For each recommendation, BETO has provided a general response, followed by some specific examples of how the feedback will be integrated into the technology area covered in this session.

Recommendation 1: Independent assignment of TRL.

The program thanks the reviewers for their insightful review and valuable recommendations regarding the assignment of TRLs for projects in our portfolio. As we are committed to continuously improving our processes to ensure accuracy and consistency in TRL assessments, this is an excellent suggestion; it will allow for more realistic cross-portfolio analysis.

Based on your suggestion, we recognize the importance of having an entity outside the project teams, such as the technology manager, assume the responsibility of assessing and assigning TRLs. This approach will help eliminate potential biases and provide a more objective evaluation of the TRL.

To address the concern of skepticism among reviewers about self-assessed TRLs, we acknowledge the need for a concrete example as a benchmark to guide the assessment process. Providing a clear reference point will enhance the reliability of TRL assignments and ensure that they better align with the reviewers' perception of the project's technology status.

BETO understands that there might be some subjectivity in the TRL assessment process, but having a single assessor for the entire portfolio will indeed promote greater consistency across projects for the reviewers. We are keen on implementing this approach to maintain uniformity and fairness in our evaluations.

In addition, we agree that engaging the PI and research team in a dialogue to reconcile the TRL will be a valuable educational opportunity. This open discussion will foster better understanding and communication among all stakeholders and will lead to more accurate and meaningful TRL assignments.

Recommendation 2: Encourage project teams to perform LCA and TEA early in the project.

BETO thanks the reviewers for recognizing the importance and effectiveness of detailed LCA and TEA for the success and impact of projects.

We completely agree with your recommendation to encourage project teams to perform LCA and TEA early in the project's life cycle. By integrating these assessments from the beginning, we can better steer our choices and ensure that our decisions align with the most sustainable and economically viable options. We have begun requiring these as milestones within each budget period for our more recently funded projects.

The reviewers' suggestion to utilize LCA and TEA in individual go/no-go decisions is an excellent approach that is currently being adopted by project teams. By making them an integral part of our decision-making process, we have begun to institutionalize their importance and ensure they become standard practice across projects.

Moreover, we recognize the potential benefits of promoting cross-project sharing of LCA/TEA boundaries and assumptions. Enhancing consistency in these aspects will not only streamline the review process but also empower technology managers and reviewers to make more accurate comparisons across different projects, leading to better-informed decisions throughout the life of the project and across the portfolio.

Recommendation 3: Encourage engagement of teams across the portfolio.

The program thanks the reviewers for their insightful suggestion to encourage the engagement of teams across our project portfolio. This suggestion perfectly aligns with our goal of fostering collaboration and communication to maximize the potential synergies and shared interests among projects.

Building bridges between projects is an excellent strategy to promote effective communication and collaboration. Your hypothetical example of the all-PET multilayer film project engaging with other PET recycling projects to understand key end-of-life issues is a compelling illustration of the potential benefits that can arise from such interactions.

To implement this approach, we will actively encourage project teams to identify areas of natural synergy and shared interests with other projects. By fostering open dialogue and knowledge exchange between teams, we can enhance the overall effectiveness and impact of our portfolio initiatives.

Further, we recognize the significance of sharing best practices and lessons learned among projects. Encouraging such cross-pollination of ideas will not only strengthen individual projects but also contribute to the advancement of the entire portfolio.

We genuinely appreciate your valuable input and will make concerted efforts to promote engagement and collaboration among teams across our portfolio.

UPCYCLING OF CFRP WASTE: VIABLE ECO-FRIENDLY CHEMICAL RECYCLING AND MANUFACTURING OF NOVEL REPAIRABLE AND RECYCLABLE COMPOSITES

Washington State University

WBS:	2.2.3.400
Presenter(s):	Jinwen Zhang
Project Start Date:	10/01/2019
Planned Project End Date:	06/30/2023
Total Funding:	$2,051,949

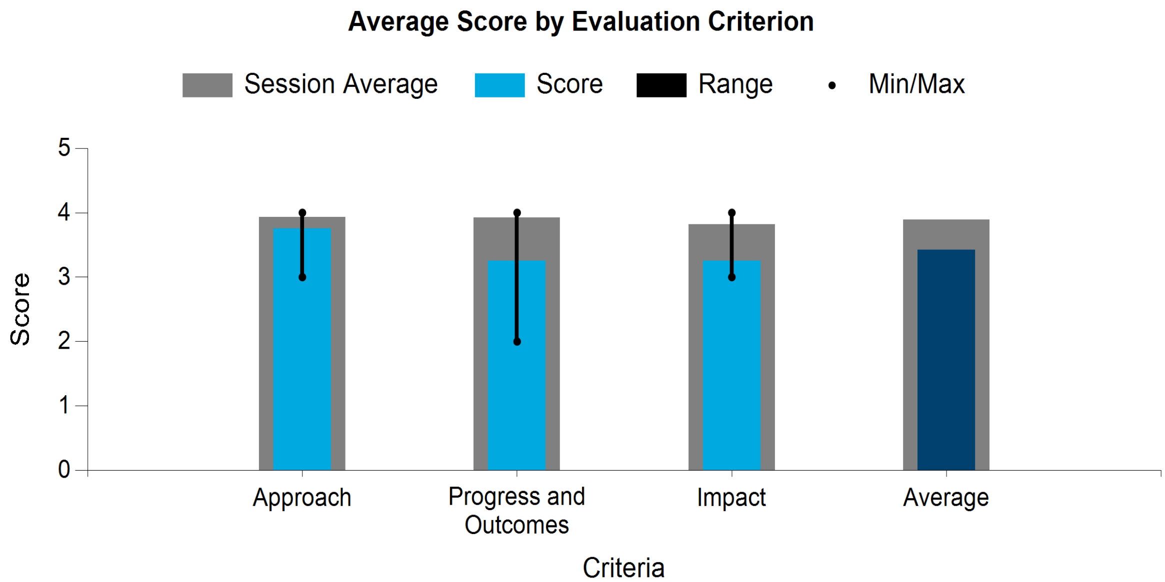
PROJECT DESCRIPTION

A team of researchers led by Washington State University will collaborate on a project entitled "Upcycling of Carbon-Fiber-Reinforced Polymer (CFRP) Waste: Viable Eco-Friendly Chemical Recycling and Manufacturing of Novel Repairable and Recyclable Composites," sponsored by the DOE Office of Energy Efficiency and Renewable Energy (EERE). In this project, the researchers aim to develop a viable chemical recycling technology for carbon-fiber-reinforced epoxy composite (CFEP) waste that is eco-friendly, energy-efficient, and cost-effective in breaking down the matrix polymer structure and makes use of both recovered carbon fiber and decomposed matrix polymer in new advanced composite manufacturing.

The rapid growth of the polymer composite market also propels researchers to find value-added applications for out-of-date prepregs, manufacturing scraps, and end-of-life components. At present, most polymer composite wastes are disposed of by burning or landfilling. To make use of the residual value and reduce the burden to the environment, various mechanical, thermal, and chemical approaches have been attempted to recover the fiber, matrix, or both; however, these current practices exhibit a lack of low-cost effectiveness, are energy-inefficient, generate secondary waste, and bring new pollution problems. In this project, the research team will develop a new CFEP recycling platform that addresses all the existing problems with current recycling methods and will introduce high-value polymer materials based on the recyclates. The key innovation is in the integration of the mild chemical recycling of CFEP and the preparation of new composites.

The success of this project will address the most significant cost/technology barriers for thermosetting composite recycling. With this technical research success, the developed technology will move from the lab scale to the small pilot scale in collaboration with commercial partners. We expect to advance the technology from the current TRL of 2–3 to TRL 4–5 by the end of this project.

The project is led by Washington State University professor Jinwen Zhang, and the major team members include Tuan Liu and Michael Wolcott, both from Washington State University; Long Jiang of North Dakota State University; and Kevin Simmons of Pacific Northwest National Laboratory (PNNL).



COMMENTS

- Recycling of carbon-fiber-reinforced plastics is energy-intensive, not cost-effective, and requires harsh conditions and secondary waste. The team is aiming to develop an eco-friendly, energy-efficient, and cost-effective chemical recycling technology to address these issues. There has been great progress in this review period. The project is on track, and the team is ahead of schedule. There is always a question about carbon fiber recycling in terms of LCA. The team should run an LCA and compare their results with other recycling methods and carbon fiber from lignin. Cost is still a challenge for implementing the recovered carbon fiber in composites applications, and therefore the team should focus on cost reduction items in their approach for scalability and transferability. The mechanical and thermal properties of recovered carbon fiber were not presented. It would be great to see the retention or decrease in the mechanical properties of the recovered carbon fiber. The PI did not present the DEI strategy and progress.

- The project has made good technical progress in defining process conditions to recover both carbon fiber and resin from carbon fiber automotive, wind, and aerospace composites. The PI has gone beyond the statement of project objectives and developed a one-step swelling-decomposition process and an atmospheric pressure process. These are both important for reducing the environmental impact. Is this process too messy to scale up industrially? It would be interesting to understand the cost implications of the vitrimer composites. Not much was shared on the vitrimer composite work. Further work should include active participation of industry partners and understanding of the durability and recyclability of the vitrimer composites.

- This project provides a good approach to a difficult recycling problem and advances the goals of the program with good progress toward the project milestones. There has been good collaboration among academia, the labs, and industry to complete the project, with appropriate application of TEA to validate the costs of the process. It would be useful to have more complete data on the reusability of the recovered carbon fiber to determine whether the recycling process deleteriously affects the physical properties of a new composite made with recycled fibers. The impact would be significantly greater if the fibers were not being downcycled during this process, and it is not apparent that they retain their performance. The disposition of the degraded resin should be described better, as it was not clear what would become of that material (whether a recovery of chemical value for new resins or just as fuel value).

- The team needs to analyze the environmental impact of their process to be able to judge if it is indeed eco-friendly. I would suggest preparing a TEA and LCA that compares the process to virgin material (is it cheaper/better for the environment to use the recycling process versus starting with new material?). The team did not build a prototype of its process to scale beyond the bench scale with their current system. I appreciate that the team is talking to Boeing and Toray about this upcycling method and is continuing the conversation to further scale up this method. I would suggest that the team further engage its industry partners to help with scale-up as well as verify that its recycled materials can be reused in the targeted applications.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the comments from the reviewers. We did not propose an LCA study in the original proposal. During the implementation of the project, we also obtained permission from the project manager to not pursue the LCA, as the chemical recycling proposed in this project is unprecedented and we did not have any reference for doing the LCA. The recovered carbon fiber retained approximately 91% of the original carbon fiber's strength and exhibited almost identical thermal stability. We have recently identified a new solvent system that is eco-friendly, inexpensive, and can be used for chemical recycling of CFRP below 200°C at ambient pressure. We are very hopeful that this new resin system will make the recycling process more economic. We will continue to engage with related industrial companies for potential collaboration for technology transfer. Our industry partner in this project, Global Fiberglass Solutions, is a minority-owned small company in Washington state. We have also trained an American Hispanic student for his master's study on this project for 2 years.

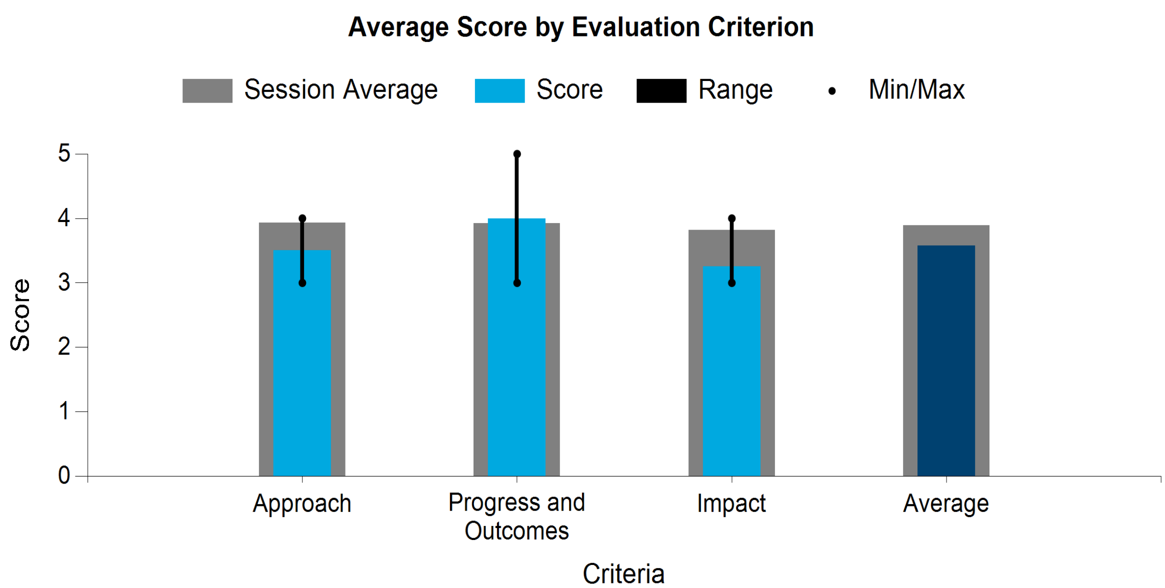
DESIGN AND DEVELOPMENT OF BIO-ADVANTAGED VITRIMERS AS CLOSED-LOOP BIOPRODUCTS

University of California, Berkeley

PROJECT DESCRIPTION

WBS:	2.3.2.219
Presenter(s):	Jay Keasling
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2023
Total Funding:	$2,497,327

Plastics in use today are predominantly single-use and are rarely recycled. The linearity of their life cycle is not only wasteful from a resource and energy perspective but has also resulted in environmental stresses with more than 6 billion metric tons of plastic waste. The goal of this project is to elucidate design rules by which life cycles for plastics become circular and therefore sustainable. We focus our efforts on a new class of dynamic covalent polymer networks, known as vitrimers, which combine the processing and recycling ease of thermoplastics with the performance advantages of thermosets. Regarding circularity, most vitrimers are differentiated from classical thermosets in that they can be chemically de-polymerized, typically into small molecules or short oligomers, including dimedone, ß-keto-d-lactone (BKDLs), and diacids in this project. For decades, the microbial production of commodity chemicals has been limited in the diversity of the molecules produced by natural or modified enzymes. Our technology of recombining the Type I polyketide synthases demonstrates a promising strategy for the synthesis of diverse molecules, including BKDLs and diacids. With computational materials genomics of vitrimers and TEA and LCA for bioproducts, we can design and develop infinitely recyclable and therefore closed-loop polymeric bio-based materials for potential commercialization.



COMMENTS

- The team’s technology of recombining the Type I polyketide synthases demonstrates a promising strategy for synthesizing diverse molecules, including BKDLs and diacids. Using this approach, the team can design next-generation sustainable plastics and composites. The team also incorporated computational materials genomics of vitrimers and TEA and LCA for bioproducts. They selected the right polymer to work on this proposal. There is a lack of research in PU foams in terms of recyclability/circularity of plastics recovered. There has been some progress in this review period. The project is still in the development stage. The TRL should be updated at the end of the project. The PI and the team need to meet and have a serious discussion with their industry partners for the target applications. It is very difficult to pass the requirements for automotive seating. They should focus more on under-the-hood and under-the-carpet foam applications. Achieving PU foams with >75% biomass content and meeting all the durability and design requirements for the final PU applications is extremely difficult. The PI did not present the DEI strategy and progress.

- The concept of infinitely recyclable poly(diketoenamine)s, as vitrimers, replacing petrol-based chemicals like PUs is innovative and addresses an unmet need for the circularity of cross-liked polymers. As such, the team has a difficult road ahead in changing materials and systems that have long been in place, scaled, and optimized. PU foams for the applications identified (automotive seating and mattresses) have an exceedingly difficult list of properties to meet, including density, odor, cell size, compression modulus, compression set, fogging, and tear. The characterization and material properties of the isocyanate, polyol, and novel foams were not provided. Although original equipment manufacturers have shown interest, they should provide specifications for seating foams as a control so that materials can be tailored to meet these requirements. There should be identified partners throughout the supply chain (Tier 1, 2, 3). It is unclear how much this technology could supply the 21 million ton/year PU market as far as scalability. It might be better for the project to focus on foams that have lower performance requirements, such as automotive headliner foams.
- Very good progress has been made on this well-managed project to provide an alternative recycling process for PET. The project has made appropriate use of TEA and LCA to inform the work and to demonstrate potential viability for such a process. There has been excellent collaborative work between academia and the labs to achieve the progress that has been made to date. The application of *in situ* product recovery is an innovative approach to recovering valuable products from the process, and there is a strong sense of industrial practicality in the upstream process steps (including extrusion) that were investigated.
- The team has fulfilled the performance metrics as laid out in its proposal. I appreciate the team's approach to creating novel, recyclable vitrimers. To enable translating this technology into industry, I would implore the team to quantify the processability of their plastics as well as the foaming of their plastics. The proposed material is economically and environmentally viable at 99% recyclability. To further this project, the team should investigate with industry partners ways to realize these very high recycling numbers.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for the very positive comments. Lawrence Berkeley National Laboratory is negotiating a license to this technology with multiple companies. We are looking beyond seating for automobiles to several other important applications.

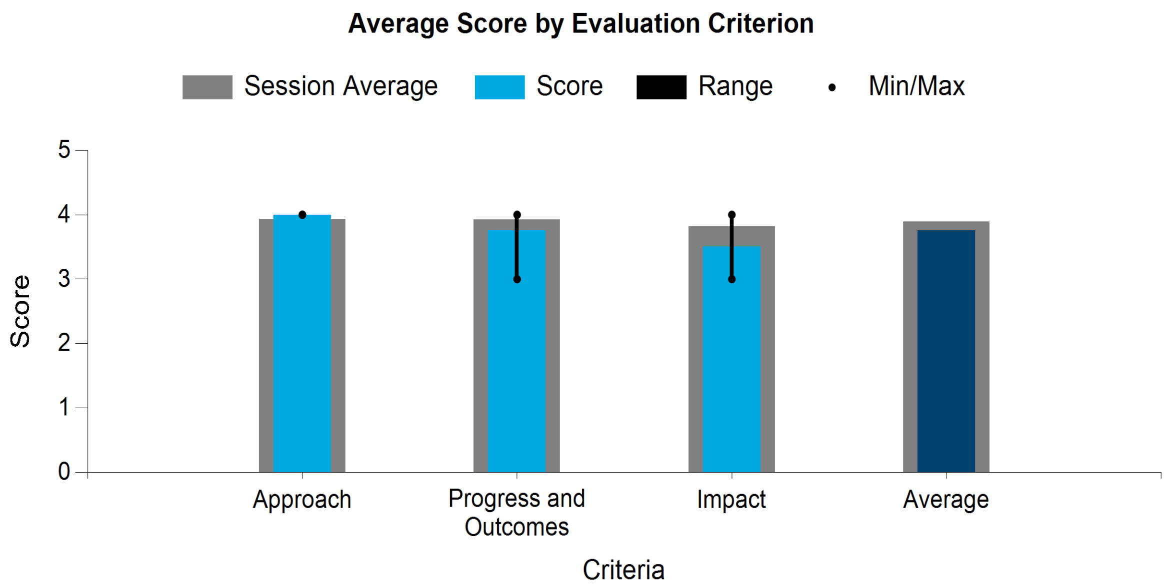
BIOCONVERSION OF HETEROGENEOUS POLYESTER WASTES TO HIGH-VALUE CHEMICAL PRODUCTS

University of Massachusetts Lowell

PROJECT DESCRIPTION

WBS:	2.3.2.224
Presenter(s):	Margaret Sobkowicz-Kline
Project Start Date:	10/01/2019
Planned Project End Date:	06/30/2023
Total Funding:	$1,921,237

This project aims to discover, evaluate, and develop pathways for the economic biochemical recycling of waste polyesters into small-molecule products used in the chemicals and materials industries. A major hurdle in recycling plastics to high-value chemicals is the energy intensity of the process, which could be improved using microbial deconstruction. The aims of the project are to (1) study efficient pretreatment strategies to prepare diverse polyester wastes for deconstruction, (2) develop optimal enzyme combinations for the production of terephthalic acid (TPA) from PET waste, and (3) scale up reactor design for high-efficiency product recovery. The project will enable industry to deploy high-performing drop-in chemicals as an alternative to conventional unsustainable sources.



COMMENTS

- The team tried to develop a biochemical conversion process for the microbial production of specialized degradation enzymes for recalcitrant polyesters as well as bioconversion of the degradation products to high-value-added chemicals, guided by TEA. The team also evaluated different PET waste streams and characteristics for degradation. There were improvements in the minimum selling price and environmental impact resulting from lowered electricity costs for pelletizing versus cryogrinding for recycled terephthalic acid (r-TPA). There has been some progress in this review period. The project is on track. The PI and the team should look at other challenging post-consumer PET wastes, such as automotive waste (headliner and seat fabric, under-body shield and wheel liner, carpet), carpets, and colored textile wastes. If they can focus on these wastes that are not easily recycled (contamination and used chemicals for coloring), that could be a true game-changer. As far as I know, the enzymes digest the PET and leave the rest. The team should also increase their engagement with their industry partners to understand materials and cost requirements. A detailed DEI plan will be great.

- The project has made progress toward the goal of addressing the enzymatic recycling of PET mixed waste to TPA. The PI has a strong DEI plan, including active bystander training. Progress has been made in quantifying the mechanical properties of a wide variety of PET waste streams, identifying appropriate enzymes, and exploring pretreatment through melt processing. Real-life PET mixed waste streams will include a vast selection of dyes, colorants, and other additives. How these will affect both the extrusion process and the enzymes and yield of TPA should start to be addressed. Recycled materials with colorants (generally black because of mixed colors) are of much lower value than a purified product that can be recolored. It is unclear whether there is a higher level of engagement between the researchers and the companies that provided PET samples. Understanding their needs and challenges could help refine the project goals to ensure TRL 4–5 at the end of the project.

- This project provided a very innovative approach to developing high-value products from waste streams. It made excellent use of computational methods and molecular biology to produce new molecules that could have a significant impact on a developing bioproduct market. The project made excellent progress toward its milestones and showed a very good collaborative effort across the labs and academia. The progress through scale-up in fermentation was excellent, and the TEA and LCA were appropriately applied. This project could have benefited from more interactions with an industry partner. The suggested end use for the technology (flexible foams) is a noble target but one for which practical advice on the probabilities of reaching that target would have been a benefit.

- The team has presented a viable strategy to recycle polyester waste. I appreciate that the team has already tried feed streams other than bottle flake, including mylar film and textiles. I suggest that the team work with material recovery facilities (MRFs) and source real-world recycling streams to prove the translatability of their approach and test the influence of additives and dyes on their enzymes. On the commercialization side, the team is ready to move to work on reactor design, scale-up, and system integration. I suggest that the team reach out to industry partners to help with scale-up and integration as well as with potential offtakers of their products (TPA, etc.).

PI RESPONSE TO REVIEWER COMMENTS

- Thanks to the peer reviewers for their thoughtful comments on our project. We identified two primary topics that the reviewers brought up, and we will respond to them here. On the subject of diverse PET waste sources: We agree that this technology would be particularly useful for mixed and contaminated waste streams. The project team has preliminarily evaluated some diverse PET sources for feedstocks in the enzymatic depolymerization process, including textile waste, film, and metallized film. There are two complications that prevent more in-depth investigations in this area. First, our extrusion pretreatment process cannot handle low bulk density materials without a densification step. The extrusion of textiles or fibers is only possible at a very small scale because the material does not flow freely in solids handling equipment. The other complication is the influence of unknown contaminants on enzyme activity. This would be a very interesting area to explore in depth, but because so many factors could be influenced, model contaminants should be explored in a systematic way first. Thanks to the peer reviewers' suggestions, we plan to run some experiments in standard reactor conditions with PET textile feedstocks containing colored contaminants in the final months of the project. On the subject of industry partners: We appreciate the suggestion to look toward commercial partners for this technology. We will discuss reactor scale-up with our partners at the National Renewable Energy Laboratory (NREL) to understand how our innovations could be translated. We also plan to meet with Unifi, our source for PET textile grade scrap, to discuss their interest in supporting this project through the study of more diverse waste sources.

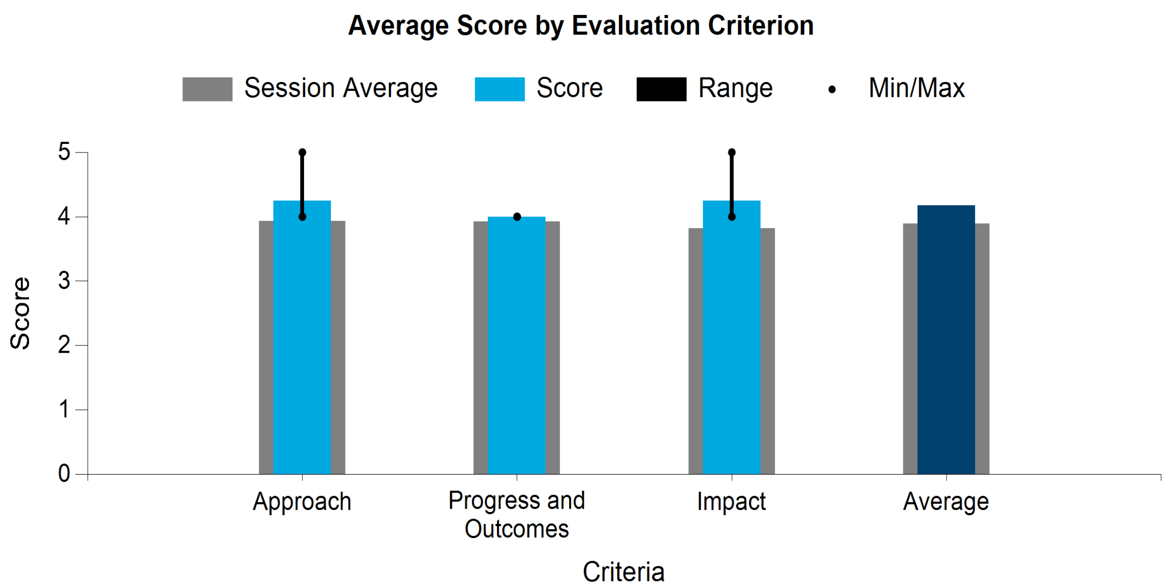
HIGH SOLIDS IN SITU PRODUCT RECOVERY; THE NEXT GENERATION OF ARRESTED ANAEROBIC DIGESTION TECHNOLOGY

Quasar Energy Group, LLC

PROJECT DESCRIPTION

WBS:	2.3.4.210
Presenter(s):	Xumeng Ge
Project Start Date:	10/01/2021
Planned Project End Date:	04/30/2025
Total Funding:	$4,380,000

This project aims to scale the high-solids *in situ* product recovery (ISPR) system (patent application no. 63/020,598) developed by NREL to produce >1.5 kilograms of volatile fatty acids (VFAs) from high solid food waste and subsequently to produce >1 kilogram of sustainable aviation fuel (SAF). Wet waste streams are available at zero or even negative cost and generate significant GHG emissions when landfilled, making them an attractive feedstock for producing cost-advantaged, carbon-negative biofuels. Arrested anaerobic digestion (AAD) can convert wet waste into VFAs, a chemical intermediate for SAF production via ketonization and hydrodeoxygenation; however, this process needs an advanced separation system to continuously extract soluble VFAs from sludge-like fluids with solids present. Due to separation challenges in handling solids and controlling energy consumption, AAD technology has seen limited commercial success in biofuel production. The ISPR system can potentially address these two hurdles, allowing the use of high solid food waste with AAD technology and improving energy efficiency by more than tenfold. This project will scale this system for a first-of-a-kind demonstration to produce VFAs, and subsequently SAF, from high solid food waste with a positive energy balance. We have developed a process model with cost analysis between the proposed system and the risk mitigation strategies. We have carried out pilot-scale system construction and commissioning with 80% completion in build-out and 60% completion in equipment commissioning. We have done feedstock characterization with the preliminary evaluation of biological conversion.



COMMENTS

- The project is on track. The team is trying to separate VFAs from digesters and produce an SAF product using NREL-patented high-solids separation technology. Previous and planned DEI activities look good.

- The DEI plan does not mention the number of interns that will be recruited; however, the team itself is diverse. The objective of the project is to demonstrate NREL's patented process for high-solids food waste separation to separate VFAs that can be turned into SAF. There are two approaches that will be researched: (1) rotating ceramic disk filter followed by hollow tube filter and (2) vibrating membrane followed by emulsion separation membrane. The TEA data and construction demonstration build-out of both processes are close to complete, along with feedstock characterization. The process models are complete and on schedule. The TEA and LCA show significant potential value (lower-cost separation and ~5/gallon VFA) and a carbon-negative footprint. Good progress has been made, and this is a good project.
- This scale-up project is well managed and has a thoughtful approach that should lead to the successful completion of the project objectives. Reducing the costs associated with the separations required for SAF production will have a significant impact on achieving the department objectives. The project shows good collaborations between labs and includes industry partners in useful ways. Risks that may require more attention to mitigation include ensuring that the separations reflect the actual feed, whether it is live broth or some other source, because small changes in that feed could have a deleterious impact on the process. This is exacerbated by the variability of the wet waste feed stream. The post-bioprocessing step appears to be less developed than the basic separation, and the team should consider decoupling the effort to ensure that the proper focus is kept.
- I appreciate that the team is working closely with their industry partners, who are supplying the equipment parts of the separation system. I appreciate that the team has identified a downstream partner, Alder, that is planning to offtake the product of their separation. I appreciate that the team is working on its TEA and LCA during the whole lifetime of the project. I would love to learn more about how resilient the process is for waste streams from different sources and whether the team can find an industry partner to produce food waste. This team's assessment of the starting TRL as 3 is accurate, and their target of TRL 5 seems realistic.

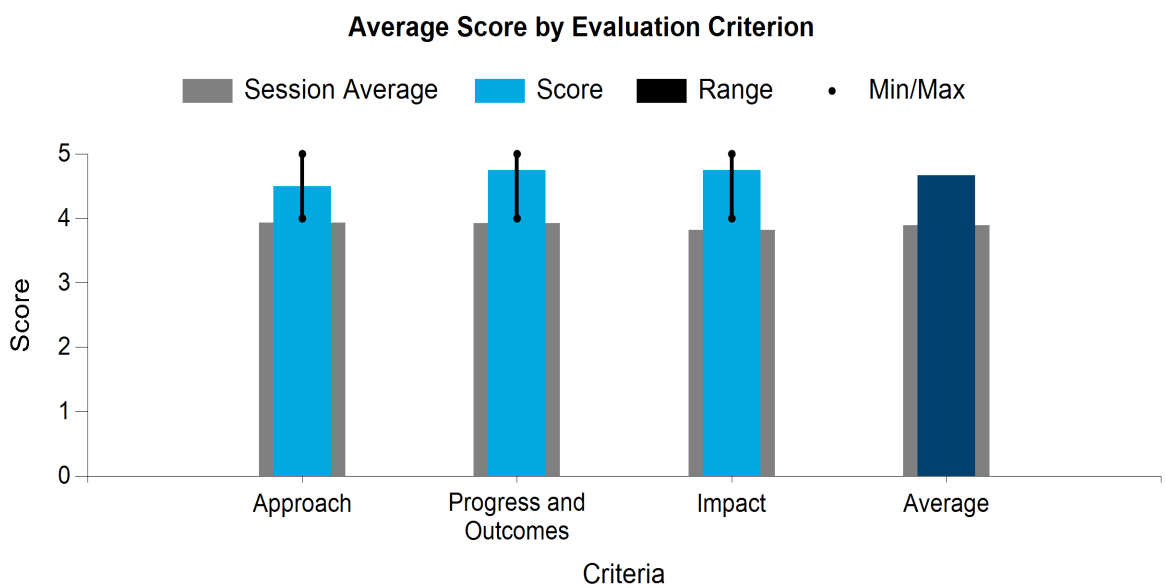
PI RESPONSE TO REVIEWER COMMENTS

- We thank the review panel for the positive comments and constructive input. We are incredibly excited about the potential for this project to be successful in the coming months as activities ramp up in all the tasks. In response to the comment about the number of interns that will be recruited, Quasar Energy Group (QEG) plans to hire two interns from local institutes in Budget Period 3 (BP3). Regarding the comment on using actual feedstocks—we completely agree on the need to use real feedstocks during commissioning to ensure a successful demonstration and accurate integration, especially between the anaerobic digestors and the separations train. This has been planned and will be happening in the coming months. The need to start building out and commissioning all the unit operations in a parallel manner led to initially using materials other than the actual digestate for the early commissioning of the separation's unit operations. In addition, we are leveraging prior NREL results from an initial lab-scale demonstration using food waste at high solids. In terms of decoupling efforts between the post-bioprocessing and product separation steps, as noted in the approach section of the presentation, novel separation technologies are being assessed in this project. The pilot-scale vibrating membrane system developed by project partner New Logic Research has recently been commissioned and will be evaluated as an alternative to the rotating ceramic disk filter to serve as a solid-liquid separation unit. Although initially proposed to be coupled to the emulsion separation membrane system as an option, potential permutations between the two process configurations will also be considered. Regarding the comment on using different sources of waste streams—we completely agree on the need to understand the resilience of the process; however, our first objective is to demonstrate the proposed process at the pilot scale, and using a single source of waste will allow us to focus on the bioconversion-separation interface during the integration efforts. After that, and if the period of performance allows, we will use samples from the feedstock tanks of QEG's digester plants, which receive food waste streams from different sources. As for industry partners that generate food waste, QEG contracts with many of them (mainly in Ohio) and routinely works with them to treat their food waste.

CONTINUOUS BIOBUTANOL FERMENTATION INTEGRATED WITH MEMBRANE SOLVENT EXTRACTION

Archer Daniels Midland Co.

WBS:	2.3.4.212
Presenter(s):	Erik Hagberg; Jesse McVay
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$4,341,844



COMMENTS

- There has been excellent progress in this review period. The project is on track, and the team is ahead of their schedule. A business justification and a single-source material for feedstock should be addressed, and the team should look at alternative feedstocks other than pea starch. Based on the plan and progress, the team will be ready to present the infrastructure architecture that would demonstrate the process to produce 100 kilograms with 100 hours of continuous operation at the end of the project. The industry, national lab, and university collaboration is excellent, and the DEI plan is very clear and well executed.

- The project plan looks very solid and is integrated with the participation of partners at each step. A strong industry partner, Archer Daniels Midland (ADM), is collaborating with the team. Decision points are well defined. The DEI plan is well defined and broad (nine internships, teacher workshops, and researcher training). It may be interesting to study starches other than pea starch. Is the pea starch crude or purified (washing)? Pea starch is a growing industry, but many companies using it are struggling financially, and the amounts available pale in comparison to starches like corn. Also, pea starch is viewed as a healthier, low-glycemic-index, and non-genetically modified organism material for use in gelling foods or as a gelatin replacement (for vegetarians). There may be resistance from a media standpoint in using more precious food sources for aviation fuel and chemicals. Pea starch is also high in amylose, making it more resistant to digestion. This could be a benefit for human health as well. I wonder if you would see any effects or efficiencies in your process (hydrolysis) using other starches?

- This project has the potential to be very impactful in reaching the department goals for SAF, and it illustrates an excellent collaborative relationship with industry partners. Each party's role is understood, and the division of labor is very sensible. One weakness in the approach is the focus on pea starch. Volumes were not presented, but the amount of pea starch available for fuel production relative to the demand should be considered in order to assess the value of the technology. To meet the fuel volume target, many more sugar sources will be required, not just pea starch. That risk should be relatively low, as changing the feedstock should not have a large impact on the fermentation process.

- The graphic on slide 5 showing which industry partners are supplying which materials and equipment/expertise is extremely helpful. I would suggest that all projects with milestones around partnering, sourcing real-world feedstocks, or working with offtakers should present an equivalent slide. I appreciate that both Gevo and ADM have plans to expand their SAF collaboration and deploy capital. The team is strongly partnering with Gevo, which will be the offtaker of isobutyric acid to use it as a starting material in SAF production. How much pea starch is available? I would suggest that the team explore other feedstocks to make the process more widely useable.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the peer reviewers for their thoughtful comments. All reviewers recognized the feedstock, pea starch, as a potential weakness in the project's approach due to its relatively low volume as well as its potential human nutrition applications. The approach for selecting pea starch, a protein production residue, was centered around three basic assumptions: (1) Alternative, plant-based proteins will grow significantly in the future (reaching 65 million tons per year by 2035, based on some estimates); (2) protein produced from legumes and grains will generate carbohydrate byproduct streams as their protein is recovered (from 0.5–2 kilograms carbohydrate per kilogram protein, depending on source); and (3) pea starch is a reasonable representative carbohydrate stream from these alternative proteins. The focus on one carbohydrate byproduct from protein production allowed the team to investigate whether individual challenges from fiber, residual protein, and non-hydrolysable solids could be overcome with a relatively stable and homogenous feedstock. Initial findings showed that hydrolysis could be achieved economically and that the resultant fermentation feedstock meets the organism's needs and provides adequate nutrition. These results indicate that, in principle, starch streams from additional protein sources could be addressed as well, including from legumes (for example, lentils and chickpeas) and other low-value carbohydrate streams not appropriate for human nutrition, such as soy protein processing byproducts (soy molasses) and wheat processing byproducts (B-type starch). Traditional sources of dextrose for fermentation, such as corn—processed in either dry grinds or wet mills—could also likely be used for this fermentation with little technical risk, based on the initial results.

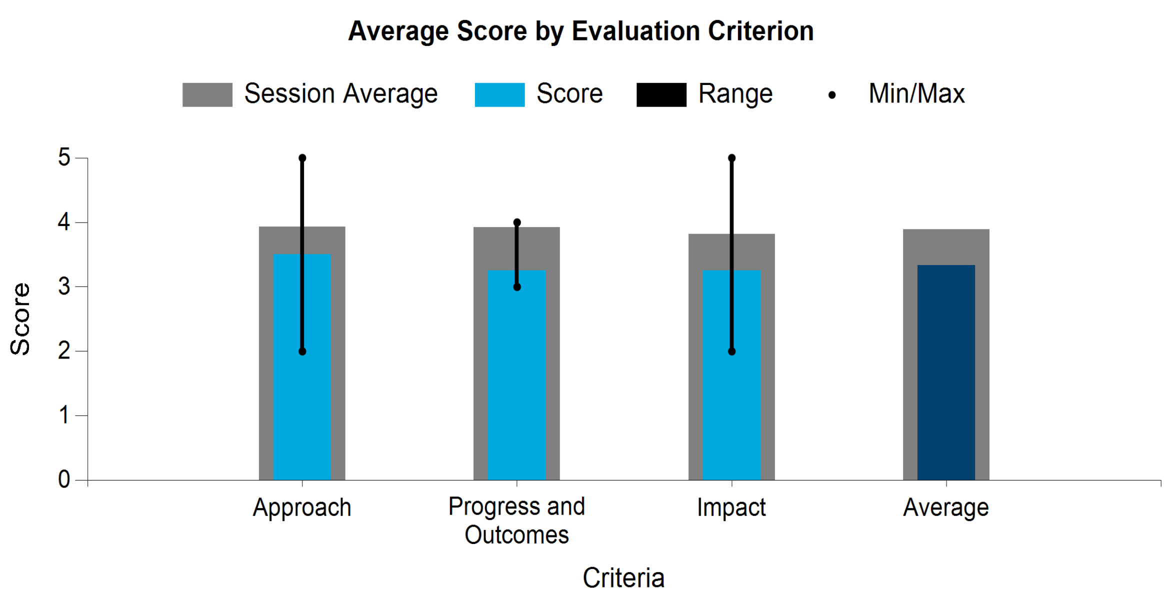
TROJAN HORSE REPEAT SEQUENCES FOR TRIGGERED CHEMICAL RECYCLING OF POLYESTERS FOR FILMS AND BOTTLES

Iowa State University

PROJECT DESCRIPTION

WBS:	2.3.4.400
Presenter(s):	Eric Cochran
Project Start Date:	10/01/2020
Planned Project End Date:	03/31/2024
Total Funding:	$2,722,420

This BOTTLE project (Topic Area 1a) will develop highly recyclable (at least 50% and up to 100%) bio-based polyesters (at least 50 wt % non-food starch-based terephthalate) that are functionally equivalent or superior to, and compatible with, PET. ADM will develop scalable pathways for processing non-food starches obtained as coproducts of vegetable protein production from peas, wheat, beans, and other crops to upgradable furan- and phthalate-based building blocks, including the furan dimethyl esters and terephthalates ADM has developed previously from corn sugars. Iowa State University will use these building blocks to design highly recyclable PET/"trojan horse" copolymers through trojan horse repeat sequences that enable quantitative chemical depolymerization triggered by specific yet mild conditions, enabling facile raw material recovery and repolymerization to virgin material. Diageo and 3M will holistically evaluate PET/trojan horses as bottles and films from the perspectives of performance, aesthetics, compatibility with existing infrastructure and recycling streams, regulatory considerations, and life cycle impacts. Promising candidates will be brought to the multikilogram scale by 3M and processed to bottle (Diageo) and biaxially oriented film (3M) prototypes for further evaluation. Diageo will evaluate bottle prototypes for suitability as packaging for its products. 3M will evaluate prototypes as carrier films, release liners, and optical films that are used for adhesive tapes and electronic devices. TEA will demonstrate the economic potential of the materials, and LCAs will model the carbon and energy savings of the PET/trojan horse copolymers over the entire life cycle. The research partnership comprises entities representing the entire supply chain of the proposed plastics, ensuring that the research and development (R&D) efforts account for all aspects of bringing a new polymer to market.



COMMENTS

- This presentation was notable for communicating in-depth scientific information in a manner that works for a broader audience (me). It also clearly noted limitations and decisions not to proceed with certain material(s), which to me provided credibility to the larger effort. My notes indicate that one of the commercial partners is now working in the kilogram range, which indicates that commercialization is being explored in accordance with the lab findings.

- The concept of trojan horse linkages for the controlled depolymerization of PET is elegant. The project team includes strong industry participation spanning the value chain, including material manufacturing (3M), packaging design and recycling (Diageo), and bio-based feedstocks (ADM). The team has clear roles and a clear communication plan. The project team is diverse and has successfully recruited students from minority-serving institutions (MSIs). It would be useful to pay continued attention to how members with different identities thrive during the project so that true inclusion can be achieved. My main concern with this project is that the risk mitigation in inadequate. Of particular concern to me are the toxicity/rational selection of trojan horse linkages from the start; benchmarking against current methanolysis/glycolysis recycling routes, as they go back to monomers rather than the expected oligomers; interaction with existing polymer processing and recycling streams; and the melt stability and moisture sensitivity of these systems. It is good that the project has ambitions to evaluate these materials' suitability for film and bottle processing, but jumping there without first screening for food contact compliance and melt stability aspects creates a large risk that the material will not be fit for application in the end. Including TEA to understand the commercial viability of this approach would be advisable early in the project. Additionally, the LCA shown focused on the impact of bio-based TPA and did not include the trojan horse linkages. This must also be included. Also, given the commercialization of several chemical recycling routes for PET (methanolysis, glycolysis, etc.) that are coming online, it would be helpful to understand the comparison with this technology and those routes as the system depolymerizes to monomers rather than the envisioned oligomers. I am also concerned about how these materials will interact with standard mechanical PET recycling streams. If they would negatively affect mechanical recycling and require sorting from that stream, it could have globally negative consequences on the recycling system for PET.

- The team has made satisfactory progress. There is a very transparent description of DEI and organization. The regular team meetings of all stakeholders (including the industry partners) are important in providing guided technical decisions. The scale-up goals for 2023/2024 indicate strong interest by industry partners and promise in the technology. The physical properties of the PETs with varying percentages of the trojan horse molecule look good. Does the team have a hypothesis-driven plan to address the barrier inferiority of the PET/trojan horse? If there is a food/liquid-contacting surface, the team should work with partners to identify appropriate in-use stability testing requirements of these new PET/trojan horses.

- I appreciate the close connections the team has to its industry partners. They are working with 3M, which wants to use their plastics; ADM as the biomass feedstock provider; and Diageo as a bottle end user, which has a bottle manufacturing pilot line and will make some bottles at the end. I would implore the team to investigate the toxicity of their plastics as well as the processability of their plastics. The easy decomposition of the plastic under the influence of water can result in decomposition of the plastic during processing. As this is a novel compound that will be in contact with food, it will have to undergo U.S. Food and Drug Administration (FDA) approval before coming to market. The team should develop a regulatory plan in order to enable commercialization.

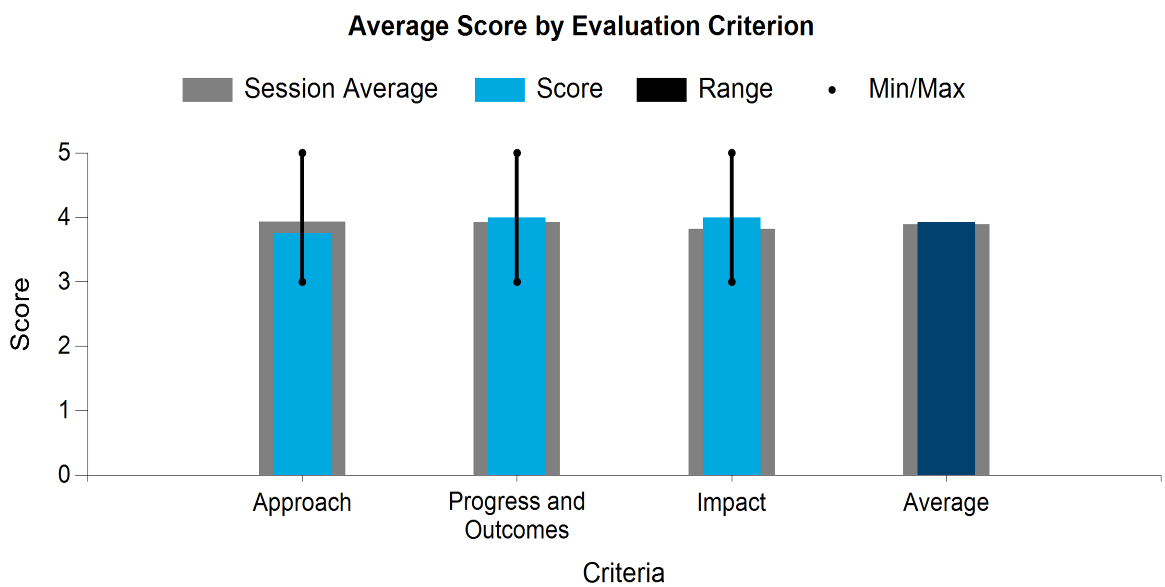
PI RESPONSE TO REVIEWER COMMENTS

- We appreciate your time, expertise, and constructive feedback on our project, "Trojan Horse Repeat Sequences for Triggered Chemical Recycling of Polyesters for Films and Bottles." The unique perspectives and insights each of you have provided are invaluable to the success of our R&D efforts. Reviewer 1, we gratefully acknowledge your positive comments about our project's concept and the diversity of our team, including the significant industry participation across the value chain. Your remarks about our attention to inclusion within the project team are well taken. We will continue to ensure that all team members, regardless of their identities, feel valued and thrive in our project environment. We also recognize the concerns you raised regarding risk mitigation, especially the need for a rational selection of trojan horse linkages from the start to avoid toxicity issues. Benchmarking against current recycling routes and understanding the interactions with existing polymer processing and recycling streams are important aspects that we will address more thoroughly moving forward. These aspects are especially important to project participant Diageo, which has firsthand knowledge of the importance of these issues. Additionally, we will study the interactions of our new materials with standard mechanical PET recycling streams to avoid any negative consequences on the recycling system for PET. The suggestion of including a TEA early in the project to understand commercial viability is acknowledged; we initiated these activities shortly after developing confidence that the trojan horse methodology had technical promise. The project is also working on a complete LCA, including the impact of trojan horse linkages. We recently added a student under Prof. Mba-Wright's advisement to strengthen this part of the project. Reviewer 2, we are glad that you found our presentation to be communicative and credible. We will continue to communicate our scientific findings in a manner that is accessible to a broad audience. Reviewer 3, we appreciate your acknowledgement of our transparency in the description of DEI and organization as well as the regular team meetings with all stakeholders. Regarding the comment relating to the barrier inferiority of the PET/trojan horse, we note that as we continue to collect better data from properly processed films, these properties are, in fact, comparable among the various compositions. We will work closely with our partners to identify appropriate in-use stability testing requirements for these new PET/trojan horses, particularly in the context of food/liquid-contacting surfaces. Reviewer 4, your appreciation of our close connections with industry partners is encouraging. We understand your concerns about the toxicity and processability of our plastics and the need for a regulatory plan for FDA approval before commercialization. We will make sure to investigate these aspects further and develop a comprehensive regulatory plan. In response to the various points raised, we would like to assure you that we will integrate your valuable advice into our project moving forward. Your constructive criticisms not only aid in the identification of potential pitfalls but also guide us toward the necessary adjustments for the success of the project. Again, thank you for your insightful feedback and for your contribution to advancing our research.

UPCYCLING PET VIA THE VOLCAT PROCESS

IBM

WBS:	2.3.4.401
Presenter(s):	Greg Breyta
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,147,090



COMMENTS

- The presenter stated a definition of closed loop wherein the project does not consider the waste produced; this is a problem either in communication or in vision. Similarly, there was either a problem in waiting until the work was completed to do LCA and TEA or—if those are not just afterthoughts—then there was a problem in the communication of how those analyses are part of the process as decisions are made. I would have appreciated more benchmarks and comparisons, particularly in visual form. Without them, it was difficult to assess the meaning and relevance of the information the speaker was attempting to share.

- This is an extremely strong project with a clear approach to transitioning the technology to pilot-scale demonstrations. Risks are clearly identified with clear mitigation strategies in place, such as reverting to a stirred tank if the extrusion reactor proves unworkable. The management and communication plan was not explicitly covered in the slides, but from the work presented, it appears that there is sufficient interaction among the project participants. My only suggestion is that more focus be put on understanding the BHET benchmarking needed to be suitable for repolymerization (what does "high-quality BHET" mean in terms of performance metrics?). The project has demonstrated substantial progress toward objectives and reducing costs, particularly with regard to the decoloring process. Additionally, the demonstration of successful recovery and decolorization for real post-consumer recycled (PCR) waste flake and fabric trimming is highly encouraging. The focus on evaluating real waste streams is excellent and should remain a focus. The rationale and approach for pursuing polybutylene terephthalate were not clear and not discussed. The project team should consider whether narrowing their focus to core BHET production would ensure faster progress. The potential to target waste streams that do not compete with the mechanical recycling of PET gives this process potential to expand the amount of PET recycled rather than displacing mechanical recycling. This focus and the emphasis on patents is appropriate for this commercialization-focused project. The suitability of BHET as a feedstock for any PET production process currently greatly lowers the barrier for adoption as well as ensures a large potential market with lower barrier of entry for recovered materials. Given the brand pledges around PCR in both fiber and bottle markets, there is a real potential for rapid adoption, and therefore near-term decarbonization impact, due to market pull if VolCat can be shown to be feasible at the pilot scale.

- I am excited by the promise of this project because of the success in demonstrating PET fabric and particles as viable substrates for upcycling. I would like to see more data about the catalyst and understand its stability, resilience, and recovery in the presence of common additives in the crude waste feed.

- The team is doing their TEA/LCA at the very end of the process. It will be too late to pivot then. There has been a baseline TEA out there, and the team is currently feeding information in that model. I would like the team to more actively engage with the TEA/LCA, especially because this project is starting at a relatively high TRL. The stated goal of the project is to develop a TEA/LCA and demonstrate reducing GHG emissions. Without being able to review the results of this analysis, it is not possible to judge the progress made toward this goal.

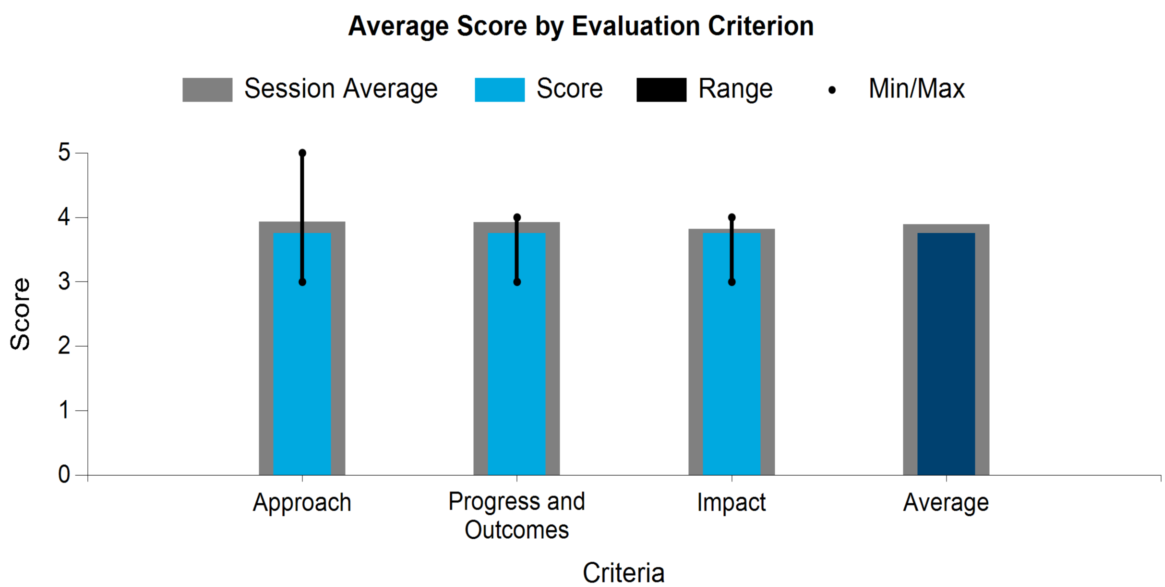
PI RESPONSE TO REVIEWER COMMENTS

- Thank you for providing feedback on my recent project review presentation for PET upcycling via the VolCat process. The comments about benchmarking the BHET have been incorporated into a new task. In this task, we are benchmarking the recycled polyethylene terephthalate (r-PET) prepared from the BHET obtained using the nominal VolCat reaction, which will then be compared with the BHET obtained using all the optimization results, e.g., the modified decolorization process in the scaled process. The production of polybutylene terephthalate is a component of the project for at least two reasons: first, as a demonstration of "upcycling" to a more valuable product than the feedstock polymer type we used to make the monomer and, second, as a demonstration that the VolCat process has broad applicability to polyesters in general (not just PET). Regarding my lack of clarity on the economic analysis/project progress feedback loop: There is already a basis TEA and LCA model prepared from data from the "nominal" VolCat process as it existed prior to the project start. The TEA model will be updated as new data permits, and we will have a final deliverable that incorporates the totality of what we learned during the project. The mid-project interim TEA was not yet prepared, so I was not able to provide a summary at the Project Peer Review. There is a task to quantify the catalyst recyclability along with conducting a purity assessment. This project was not intended to be a survey of a wide range of potential inputs to the VolCat reaction but rather to pick a number of the highest-volume viable inputs to the process that cannot be recycled by existing mechanical means. We are therefore investigating the fate of the catalyst with these inputs as a starting point.

DESIGNING RECYCLABLE BIOMASS-BASED POLYESTERS

University of Wisconsin–Madison

WBS:	2.3.4.403
Presenter(s):	George Huber
Project Start Date:	10/01/2020
Planned Project End Date:	04/30/2024
Total Funding:	$3,125,000



COMMENTS

- My notes indicate that the question of how/why waste plastics escape into the environment arose in the discussion of this presentation. The U.S. Environmental Protection Agency (EPA) has a method—the Escaped Trash Assessment Protocol (ETAP)—aimed at helping people at all levels assess and answer this question for their geographical area of interest. That data set, and other data sets with different parameters (some use weight, some use count of items, etc.), are available for use by researchers. The Q&A indicated that the researchers are not connecting to the main potential markets for their potential products, such as mulch film.

- The approach has merit in terms of identifying potential new bio-based polymers with properties superior to polybutylene adipate terephthalate (PBAT). The active engagement of partners along the entire value chain from monomer production to film production increases the likelihood of commercialization. This is due to a high level of understanding of what material property targets are needed and what monomers can be produced at scale. A particular strength of the project is the focus on the processability and rheology of the materials; however, the crystallization behavior, including rate, should be added as an area of focus. The project is making good progress on hitting the objectives set out, with routes identified to increase biomass content. Incorporating TEA/LCA from the start of the project has proven effective. The involvement of Pyran, which is commercializing 1,5-pentanediol

(PDO) production, increases the likelihood that selected polymers will be able to be produced at scale. Given the choice of PBAT as their reference material to improve upon and its widespread use in mulching films, it would seem logical to target agricultural applications with these new materials. The plan for down-selecting to focus only on the more promising materials for scale-up and evaluation is smart.

- The project has a clearly delineated technical scope coupled with a budget cycle and timelines. I am optimistic that the project has a high probability of meeting polymer physical and process targets for the next budget period verification. I am still curious about the interesting structure/property relationship of the methylene groups in the diol and where the 1,5-PDO falls off that curve. This begs more polymer structure analysis to understand it.
- I am impressed by the team's focus on bringing their plastics to market, thinking through final applications, and lining up partners to help with realizing these. I would recommend that the team test their plastics in a mulch film application as well.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for providing their helpful comments about our project. We also thank the reviewers for their very positive comments. We look forward to moving ahead with our new types of biomass-derived biodegradable plastics.
- Comment: The approach has merit in terms of identifying potential new bio-based polymers with properties superior to PBAT. The active engagement of partners along the entire value chain from monomer production to film production increases the likelihood of commercialization. This is due to a high level of understanding of what material property targets are needed and what monomers can be produced at scale. A particular strength of the project is the focus on the processability and rheology of the materials; however, the crystallization behavior, including rate, should be added as an area of focus.
- Response: We have made crystallization an area of focus and have now identified a nucleator to speed up the crystallization of our polymers. Previously, crystallization half-time at 40°C was ~30 minutes. Now, it is ~30 seconds, which is the same value for commercial PBAT at these conditions. We are continuing to explore other nucleators to see if improvements are possible.
- Comment: The project is making good progress on hitting the objectives set out, with routes identified to increase biomass content. Incorporating TEA/LCA from the start of the project has proven effective. The involvement of Pyran, which is commercializing 1,5-pentanediol (PDO) production, increases the likelihood that selected polymers will be able to be produced at scale. Given the choice of PBAT as their reference material to improve upon and its widespread use in mulching films, it would seem logical to target agricultural applications with these new materials. The plan for down-selecting to focus only on the more promising materials for scale-up and evaluation is smart.
- Response: We thank the reviewers for their comment. We are excited for the many industry partners we have on the project who are making crucial contributions.
- Comment: My notes indicate that the question of how/why waste plastics escape into the environment arose in the discussion of this presentation. The EPA has a method—the ETAP—aimed at helping people at all levels assess and answer this question for their geographical area of interest. That data set, and other data sets with different parameters (some use weight, some use count of items, etc.), are available for use by researchers. The Q&A indicated that the researchers are not connecting to the main potential markets for their potential products, such as mulch film.

- Response: We thank the reviewer for providing us with information about ETAP, and we will analyze this in the future. The ETAP tool can be used to quantify the plastic waste across time and habitat type, which provides insight into the trends for plastic waste across the United States. Based on the feedback from reviewers, we are going to focus more on mulch films for the next part of the project.
- Comment: The project has a clearly delineated technical scope coupled with a budget cycle and timelines. I am optimistic that the project has a high probability of meeting polymer physical and process targets for the next budget period verification. I am still curious about the interesting structure/property relationship of the methylene groups in the diol and where the 1,5-PDO falls off that curve. This begs more polymer structure analysis to understand it.
- Response: In work leading up to the current DOE-funded work, Ph.D. student Lei Zheng (University of Massachusetts Amherst, 2022, advised by John Klier) described the effects of PDO structure on macro properties, including thermal transitions, crystalline structure, crystalline behavior, mechanical properties, and biodegradation. We have continued this line of inquiry. We have also found data from other literature sources at higher aliphatic diol contents that suggest more of an even-odd effect than originally thought. We will be adding crystal size to our analysis via small-angle X-ray scattering measurements as well. We will provide this information to DOE in our next report but cannot paste graphics into the response to reviewers.
- Comment: I am impressed by the team's focus on bringing their plastics to market, thinking through final applications, and lining up partners to help with realizing these. I would recommend that the team test their plastics in a mulch film application as well.
- Response: We are going to focus on mulching film applications in the future as well. Amcor has agreed to produce several mulching films, which we will test.

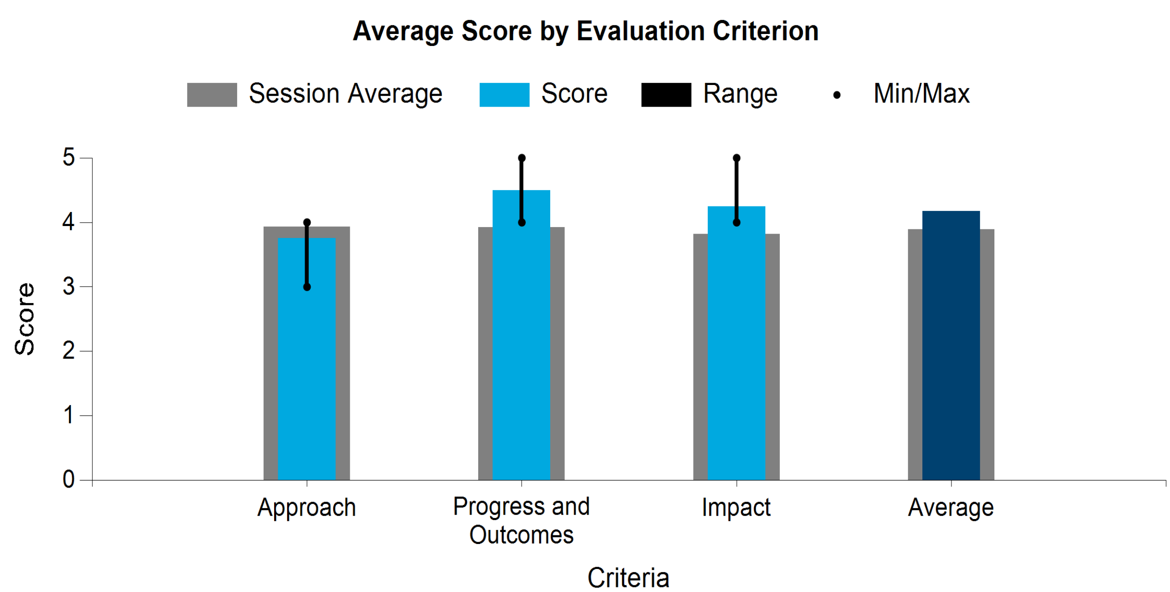
SYNTHESIS AND ANALYSIS OF PERFORMANCE-ADVANTAGED BIOPRODUCTS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.4.501
Presenter(s):	Gregg Beckham; Laura Hollingsworth; Megan Krysiak; Michelle Reed
Project Start Date:	10/01/2017
Planned Project End Date:	09/30/2023
Total Funding:	$520,000

This project focuses on the synthesis and analysis of PABPs. We have established collaborations with other BETO-funded projects and academic and industry collaborators to source new molecules that have promising manufacturing pathways and that could serve as performance-advantaged biochemicals or biopolymers. We conduct synthesis and characterization of biochemicals and biopolymers alongside TEA and LCA to estimate their cost and environmental impacts relative to incumbent materials. As part of the project, Linda Broadbelt and Brent Shanks are developing computational pathway prediction tools to identify optimal production pathways for bio-based compounds via biological and chemo-catalytic transformations. When coupled to the Polymer Inverse Design (PolyID™) tool from the Inverse Design Project, these tools will ultimately enable a narrowing of the design space for PABPs. From FY 2021–FY 2023, we described a framework for benchmarking PABPs, estimated the energy and GHG emissions for commodity organic chemicals, developed performance-advantaged nylons and polyesters from beta-ketoadipic acid (beta-KA), and produced lignin-based plasticizers. We have shown that aromatic amines can be used in performance thermosets and that polyhydroxyalkanoates with cross-linked side chains can exhibit rubber-like properties, along with repair and degradability. We are actively working with industry partners on the scale-up and validation of multiple PABPs.



COMMENTS

- There has been some progress in this review period. The project is on track. The team developed new PABPs for polymers and chemicals with viable, economic, and GHG-advantaged manufacturing pathways. There is cross-collaboration with other teams. It is clear that incorporating beta-KA in PET and PBAT enhances polymer properties, recyclability, and biodegradation. It would be also great to understand the effects of beta-KA on the barrier properties and transparency of the final polymers. Active technology transfer with a startup company (textile major) for nylon-6,6 incorporated with beta-KA is a really important step. The team should investigate and find the mechanism for improving the water absorption behavior of nylon-6,6 incorporated with beta-KA. It is also important to find target applications and industry partners for other polymers with PABPs in the early design process. The PI did not present their DEI strategy and progress.

- There was no structured DEI plan in the presentation. The lignin-derived plasticizer work is promising as an alternative for toxic phthalates. There is a real need for lower-toxicity small-molecule additives such as plasticizers, flame retardants, and per- and polyfluoroalkyl substances (PFAS) replacements. On incorporating beta-KA into nylon 6,6: Is there a need for a higher glass transition temperature (Tg) in textiles? The success of the project may be more likely with small-molecule development versus new polymers, which are very difficult to implement from cost, risk, and change perspectives. Will these new polymers produce yet another material at end of life to separate out for special handling? There was good collaboration with the computational group and with several industry partners. The industry partners can help you to determine which properties to home in on for each application—most times, cost will be a major factor. Instead of a 25% cost increase, they won't be interested until there is at least a 15% cost savings because of all the transition and investment required. The additives, however, can be more readily changed, and the lower toxicity of bio-derived additives will help them sell their product to consumers and continue to do business with health and safety regulations. What about heat and light stabilizers from bioprivileged molecules?
- This project is well organized and shows excellent collaborative work with academic and lab partners. This range-finding work is important for extending the possible technical and market reach of bioproducts and further demonstrates the utility of bioproducts in a range of applications. There has been excellent use of TEA and LCA as a means of quantifying the relevance of these new products for comparison to incumbent products. For future work, I would suggest more industry involvement to help validate target identity and performance requirements.
- The team has screened an impressive number of different structures to identify moieties that can be procured at reduced cost and with lowered GHG emissions. The project seems to be at a point where the team can move from a wide screen to focusing on its "winners" and pushing them to higher TRLs. I am impressed that the team identified a beta-KA-containing polymer that degrades favorably and that the team is planning to scale it up. I appreciate that the team is working on several patents and is working with a startup company and textile major to scale up production of their performance-advantaged nylons from beta-KA. I would like to see the team continue the commercialization of this polymer. As this project is coming to an end, it would be worthwhile to explore whether next steps should target pushing commercialization of this project's lead candidates or continue on discovery work. I see merit in both and would suggest a two-pronged approach. First, proof out the platform by continuing scale-up and commercialization of the lead candidates. In parallel, use an analysis/experimental data science cycle platform to discover additional PABPs. I would be more specific in the desired metrics for this second set of PABPs by continuing to focus on the team's analysis that showed opportunities in heteroatom-containing chemicals, which exhibit the highest energy/GHG emissions of all chemical classes studied here. As the team is already working with industry partners to scale up the existing material, I would love to see validation of this need with industry partners before further synthetic efforts are taken.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the positive and constructive feedback from the review panel. In terms of nylon properties, we will work with our industry partners to address the excellent feedback that was provided. The work on incorporating beta-KA into nylons was originally intended to focus on applications where higher glass transition temperatures would be useful (e.g., in automotive applications). In terms of DEI, we are drafting our formal DEI plan for FY 2024–FY 2026, but we have had impacts with workforce development, MSI outreach, and open-source tools. We agree that small molecules offer a new and exciting direction for formulated products, and we have shifted a substantial part of our portfolio in that direction. The heat and light stabilizer concept is also excellent—we will look into that. In terms of the comment regarding more industry involvement, we are actively working with industry. It is also notable that this is a fairly small project, and we are attempting to increase our industry engagement activities through supplementary programs like Energy I-Corps, the Technology Commercialization Fund, the West Gate Program, etc. We have active collaborations with companies as well as ongoing technology transfer. Last, we appreciate and agree with the concept of a two-pronged approach, wherein one project goal is to keep the discovery pipeline full and the other is focused on transitioning winners out of the discovery pipeline to larger scales, including with industry partners.

RESIN: RESPONSIBLE INNOVATION FOR HIGHLY RECYCLABLE PLASTICS

Northwestern University

PROJECT DESCRIPTION

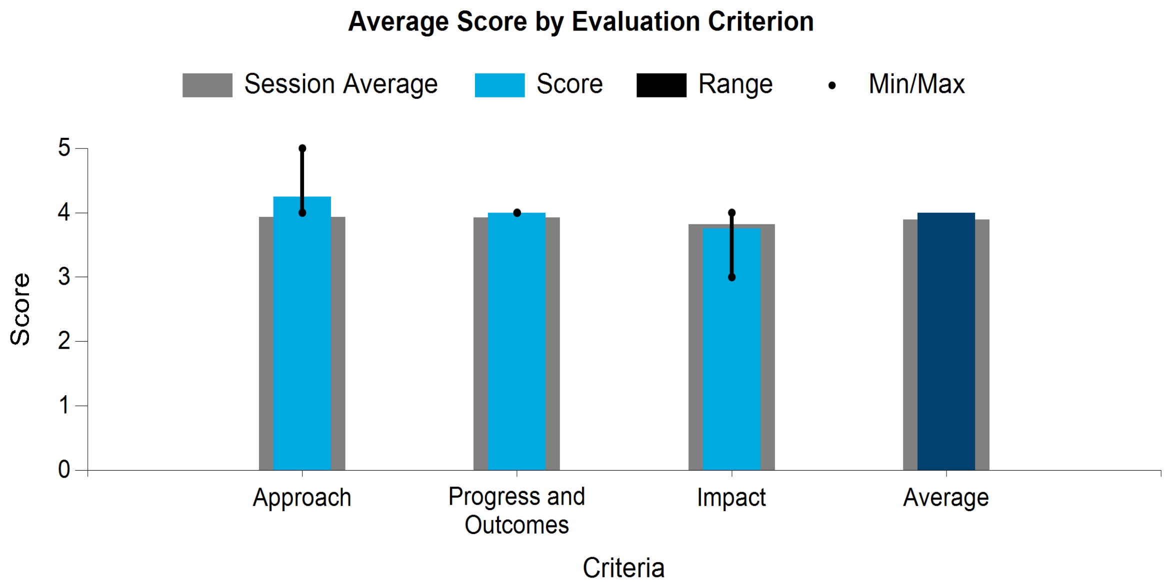
WBS:	2.3.4.607
Presenter(s):	Linda Broadbelt
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2023
Total Funding:	$3,156,484

As far as objectives, we are developing a responsible innovation approach that marries computational-based approaches with experiments to design materials that achieve high polymer recyclability and benign degradation products at end of life (EOL). We target the PU family of polymers, which ranks sixth in worldwide production, at 36 billion pounds produced in 2016, and has a 6% annual growth rate. PU is not recycled at any significant level when made of linear chains (thermoplastics) or cross-linked networks (thermosets). The state of the art (SOA) is 0% recovered monomers for PU.

The Northwestern University and Argonne National Laboratory team, in collaboration with its industry partners, focuses its efforts on the responsible recycling of bio-based PU-like materials, namely, bio-based polyhydroxyurethanes (PHUs) and polythiourethanes (PTUs), that offer the possibility of recovering value and improving sustainability in two ways: (a) recovery of monomer from spent materials, whether thermoplastics or thermosets, and (b) reprocessability of spent networks with full recovery of cross-link density and associated properties after reprocessing. Our approach is designed to meet the monomer recovery challenge as well as put thermosets on par with thermoplastics, where the melt-state reprocessing of spent polymer into recycled high-value products that meet original use guidelines is the most energy-efficient and responsible method of recycling.

In terms of approach, the overall design framework begins with biomass-derived intermediates as starting molecules. A computational framework for reaction pathway design is applied to this to generate potential monomers. These monomers are used to synthesize PHU and PTU that can be reversibly thermally reprocessed (chemically recycled) for their original use. Experimental studies and kinetic Monte Carlo simulations are used to explore conditions for optimal chemical recycling. Experimental design and kinetic Monte Carlo simulations of monomer recovery for PHU and PTU are also conducted, exploring conditions for high monomer yield. Environmental and economic analyses are being conducted in concert with these studies. Risk assessment for environmental performance is used to understand the potential impacts of the plastics’ disposal pathways and the exposure analysis of the polymers and their monomers. Testing for EOL properties involves both engineered and natural environments. Finally, LCA and TEA are done to assess alternatives, explore economic feasibility, and evaluate sustainability.

In terms of impact, the project impacts multiple fronts. We have achieved chemical recyclability of 25% monomer recovery. We are developing modeling and analysis tools to guide the production and recycling of PHUs and PTUs that are at least 50% biomass-derived, benign at EOL, cost-effective, and less energy-, GHG-, and water-intensive than baseline PUs. An additional focus is to develop PHUs and PTUs that exhibit equivalent or improved properties compared to conventional PUs. Further outcomes of the project are publicly available tools for PHU and PTU design for recyclability, performance, and benignity that can be evolved to cover other types of polymers and publicly available cost and environmental assessment tools for recyclable bio-based polymers. A critical outcome is the demonstration of the successful design of a market-relevant polymer while incorporating key performance requirements and EOL considerations that can be replicated for other polymer types.



COMMENTS

- The prominence of the EOL property testing was much appreciated, and I would encourage that to be part of other projects as well.

- The proposed tasks and interplay between activities are well thought out, and the project is clearly aligned with FOA goals. It is highly ambitious, spanning new bio-based monomer discovery, novel polymer synthesis, and a novel prospective risk model for new polymers' life cycle. Having a clear framework for how to navigate this extremely broad space is critical for keeping the project focused and progressing. The fact that the project pivoted after guidance from the industry partner on the need to test foaming is encouraging and increases the likelihood of a commercial fit for these materials. Strengths of the project are the strategic risk assessment framework, the focus on understanding EOL degradation, and the use of TEA/LCA to identify monomers with the largest benefit for a bio versus fossil route. The focus on engaging industry collaborators and the full supply chain focus with the Greenhouse Gases, Regulated Emissions, and Energy Used in Technologies (GREET) model increases the chances of commercialization. The insight gained into critical properties for environmentally benign target products (Milestone 4.5) will be valuable in assessing other proposed biodegradable TPU systems. Likewise, the dissemination of the molecular discovery efforts will allow insights to be leveraged beyond this project for other development efforts in this space. The dynamic bonds leveraged for reprocessing (assessed by multiple pressing cycles) will also lead to substantial differences in flow behavior during processing. To understand the application space for these new materials, it would be useful to keep a keen eye on the rheological requirements for processes to flag potential roadblocks and to work with industry partners to focus on the most promising application space to evaluate material potential. The materials can foam and then be reprocessed into film, but due to the foaming mechanism, they cannot be re-foamed, meaning that a different application would need to be identified for recovered material unless chemically recycled.

- The PIs responded to and addressed the substantial concerns in the 2021 review. This is an aggressive and detailed analysis of these PU derivatives and promises to deliver a very comprehensive product. This project seeks to identify derivatives that bring higher functional value to suppliers and an additional sustainability benefit. The blueprint has the potential to have a greater industrial impact and pull. I am pleased that the team has an excellent understanding of risk areas and mitigation strategies in place. The work to date is reassuring. There is still a question as to whether, with full transparency and guidance from industry partners, these designed bio-phased PUs will gain entry and sufficient traction to enter the market, when there are always hurdles for business adoption.

- The close collaboration with industry is fantastic. The team is taking on the feedback that they need to produce a foam. The team is transferring material to Dow, producing co-publications, and receiving samples from Dow and Jenner. Close collaboration in this field of work is great preparation for bringing these technologies into the real world.

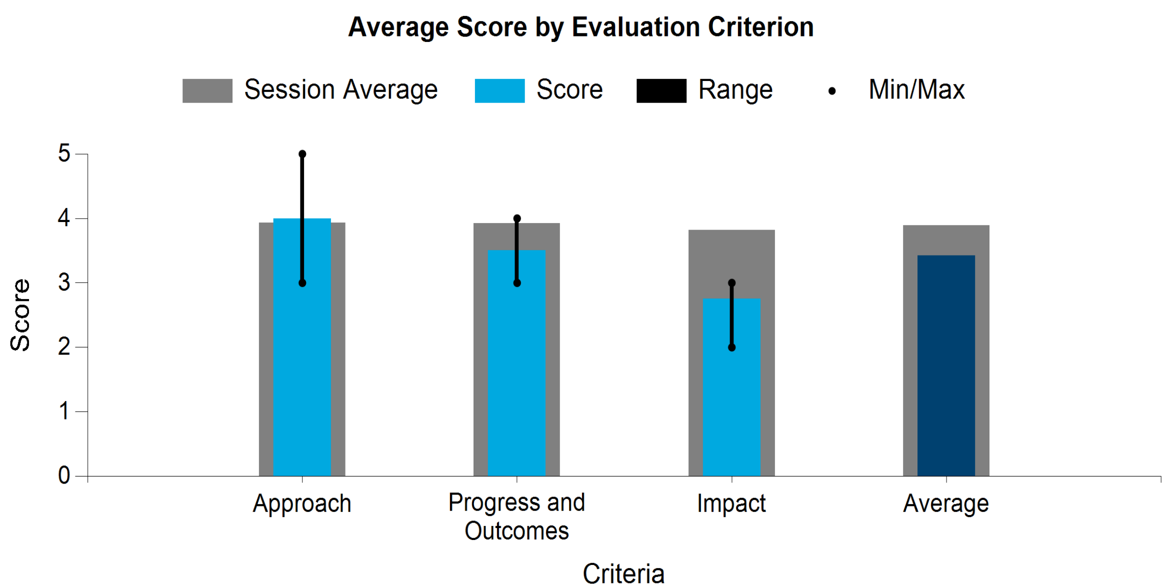
PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' positive and insightful comments regarding our project. We are particularly excited that they noted the strong partnership with industry and how the input of industry partners was critical in guiding, and indeed pivoting, the focus of our project. We are grateful that the reviewers appreciated how our team collaborated to bring a combined systems-level and focused science approach to a grand challenge, providing a model for the future. We would also like to note that DOE's support for a tightly integrated project among a university, a national laboratory, and industry that adopted a cradle-to-grave approach and was supported by detailed risk analysis, LCA, and TEA was greatly appreciated.

MULTI-UNIVERSITY CENTER ON CHEMICAL UPCYCLING OF WASTE PLASTICS (CUWP)

University of Wisconsin–Madison

WBS:	2.3.4.613
Presenter(s):	George Huber
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2025
Total Funding:	$12,500,000



COMMENTS

- The overall project structure and organization is clear. There is a clear logic to the interplay between the different focus areas as well as a clear management structure. My main concerns with the project are related to engagement with the wider ecosystem (MRFs, recyclers, and companies engaged in the pyrolysis space as well as other DOE consortia and institutes), such that the research activities are adding value and insight to the space and not duplicating information that already exists. Enhancing our understanding of pyrolysis is only impactful if it is connected with a path to commercialization. It seems like an excellent opportunity to build bridges between BOTTLE and Chemical Upcycling of Waste Plastics (CUWP), with their different research portfolios, to accelerate the entire polymer circularity space. Additionally, it may be fruitful to engage with the Reducing Embodied Energy and Decreasing Emissions (REMADE) Institute and the Biomass Feedstock National User Facility for opportunities and limitations on MRFs and sortation. In order to realize the ambition of being a global leader in plastic recycling technology R&D, wider and more intentional engagement is needed. A particularly nice output from the project is the view on what infrastructure is needed and how to optimally locate it. A stronger environmental justice lens for this analysis is recommended to avoid locating facilities in areas with already disproportionate burdens. For the educational aspect of the project, tracking the impact of materials would be valuable. Are the fact sheets or course materials being used by organizations outside CUWP? Which groups are being reached successfully, and which need different approaches? Understanding the reverse supply chains and the composition of recycling streams is critical, and it is good that this is part of the project focus; however, I am concerned that there was no mention of reaching out to other actors in this space. For example, the team could engage with surveys such as the Recycling Partnership's Residential MRF Survey, Stina's Annual Plastic Recycling Survey (https://stinainc.com/view/annualrecycling), Resource Recycling Systems' recently completed film recovery survey for California, and BOTTLE's analysis of plastic recycling systems ("Quantification and Evaluation of Plastic Waste in the United States"). Hand sorting a few bales is hugely time-intensive and yields low statistical power insights. Engaging with the recycling infrastructure to understand composition will be more fruitful. I fail to understand how the results of testing molded tensile bars from the bale is advancing understanding; this is something that is actively done at recyclers in this space, and it feels like engagement with them would be more useful. The solvent targeted recovery and precipitation (STRAP) work is among the strongest from the project, with partners interested in commercialization and scale-up work ongoing. As there are other solvent-based recovery technologies coming into the market, such as Pure Loop, understanding the TEA/LCA for STRAP against the wider landscape is critical. It is worth considering how insights into the variability of waste streams with location, season, and potentially long-term material shifts would impact the sizing, location, and design of STRAP facilities.

- The wide collaboration is impressive. The focus on pyrolysis is not innovative. The impact of the ML database is not clear. It was unclear whether the solvent analysis includes the costs to dispose of waste solvent (it should). The work sorting bales was done by hand by a graduate student and does not seem to be replicable in any scalable, financially viable way. I would like to know how they identify the number of the matrix plastic; that seems important and difficult.

- The absence of synergy between teams noted in the last review was addressed with regular meetings with constituencies within the consortium. I applaud the strengthening of the CUWP management structure and the existence of a board with representation from all stakeholders, including the IAB. Recovery from multilayers seems particularly solvent-intensive. The STRAP process is excellent, and I would like to see a validation step—a side-by-side comparison of STRAP-recovered polymers against virgin polymer in a multilayer film food application as a way to demonstrate equivalency in performance. One point of concern: The economics modeling that shows value in siting pyrolysis plants in high-population-density areas raises my concern for having a rigorous study of the impact through an environmental justice lens. I would encourage the investigators to engage with entities to thoroughly vet the potential environmental impact on the adjacent communities.

- For the research-focused aspect of the program, it would be great to collect data on the number of students that have attended the class, the number of undergraduate researchers that are sponsored, and the number of students that have participated in the exchange program. Bringing samples to share is fantastic! I believe that writing a review article at the beginning of the funding period is a great idea and could be included in several of the other funding programs. I think it is a very positive sign that the individual steps are building on each other, e.g., using the actual pyrolysis oils in the zeolite-guided conversion. This is important to demonstrate the full life cycle of the material.

PI RESPONSE TO REVIEWER COMMENTS

- We would first like to thank the reviewers for their kind comments about CUWP. We are very grateful to DOE for supporting this work. We are excited about everything that CUWP has accomplished to date, and we look forward to continuing to address the scientific and engineering challenges with plastic recycling. In the following, we offer our responses to the main comments by the reviewers.

- Comment (Reviewer 1): The overall project structure and organization is clear. There is a clear logic to the interplay between the different focus areas as well as a clear management structure. My main concerns with the project are related to engagement with the wider ecosystem (MRFs, recyclers, and companies engaged in the pyrolysis space as well as other DOE consortia and institutes), such that the research activities are adding value and insight to the space and not duplicating information that already exists.

- Response: Thank you for this comment. We received feedback from several companies engaged in plastic pyrolysis during the CUWP Annual Meeting. These companies are already part of the CUWP IAB. We will invite companies that own MRFs (like Waste Management) to participate in CUWP's IAB and are open to engaging with the wider ecosystem.

- Comment (Reviewer 1): Enhancing our understanding of pyrolysis is only impactful if it is connected with a path to commercialization.

- Response: We agree that the impact of any technology is measured by its eventual commercialization. Several of CUWP's IAB members are advancing pyrolysis to commercialization, including Anellotech, Braskem, Frontline, GSF, Ketjen, Saudi Basic Industries Corporation, and GAL Group. Independent of the efforts of CUWP, a number of companies are attempting to recycle or upcycle waste plastics via thermal depolymerization, including Agilyx, BASF, Brightmark Energy, ExxonMobil, Full Circle, Freepoint Eco-Systems, Nexus Fuels, Plastic2Oil, Plastic Energy, Renewlogy, and RES Polyflow. The CUWP IAB members are interested in advancing the current state of technology in pyrolysis to improve its technical and economic prospects for processing waste plastics into value-added products. Our experimental and computational studies on thermal depolymerization help overcome the challenges of plastics upcycling identified by TEA/LCA performed at CUWP. We also have a patent application on pyrolysis technology and are working with CUWP members to understand how it could be commercialized.

- Comment (Reviewer 1): It seems like an excellent opportunity to build bridges between BOTTLE and CUWP, with their different research portfolios, to accelerate the entire polymer circularity space. Additionally, it may be fruitful to engage with the REMADE Institute and the Biomass Feedstock National User Facility for opportunities and limitations on MRFs and sortation.

- Response: Further interaction with researchers within this space is indeed an important goal. In the near term, several members of CUWP will be attending the Plastics Recycling Gordon Research Conference in summer 2023, which will promote discussion with a variety of researchers (including those affiliated with BOTTLE and REMADE). We also plan to organize a mini symposium as part of the American Institute of Chemical Engineers annual meeting to establish further connections between groups.

- Comment (Reviewer 1): In order to realize the ambition of being a global leader in plastic recycling technology R&D, wider and more intentional engagement is needed.

- Response: DOE has limited us to partners that have operations in North America. We have attended international conferences and will continue to do so; however, DOE will have to give us permission to engage with the recycling community outside of North America.

- Comment (Reviewer 1): A particularly nice output from the project is the view on what infrastructure is needed and how to optimally locate it. A stronger environmental justice lens for this analysis is recommended to avoid locating facilities in areas with already disproportionate burdens.

- Response: Our computational models will be adapted to account for constraints on technology locations; here, it will be interesting to understand the interplay among environmental justice, carbon emissions, and economics (that might result from higher transportation demands). We are also currently developing a computational model to evaluate the impact of new recycling technologies on social justice in Mexico.

- Comment (Reviewer 1): For the educational aspect of the project, tracking the impact of materials would be valuable. Are the fact sheets or course materials being used by organizations outside CUWP? Which groups are being reached successfully, and which need different approaches? Understanding the reverse supply chains and the composition of recycling streams is critical, and it is good that this is part of the project focus.
- Response: We have provided the fact sheet to plastic converters and the media. We have provided the course material on plastic recycling to professors at universities outside of CUWP.
- Comment (Reviewer 1): I am concerned that there was no mention of reaching out to other actors in this space. For example, the team could engage with surveys such as the Recycling Partnership's Residential MRF Survey, Stina's Annual Plastic Recycling Survey (https://stinainc.com/view/annualrecycling), Resource Recycling Systems' recently completed film recovery survey for California, and BOTTLE's analysis of plastic recycling systems ("Quantification and Evaluation of Plastic Waste in the United States"). Hand sorting a few bales is hugely time-intensive and yields low statistical power insights. Engaging with the recycling infrastructure to understand composition will be more fruitful. I fail to understand how the results of testing molded tensile bars from the bale is advancing understanding; this is something that is actively done at recyclers in this space, and it feels like engagement with them would be more useful.
- Response: Thank you for the comments and suggestion. We are currently working with multiple MRFs and recyclers across the country. We do not have data on the composition and performance of sorted mixed waste landfill plastics. There is also no compositional data on mixed #3–#7 bales (in the United States), and as result, there is no performance data on the properties of sorted #3–#7 mixed bales. The process for sorting a whole bale is necessary to understand the entire composition, which, in turn, allows for implementation of ASTM International D5231 for sampling mixed waste for further processing. Per ASTM, washing, pelletizing, and molding is the globally accepted method for understanding the mechanical properties of these landfill-diverted mixed waste plastics for downstream operations. This characterization via injection molding helps MRFs understand which markets are suitable for these currently landfilled mixed waste bales. The injection process is a critical step in the optimization of new polymer delivery systems for the thermal oxo-degradation and pyrolysis teams. MRFs and recyclers do not mold test strips on #3–#7, and very little (if any) of this work is done by recyclers on recovered materials for characterization. Very limited characterization is done at converters on bales that have established markets. We have active relationships with six MRFs across the country. We have completed site visits at four MRFs and are planning to visit two more in late summer and early fall 2023.
- Comment (Reviewer 1): The STRAP work is among the strongest from the project, with partners interested in commercialization and scale-up work ongoing. As there are other solvent-based recovery technologies coming into the market, such as Pure Loop, understanding the TEA/LCA for STRAP against the wider landscape is critical. It is worth considering how insights into the variability of waste streams with location, season, and potentially long-term material shifts would impact the sizing, location, and design of STRAP facilities.
- Response: We appreciate the positive comment. We have compared STRAP to two competing solvent-based recycling processes (PureCycle and CreaSolv) based on information in the literature. We believe that STRAP has potential advantages, and we have applied for intellectual property (IP) in these areas. Moreover, we have already hosted a representative from CreaSolv at a CUWP seminar to exchange ideas and learn about their technology. We will host a representative from PureCycle as a seminar speaker in

summer 2023. These conversations have already been helpful in understanding potential challenges, and possible solutions, that will be faced during scale-up of STRAP.

- Comment (Reviewer 2): The wide collaboration is impressive. The focus on pyrolysis is not innovative.
- Response: A more accurate characterization of plastics pyrolysis is that it is not a new technology; however, innovation can occur at any stage in the life cycle of a technology. Pyrolysis has been attractive to industry for many years because of its robustness in handling diverse plastic wastes and its ability to process those wastes at relatively high rates; however, pyrolysis faces distinct challenges that call for innovation in energy efficiency, contaminant neutralization, and products that have higher value than fuel oil. The CUWP pyrolysis program is targeting these challenges through studies on generating high-value olefins, aromatics, and even oleochemicals from waste plastics and eliminating external energy demand through autothermal operation. These innovations, along with emerging policies mandating better management of waste plastics, will make pyrolysis economically and environmentally attractive.
- Comment (Reviewer 2): The impact of the ML database is not clear.
- Response: Using characterization data collected by each MRF for landfill-diverted waste, we will establish an ML database that can be used to identify optimized pathways for each feedstock. The database will be used to determine the suitability of different waste streams for different processing pathways (particularly STRAP versus pyrolysis). The goal will also be to predict costs and emissions associated with such processing.
- Comment (Reviewer 2): It was unclear whether the solvent analysis includes costs to dispose of waste solvent (it should).
- Response: Currently, the TEA model does not account for waste solvent disposal, as we assume a high solvent recycling rate; however, we agree that this is an issue that needs to be considered, and it will be handled in our future models.
- Comment (Reviewer 2): The work sorting bales was done by hand by a graduate student and does not seem to be replicable in any scalable, financially viable way. I would like to know how they identify the number of the matrix plastic; that seems important and difficult.
- Response: Hand sorting is the accepted ASTM method for analyzing municipal solid waste (MSW) from landfill-diverted materials. The hand sorting is not intended to be scaled for MRFs or recovery facilities but instead used for analysis of a bale for research and data collection; however, most MRFs and recovery facilities are using manual sorting of recovered waste, especially MRFs in rural areas. As previously stated, we are currently working with multiple MRFs and recyclers across the country, and data on composition and performance of sorted mixed waste landfill plastics is not known. There is no compositional data on mixed #3–#7 bales (in the United States), and as result, there is no performance data on the properties of sorted #3–#7 mixed bales. The process for sorting a whole bale is necessary to understand the entire composition, which, in turn, allows for the implementation of ASTM D5231 for sampling mixed waste for further processing. Per ASTM, washing, pelletizing, and molding is the globally accepted method for understanding the mechanical properties of these landfill-diverted mixed waste plastics for downstream operations.
- Comment (Reviewer 3): The absence of synergy between teams noted in the last review was addressed with regular meetings with constituencies within the consortium. I applaud the strengthening of the CUWP management structure and the existence of a board with representation from all stakeholders, including the IAB. Recovery from multilayers seems particularly solvent-intensive. The STRAP process is excellent, and I would like to see a validation step—a side-by-side comparison of STRAP-recovered

polymers against virgin polymer in a multilayer film food application as a way to demonstrate equivalency in performance.

- Response: We agree with the reviewer, and we are already working on characterization of STRAP-recovered polymers to compare against virgin resins (as a collaboration between Topic Area 2 and Topic Area 5). Our data show that key properties of the recovered resins—including molecular weight distributions, thermal properties, and melt flow indices—are very similar to virgin resins. We have further scaled up the production of STRAP materials to recreate a cast polyethylene film for comparison to films from virgin resins. We will continue to incorporate such comparisons in our future studies.
- Comment (Reviewer 3): One point of concern: The economics modeling that shows value in siting pyrolysis plants in high-population-density areas raises my concern for having a rigorous study of the impact through an environmental justice lens. I would encourage the investigators to engage with entities to thoroughly vet the potential environmental impact on the adjacent communities.
- Response: We agree with the reviewer. Our computational models will be adapted to account for constraints on technology locations; here, it will be interesting to understand the interplay among environmental justice, carbon emissions, and economics (that might result from higher transportation demands). We are also currently developing a computational model to evaluate the impact of new recycling technologies on social justice in Mexico.
- Comment (Reviewer 4): For the research-focused aspect of the program, it would be great to collect data on the number of students that have attended the class, the number of undergraduate researchers that are sponsored, and the number of students that have participated in the exchange program.
- Response: Thank you for this comment. We will collect the data and provide this information in future reports.

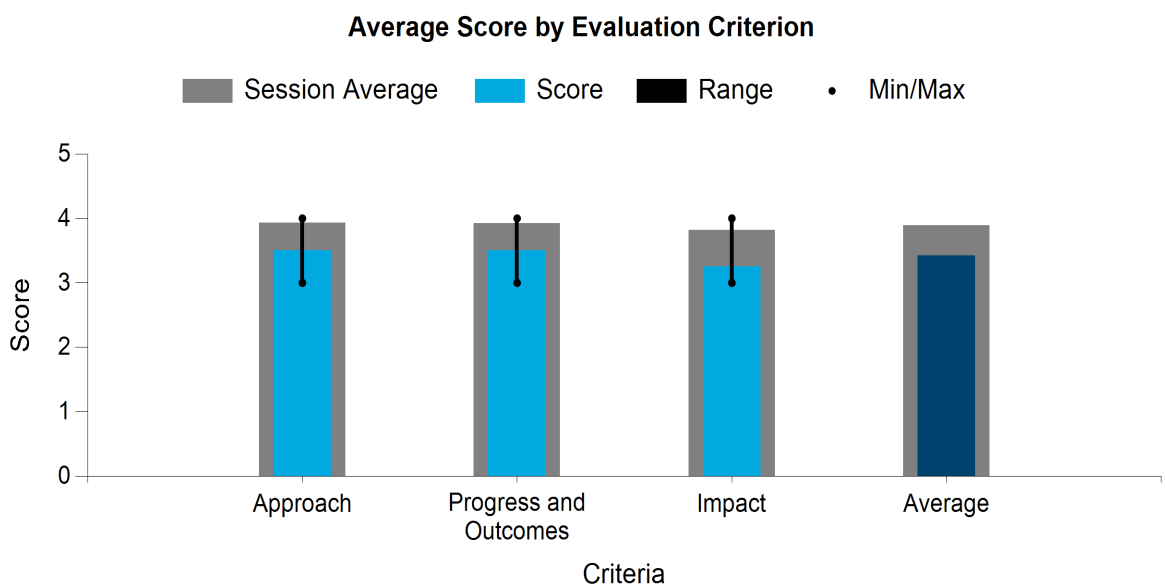
PRODUCTION OF HIGH-PERFORMANCE BIODEGRADABLE POLYURETHANE PRODUCTS MADE FROM ALGAE PRECURSORS

University of California San Diego

PROJECT DESCRIPTION

WBS:	2.3.4.615
Presenter(s):	Michael Burkart
Project Start Date:	01/01/2021
Planned Project End Date:	02/28/2024
Total Funding:	$2,500,000

For this program, we are adapting and scaling chemistry to convert algae oil into monomers for PU products, with a focus on TPUs. We previously developed routes to prepare both components of PU materials—polyols and diisocyanates—from renewable sources. We also showed that our PUs can biodegrade under compost conditions. We are expanding on these to increase the renewable content and the algae content, as well as ensuring that our TPUs retain biodegradability. We are preparing polyols with 80%–100% renewable content and ensuring that they retain properties as drop-in replacements for manufacturing. We have scaled a flow chemistry process for diisocyanate preparation and are optimizing it for yield and purity. To date, by combining these processes, we have prepared TPUs with a bio-content of 85% and an algae content of 61%. These materials show excellent physical characteristics, on par with commercial petroleum TPUs. We have initiated a route to a second algae-sourced diisocyanate via enzymatic epoxidation of polyunsaturated fatty acids. We have prepared a variety of product prototypes with renewable and biodegradable TPUs, including injection molded cell phone cases, coated fabrics, and 3D-printed filament. Finally, we have initiated TEA and LCA on the scaled processes.



COMMENTS

- Although key risks are identified, the proposed mitigations are very high level. A deeper explanation of how these technical challenges would be overcome would improve the chances of success. The general logic of the project is clear; however, the potential material design space is vast, and there does not seem to be a methodical approach to how it will be explored (e.g., what we *should* make from the range of what we *can* make). Interaction with other projects focused on developing biodegradable TPU-like materials could increase the probability of success. The novelty and strength of the project are in the synthetic routes from algae to diisocyanates and novel polyols. This aspect is well done and is progressing. The application and material performance aspects are significantly weaker. How does using heptamethylene diisocyanate (7HDI) for a TPU impact properties relative to the dominant isocyanates used in the market (such as methylene diphenyl diisocyanate (mdi) and others)? The slower reactivity could be a showstopper for commercialization or could limit the range of applications. Engaging an industry partner in the TPU space to give guidance and feedback here would increase the potential for commercial success. There is a huge variety of thermoplastic TPUs in the world that have been optimized for different processing or application spaces. The application space for these new proposed materials feels naïve (phone cases, watches)—these applications are highly cosmetic (color, feel, surface finish), which plays a key role in their potential success. Working with industry to gain more insight into how to match TPU physical and chemical properties to application spaces would increase the likelihood of identifying application spaces where the commercialization of these materials may be feasible. Finding a partner who is currently active as a TPU supplier or utilizer would strengthen the impact potential. Additionally, the logic of making these applications biodegradable rather than recyclable is not obvious. Identifying applications where the use is inherently dissipative (e.g., agriculture, paint) would be a stronger case. Similarly, the end-of-project milestone needs a sharper definition of performance and TEA/LCA to demonstrate industrial potential.

- The risks and mitigation slides at the beginning did not embody the risks and mitigation approaches described in the rest of the presentation. The approach slide needed to be reformatted to convey the intended information. The presentation became more informative at slide 8. I did not see information on communications, either within the project team or with entities outside the project team, including commercialization.

- Applying LCA/TEA upfront would be beneficial to point out critical steps that might be detrimental in scale-up and environmental impact. The team has shown progress in making the prepolymers, but process optimization is required to address slow polymerization. In terms of synthesis of diisocyanate, the team achieved very good yields of the diisocyanate product. The prototypes were impressive. How are the commercial project partners, BASF and PepsiCo, engaged to drive toward a commercially robust process with a targeted application that is realistic? On the initial biodegradation analyses: Are the tests performed with virgin polymer, or are they formulated with appropriate stabilizers for the intended applications (e.g., stabilizers typical for oxidation, thermal stability, and so on)?

- The team has made great progress toward developing their flow reactor and is close to reaching their productive target of grams per month. I applaud the team for producing application prototypes and believe that their plan to bring in industry partners to further this effort is essential. I would recommend that the team start their TEA/LCA as soon as feasible and integrate the learnings from the analysis back into the development of the flow reactor.

PI RESPONSE TO REVIEWER COMMENTS

- Comment: Although key risks are identified, the proposed mitigations are very high level. A deeper explanation of how these technical challenges would be overcome would improve the chances of success. The general logic of the project is clear; however, the potential material design space is vast, and there does not seem to be a methodical approach to how it will be explored (e.g., what we *should* make from the range of what we *can* make). Interaction with other projects focused on developing biodegradable TPU-like materials could increase the probability of success.

- Response: The full BOTTLE team, including both the University of California San Deigo and Algenesis teams, meets weekly to discuss goals, progress, and applications. Algenesis has clear goals for metrics for specific materials, specifically TPUs suitable for injection molding (for heel counters and other TPU-based footwear materials) and fabric coating. Unfortunately, the presentation format did not allow for a full discussion of these product developments.

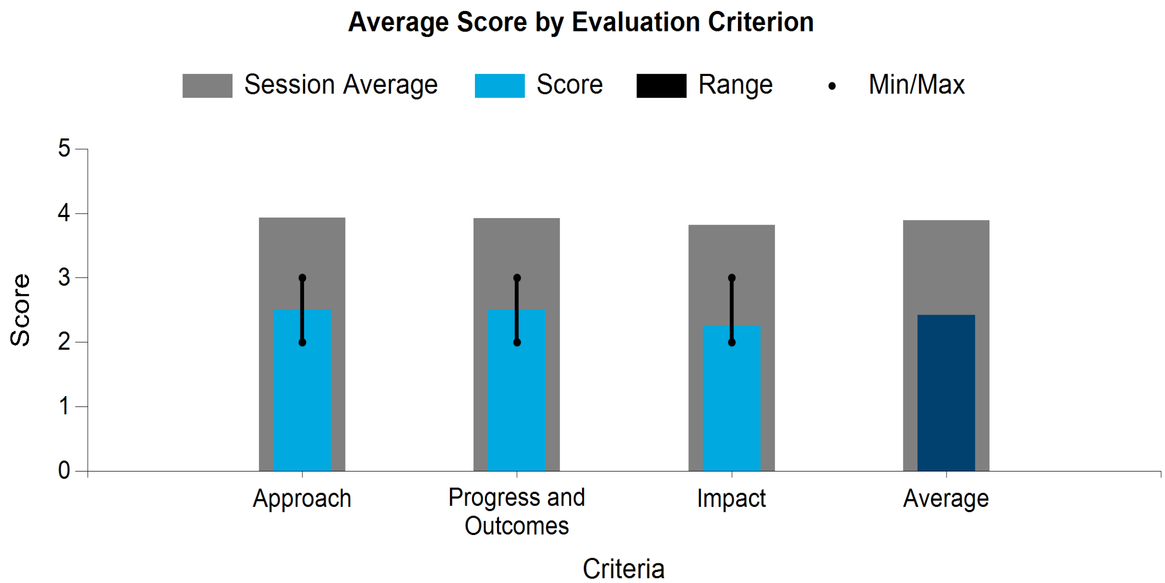
- Comment: The novelty and strength of the project are in the synthetic routes from algae to diisocyanates and novel polyols. This aspect is well done and is progressing. The application and material performance aspects are significantly weaker. How does using 7HDI for a TPU impact properties relative to the dominant isocyanates used in the market (such as mdi and others)? The slower reactivity could be a showstopper for commercialization or could limit the range of applications.
- Response: Both aromatic diisocyanates and aliphatic diisocyanates are used in commercial TPUs. Aliphatics have lower reactivity in general; therefore, TPUs must be cured prior to use. This is standard for the industry. 7HDI appears to be a drop-in replacement for other aliphatic isocyanates, such as hexamethylene diisocyanate (6HDI). According to our preliminary formulations and experiments, 7HDI reacts nearly identically to 6HDI. We believe that any differences in TPU material metrics can be addressed by formulation optimization, an area of significant expertise for Algenesis.
- Comment: Engaging an industry partner in the TPU space to give guidance and feedback here would increase the potential for commercial success. There is a huge variety of thermoplastic TPUs in the world that have been optimized for different processing or application spaces. The application space for these new proposed materials feels naïve (phone cases, watches)—these applications are highly cosmetic (color, feel, surface finish), which plays a key role in their potential success.
- Response: Algenesis has been working with large TPU manufacturers and users. For instance, the large engineered polymer company Trelleborg recently announced a collaboration with Algenesis for production of coated fabrics (https://www.trelleborg.com/en/engineered-coated-fabrics/media/trelleborg-partners-with-algenesis-to-create-sustainable-thermoplastic-polyurethanes). Therefore, we have an active engagement with product development and with end users.
- Comment: Working with industry to gain more insight into how to match TPU physical and chemical properties to application spaces would increase the likelihood of identifying application spaces where the commercialization of these materials may be feasible. Finding a partner who is currently active as a TPU supplier or utilizer would strengthen the impact potential.
- Response: We have industry partners who are actively interested and engaged in our research and downstream products. This includes cost-share partners PepsiCo and BASF. We have access to these companies to get feedback and advice, and we have had regular (monthly) interactions with members of their teams.
- Comment: Additionally, the logic of making these applications biodegradable rather than recyclable is not obvious. Identifying applications where the use is inherently dissipative (e.g., agriculture, paint) would be a stronger case.
- Response: It has become increasingly clear to us that recycling is not going to save our planet from the dangers of plastic waste. It has been reported that less than 5% of recyclable plastic is ever actually recycled, and that all plastics (even recycled ones) can end up as microplastics in our waterways and oceans. Microplastics can now be found in every animal on the planet, in all human organs, and all over the world (from the Arctic to the Himalayas.) Only biodegradable materials will solve this problem. We will make sure future presentations drive these facts home.
- Comment: The end-of-project milestone needs a sharper definition of performance and TEA/LCA to demonstrate industrial potential.
- Response: The TEA/LCA portion of this project has been slated to take place at the end of the program. We will ensure that performance and industrial potential are clarified in this work.

- Comment: The risks and mitigation slides at the beginning did not embody the risks and mitigation approaches described in the rest of the presentation. The approach slide needed to be reformatted to convey the intended information. The presentation became more informative at slide 8.
- Response: We apologize that these were not clarified in the presentation. Unfortunately, the slide template does not allow for great communication of these concepts, nor many of the most exciting aspects of the research.
- Comment: I did not see information on communications, either within the project team or with entities outside the project team, including commercialization.
- Response: We meet weekly to discuss the BOTTLE project with the entire team from both the University of California San Deigo and Algenesis. We have separate LCA/TEA meetings with the University of California San Deigo every two weeks.
- Comment: Applying LCA/TEA upfront would be beneficial to point out critical steps that might be detrimental in scale-up and environmental impact.
- Response: We are performing these TEAs now as part of the final task and final budget period.
- Comment: How are the commercial project partners, BASF and PepsiCo, engaged to drive toward a commercially robust process with a targeted application that is realistic?
- Response: BASF and PepsiCo are cost-share partners who have supported our research through their academic outreach arms—so they are interested, but their product development teams are not yet engaged. Regardless, we have regular interactions with their scientists and discuss applications for most interactions.
- Comment: On the initial biodegradation analyses: Are the tests performed with virgin polymer, or are they formulated with appropriate stabilizers for the intended applications (e.g., stabilizers typical for oxidation, thermal stability, and so on)?
- Response: The tests are done with virgin polymer. Certain additives are used to make the formulations, but they do not include stabilizers as the reviewer suggests, because many of those have been developed to hinder biodegradation and are not consistent with our desired applications.
- Comment: The team has made great progress toward developing their flow reactor and is close to reaching their productive target of grams per month. I applaud the team for producing application prototypes and believe that their plan to bring in industry partners to further this effort is essential.
- Response: Thank you!
- Comment: I would recommend that the team start their TEA/LCA as soon as feasible and integrate the learnings from the analysis back into the development of the flow reactor.
- Response: As stated above, we are beginning this now.

HYBRID APPROACH TO REPURPOSE PLASTICS USING NOVEL ENGINEERED PROCESSES (HARNESS)

Battelle Memorial Institute

WBS:	2.3.4.616
Presenter(s):	Kate Kucharzyk
Project Start Date:	05/01/2021
Planned Project End Date:	04/30/2024
Total Funding:	$2,499,778



COMMENTS

- I agree that there is a great need for foam alternatives. I did not get the information from this presentation that this work is making the connections necessary to achieve this. The answers in the Q&A did not provide the information missing from the presentation.
- This project has a high ambition to move from TRL 0 to TRL 6 during the course of a relatively small project in a 3-year time frame; however, the approach is inadequate for the ambition level. Success depends on multiple steps in the value chain, and it is not clear that there is sufficient engagement between the players. The project approach did not address any of the separation/process design steps needed after degradation of the foams. To date, the accomplishments are screening enzymes on a model compound for degradation and replication of a commercial recipe to form a TPU foam; however, no degradation results or feedstock preprocessing activities appear to have been started, and the LCA/TEA data shown on slide 9 appears to relate to PET, suggesting that the team is assuming the conclusions will hold for TPU. The TEA/LCA should be updated to reflect the materials and processes for this project. Focusing on high-volume polyether-urethane foams that currently do not have a viable recycling option at EOL has the potential for wide impact. If successful in recovering polyol and diamines at sufficient yield and purity, there is a clear route to reintroducing them into the market. Emphasis was put on

industry partners, but their level of commitment to moving this project forward is not at all clear and would be critical for any eventual impact.

- The progress in this early-stage project has been satisfactory—it is nice that you have a quick visual (fluorescent) screen for the degradation of the PU. The work in the next four quarters on the tasks on enzyme optimization and upcycling to PU foams will be critical to driving a desirable outcome in the go/no-go decision. Achieving this seems daunting. I am puzzled by the projections to move the project from TRL 0 to TRL 6 at the project end—this seems pretty aggressive for a program developing a proof of concept and building a key technology (e.g., PU foam degrading enzymes). It is laudable that the team has engaged key PU foam formulators to provide an appropriate specification for upcycling to industry standards. It will also be valuable to have detailed economic analyses on the polyols and diamines captured from the PU foams.

- The researchers are looking to grow from TRL 0 to TRL 6 during the course of the project. The team should submit a more detailed plan for reaching these very high TRLs. TRL 6 includes engineering development of the technology as an operational system. The major difference between TRL 5 and TRL 6 is the step up from the laboratory scale to the engineering scale and the determination of scaling factors that will enable the design of the final system. A report by the National Aeronautics and Space Administration in 2015 analyzed 131 projects funded by its Small Business Innovation Research program and found that the average time to advance from TRL 1 to TRL 2 was 1.2 years, from TRL 2 to TRL 3 was 1.4 years, from TRL 3 to TRL 4 was 2.1 years, from TRL 4 to TRL 5 was 3.4 years, and from TRL 5 to TRL 6 was 4.6 years. Based on the presented plan, the scale-up work will be done by the industry partners. I would want to understand in more detail how the industry partners will be participating. Even if the scale-up is developed by industry partners, the group leader should know the challenges and processes required. The "Upscaling of Non-Recyclable Plastic Waste Into CarbonSmart Monomers" project demonstrated a great plan to achieve very high TRL from an early project and showed the types of equipment and systems that are required.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you for the comments and for your time reviewing our project. We believe that we can advance swiftly from TRL 0 to TRL 3 once the enzymatic candidates for PE-PU degradation are found. Our team is already showing degradation of monomers and is starting to test solid feedstock material. The team has not started to work on the separation/process design steps, as these will come later in the program, once we show successful solids degradation. We do have an approach drafted for this work and are happy to share it with the reviewers. Thank you for the comment on the involvement of the industry partners. We created a slide that shows the material flow through our project team. We also have a pretty clear delineation of how the collaborators and industry partners contribute to the work. We are happy to share more information. The process that we are designing breaks down the PE-PU to the monomers. We are not clear yet about their purity and will have to determine what type of recycled foams we can make once the process continues through the next phase of the laboratory work. I apologize that we do not have information on this at the moment. The reviewers are correct that finding candidate enzymes for PE-PU degradation is not an easy task. During the first months of the project, we have spent time building our foundational capabilities, including detection and high-throughput detection assays, selection of proteins for degradation, and characterization of the industrially sourced foam material. We were also delayed by several months due to COVID, so our progress as planned is not on track. We will be requesting a no-cost extension to BP2. We will evaluate our progress (TRL 0–6) after the next milestone and will communicate with the project manager on any roadblocks. As I am reading your comments on the TRL progression, I wonder if we have used a different scale with which DOE is gauging the technology readiness. Based on our understanding, by the end of the project, our team would build a bench-scale prototype system that will be able to handle all the reactions at 10-L scale. We are not planning to bring the process to the industrial scale. We would like to seek more clarity and guidance on this issue. Thank you so much.

INFINITELY RECYCLABLE AND BIODEGRADABLE FILMS FOR IMPROVED FOOD PACKAGING

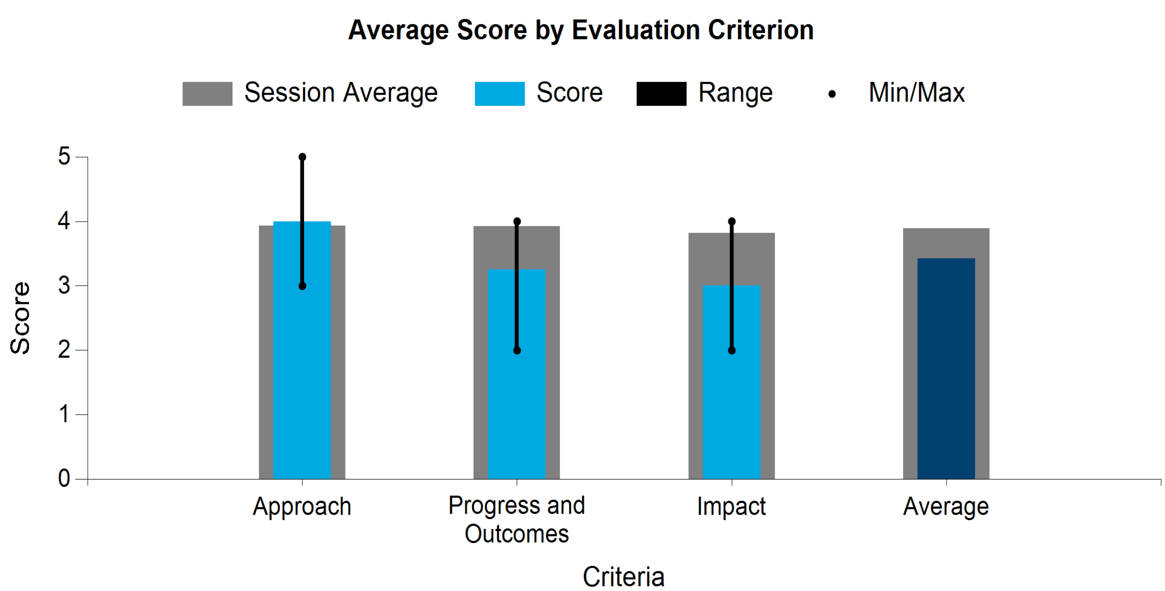
TDA

WBS:	2.3.4.618
Presenter(s):	Allison Robinson
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$2,011,426

PROJECT DESCRIPTION

Multilayer packaging is an extremely important and widely used technology; by combining many materials into a single film, the final product can have properties that are unattainable by any single material. Despite their benefits, these films generate an enormous amount of plastic waste. It is critical to transition to sustainable multilayer films, which maintain the benefits of traditional single-use packaging without producing plastic waste. This can be achieved by transitioning from today’s fossil-fuel-based polyolefins to an ester-based paradigm that uses bio-derived materials to decarbonize the packaging industry.

In this effort, TDA Research Inc., NREL, and Sulzer will work together to design ester-based films for multilayer packaging. We will optimize a compostable nanocomposite (made of surface-modified cellulose nanofibers in a compostable polymer matrix) to act as a strong food contact layer with low water vapor permeability. We will separately optimize a recyclable-by-design polymer to act as an oxygen barrier layer and as a printable outer layer. The result of this effort will be a sustainable multilayer film that is safe for food contact, has oxygen and vapor barrier properties comparable to traditional films, and is entirely compostable and/or recyclable.



COMMENTS

- The specified risks do not seem comprehensive. The connections among the partners, their roles, and the systems that the project will need to connect to prove success (obtaining inputs, having recipients for outputs) were not shown sufficiently. Each may be succeeding in their individual role, but the role distinctions and relationships were not made clear. Overall, the project appears on track with where the team is in their timeline.

- This project is focused on the formulation of polylactic acid (PLA) nanocomposites and epoxy anhydrides as barrier films. The approach is logical. The risks and mitigations are focused on project management; I would like a more detailed approach toward the technical risks and their mitigation strategies. There is a clear and appropriate mitigation strategy around food contact compliance. I feel that a large risk for this project is that the proposed material will not have the needed melt processability to compete in this space. The proposed plan of hot pressing and extrusion coating will not give sufficient insight. I recommend involving a partner with more insight in the key processing properties needed for these applications early in the project to steer development. The project team is rather process focused (TDA/Sulzer), and I fear that it lacks sufficient insights into the full value chain necessary for the introduction and successful adoption of new polymer films for this market. The project is at an early stage and is encouraged to build this broader perspective now. As the proposed work is very much a product development activity without connection to the end use and processing, I am deeply skeptical that it can be successfully commercialized. The project plan includes specific DEI milestones, and the emphasis on exposing interns to multiple career paths is good. I would like the project team to discuss what they have selected as the SOA for benchmarking their metrics; linear low-density polyethylene is very cheap, suggesting that the cost parity target may be extremely challenging to achieve. Additionally, the cost metric will be influenced by the envisioned film production method (coextrusion, lamination, blown film), and it would be good to see this full route from synthesis to film production (not just pellet production) incorporated into the evaluation metrics.

- This is a well-thought-out plan, and at this early stage, the team is on track. The team provided great details and thoughtful consideration on (a) the nuances of barrier packaging needs for each application, (b) the design and execution of the DEI plan, and (c) navigating the regulatory considerations for food contact surfaces. Also, the end-of-project milestone detailed well-defined targets.

- I appreciate that the team has a plan to use the TEA/LCA results to guide their choice of materials. The team is collaborating with an industry partner, Sulzer, to develop and optimize the manufacturing and bring this technology to market. It is fantastic that the team is already thinking about the food safety of their product and is considering the FDA process for materials in contact with food. The team will consider both composting and chemical recycling for their multilayer films. All three—TDA, NREL, and Sulzer—will develop patents for this, and the goal will be to license to Sulzer. The IP out of this DOE-funded work should not be locked into an exclusive license—especially in the field of biodegradability and food packaging, widespread solutions should be the target.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' time and feedback on our project. We are happy to see that the reviewers think that the project has a "well-thought-out plan," that "at this early stage, the team is on track," and that "the team provided great details and thoughtful consideration," as these comments highlight what we have been trying to accomplish through this FOA and overall project. Our response to the reviewers' other comments, which focused on technical risks and material baselines, is as follows. The technical risks that we discussed were focused on ensuring that the material meets the barrier property targets we initially set. The barrier properties are the primary factor that determines whether a film will be viable for this application, so this is the most important technical requirement; however, this has been significantly mitigated through our initial demonstrations, which show that we are near the targets before optimization. In our next Project Peer Review, we will discuss the technical risks and mitigations in greater detail. One reviewer had concerns that the proposed material will not have the needed melt processability to compete. The project team believes that the optimized material will be able to compete; PLA films are already produced commercially, and our work to date has not shown evidence that incorporating the cellulosic additives impacts this. Previous work with the epoxy anhydrides has demonstrated that they are sealable and that their tunability could enable the required seal at moderate temperatures, as desired (e.g., T = 50°C). To ensure that this does not prevent commercialization, we will begin investigating these concerns early in the effort, as recommended. Further, we can involve additional partners if needed (as suggested); TDA, NREL, and Sulzer all frequently collaborate with companies across the value chain and have the ability to bring in additional expertise if needed. We selected our SOA materials based on films that have moderate barrier properties and high-volume use in the market. This will allow us to have a significant impact in displacing conventional films when we commercialize our film. If our material can attain better barrier properties (which we anticipate it can), we will be able to target even higher-value films as well. We will perform TEA throughout the project, and we will include the film production method in our calculations to ensure that we are accurately assessing cost parity. Importantly, we are baselining our production against ethylene vinyl alcohol and the total multilayer performance. Marking against any variation of PE would be insufficient. This is because PE alone does not provide the proper barrier properties for food applications, and the multilayer packages derive their ideal properties in conjunction with the critical ethylene vinyl alcohol. Additionally, because we are performing TEA at multiple points throughout the development process, we will be able to change our processing methods and/or material composition as needed to ensure we reach our cost parity goals. To clarify the roles of the team members, NREL is developing epoxy anhydrides, Sulzer is optimizing their PLA formulations, and TDA is developing composites out of TDA's cellulosic additives and Sulzer's PLA. This will make two-layer materials: the epoxy anhydride and the PLA composite. All three entities will work together to combine these materials into a multilayer assembly and to assess their performance. We see this as a collaborative effort among all three team members; although we have our own specializations within the project, we will work together closely throughout the entire effort.

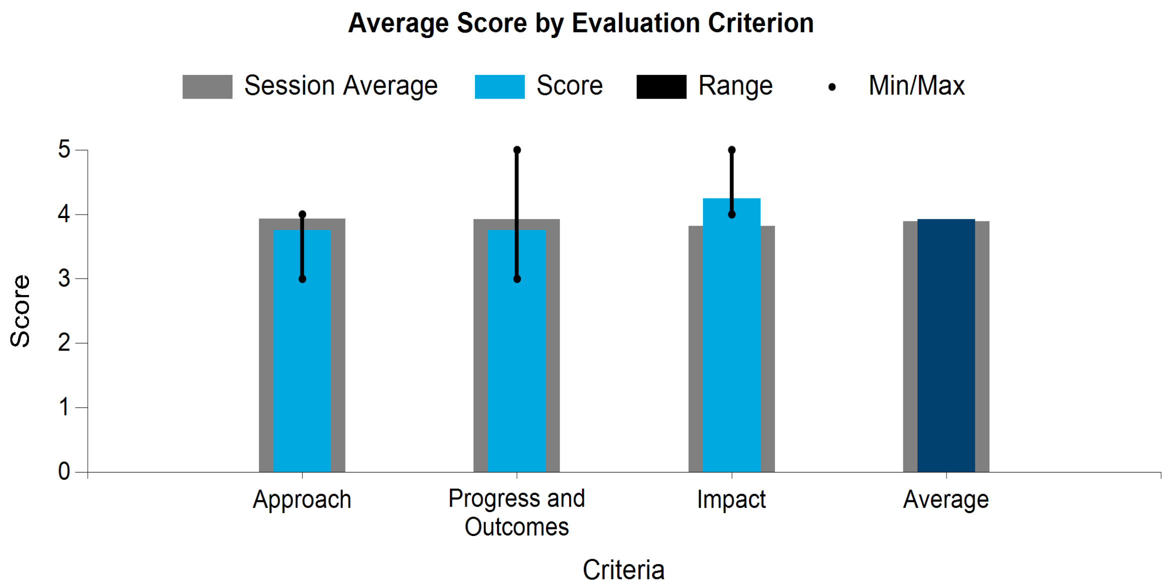
DEVELOPMENT OF INFINITELY RECYCLABLE SINGLE-POLYMER CHEMISTRY BIO-BASED MULTILAYER FILMS USING ETHYLENE/CARBON MONOXIDE COPOLYMERS

Braskem

PROJECT DESCRIPTION

WBS:	2.3.4.620
Presenter(s):	Hadi Mohammadi
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$2,500,000

Today, the majority of plastic littering the environment is packaging material. In this project, we will investigate the possibility of producing infinitely recyclable, single-polymer chemistry, multilayer films using bio-based non-alternating ethylene-carbon monoxide (CO) copolymers. We will design two multilayer films to fabricate stand-up pouches for use in packaging applications: (1) multilayer films made of one specific ethylene-CO copolymer and (2) multilayer films made of ethylene-CO copolymers with different CO content. The main recycling route for both of our proposed single-polymer chemistry, multilayer films is mechanical recycling. We will produce at least one prototype of our proposed multilayer films, which, when compared to conventional multilayer packaging, will display (1) 10% cost reduction, (2) comparable performance, (3) 60 wt % to 80 wt % recycled carbon utilization in the final design, (4) 60% energy savings during production, and (5) photodegradability. Cost-competitiveness, sustainability, and lower amounts of energy required for production will increase the value proposition for recycling multilayer films fabricated from bio-based ethylene-CO copolymer, encourage companies to invest in its recycling by decreasing the cost/benefit ratio, free landfills and oceans from its presence, and boost the economy by creating jobs in the recycling field.



COMMENTS

- Slide 5 is nice and clear. I would recommend more graphical slides. The roles of the non-Braskem partners were unclear. Is there no direct role for Braskem in DEI? The answers in the Q&A were clear and informative. I would recommend adding some of these to the presentation, as they will come up again (specifically the LCA-related questions and the existing relationship/current experience with the FDA). Braskem has recycling facility(ies) so can work out source materials internally, which is a benefit to this project in the long term. Similarly, their regular FDA food contact relationship is a useful resource.

- The project aims to produce a CO-bio-ethylene copolymer as an alternative to PE. If successful, it could have large emissions reductions given the volume of PE used. A strength of the project is the active engagement of industry partners, ranging from a material producer (Braskem) to an end user (Unilever), with converters involved via contracting. As Braskem also runs recycling facilities, there is a natural route to evaluating recyclability potential. This full supply chain vision allows clear performance metrics. Food contact compliance has been considered, but the ultraviolet stability of the proposed material is a concern. Biodegradation is not included in this project, as it has already been studied in the literature. As such, there is substantial potential for commercializing the proposed innovation. The project has a plan to address DEI both in terms of recruitment for the project as well as outreach/dissemination of the knowledge into underserved communities. The proposed tasks are logical, but as the project is just beginning, there were insufficient results to judge the quality of the approach and outcomes.

- The proposed plan for this early-stage project seems reasonable, and the engagement of two industry leaders, Braskem and Unilever, is promising. The DEI activities include hiring and educational outreach. Are these centered just at the academic institutions? Please describe the Braskem DEI commitment. How actively engaged is Unilever beyond providing specifications for the multilayer film barrier properties? It would be helpful to see more detail on the activities in BP2, e.g., the number and amount of copolymers to be produced. The technical plan seems lean, and there are a number of technical questions that are wanting. These include considerations for stabilizing these ethylene-CO-copolymers (which should be different than for polyolefin); how the discrete individual layers will be separated and reused given the mechanical recycling proposed; and an articulation of the vision for the process feed of the syngases, ethylene, and CO—from different microbial fermentations?

- This is a very early project. I appreciate that the team is working with its industry partners in developing their food contact products and has an internal group that works on this. They will work with this team to move forward with the regulatory approval. I appreciate that Braskem is open to licensing this technology to other manufacturers so that it can be deployed at scale. I would like to see a TEA/LCA of this project as well. In terms of presentation, the team could include some more graphics and data to illustrate the points they are making.

PI RESPONSE TO REVIEWER COMMENTS

- The presenter and project team would like to thank the reviewers for their thoughtful comments and suggestions. The DEI activities for this project will include hiring and educational outreach activities from academic and industrial institutions. In particular, Braskem will practice its standard hiring procedures where it prioritizes underrepresented comminutes in the interview process. Braskem will also engage in K–12 educational outreach efforts with local schools, such as PlastiVan, with a particular focus on disseminating our knowledge in MSIs and other appropriate institutions serving underserved communities. As a key partner in our project, Unilever will define the target end use for the stand-up pouches, help the team understand the packaging specifications in such applications, contribute to the design of the ethylene-CO-copolymer-based multilayer films, and test the final stand-up pouch made from virgin and recycled material in their facility. The results from the Unilever tests on our stand-up pouch prototypes will allow us to verify the performance of our solution in the target application. In terms of the number and amount of copolymers produced in BP2, we are targeting studying the copolymerization process in at least 20 different conditions with pressures from 40–200 bar, temperatures from 25°–200°C, and CO concentrations from 1%–50%. We will establish the effect of temperature, pressure, and CO concentration on activity of the designated catalyst system during ethylene/CO copolymerization while aiming to achieve a minimum catalyst activity of 500 mol(ethylene)/mol(catalyst)/h at 4 mol% CO incorporation. Regarding the recycling process, our vision is to not separate the individual layers during mechanical recycling. As our targeted solution, we will produce a multilayer film with different ethylene-CO copolymers in the layers. The balance between the mechanical and barrier properties in each layer can be adjusted by varying the CO content in each copolymer. In this design, the adhesion between the layers will be achieved through co-crystallization between the two adjacent layers. As the ethylene-CO copolymers are highly compatible, mechanical recycling of our single-polymer chemistry, ethylene-CO-based, multilayer films is expected to lead to a compatible mixture of the ethylene-CO copolymer with a CO content that is the average of all layers. After adjusting the CO content of the mechanically recycled mixture by blending it with pure PE (decreasing the CO content) or a high-CO ethylene-CO copolymer (increasing the CO content), it will be reused as a layer in the multilayer film structure. Finally, we envision producing bio-based ethylene and CO via two different routes: (1) converting sugars from corn to ethanol through fermentation, and then turning ethanol into ethylene by dehydration; and (2) producing CO from controlled combustion of biomass.

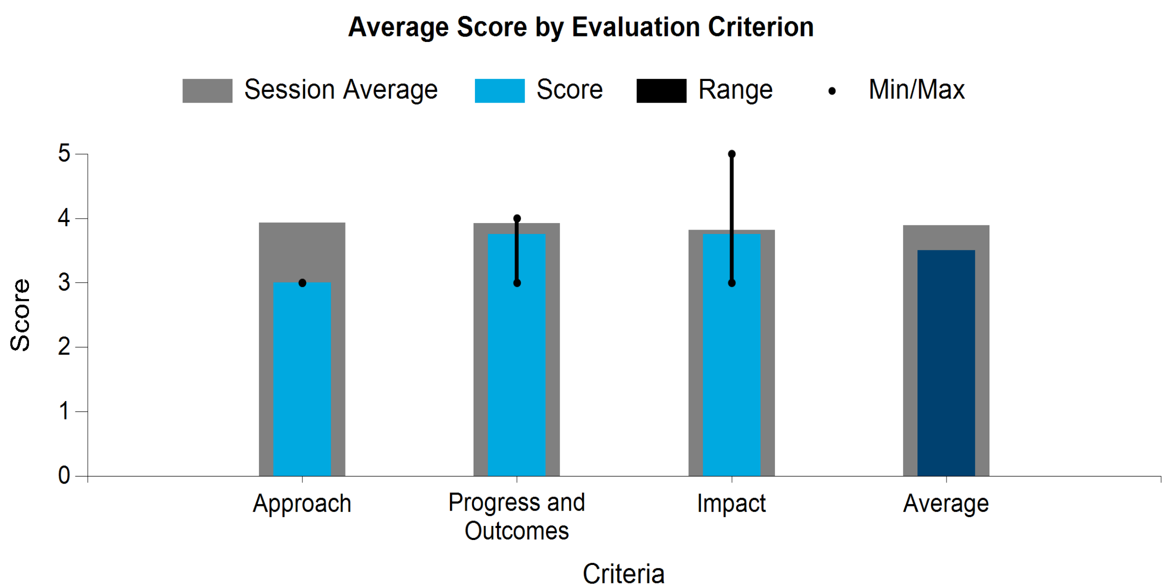
ENABLING LIGNIN VALORIZATION WITH LIQUID-LIQUID CHROMATOGRAPHY

Lignolix Inc.

PROJECT DESCRIPTION

WBS:	2.4.2.200
Presenter(s):	Eric Gottlieb
Project Start Date:	10/01/2021
Planned Project End Date:	03/31/2025
Total Funding:	$3,126,696

This project uses scale liquid-liquid chromatography for the separation and purification of lignin monomers and oligomers from Lignolix's proprietary process. The recovery of lignin products from lignin-rich reductive catalytic fractionation oils is notoriously difficult because they are chemically complex, viscous, contain fine particles, and have broad non-normal molecular weight distributions. Accordingly, these streams are not well suited for separation with traditional simulated moving bed chromatography because the high-molecular-weight compounds lead to rapid fouling of the resin stationary phase. Note also that the target products from these streams cannot be recovered with distillation due to the thermal instability of the solution. Countercurrent chromatography (CCC) is a form of liquid-liquid chromatography that is a scalable and uses the countercurrent motion of a two-phase liquid-liquid system to generate a chromatographic effect on the solvated compounds, separating them into pure components. Accordingly, CCC could represent a paradigm shift in lignin valorization through scaling and deployment in this project. It represents a single-step separation technology for these traditionally difficult-to-process streams due to its high throughput, ability to handle solids, viscous solutions, and low energy consumption. This project is developing the needed chromatography methods, solvent recycling, CCC validation, and TEA/LCA for the separation process.



COMMENTS

- The team is working on the development of continuous CCC for lignin deconstruction product streams. The team has made great progress in a short time. The project is on track. There are lots of similarities between their work and Gregg Beckham's project. I am not sure that this continuous CCC has the potential to create wider and more significant impact. The team should think seriously about feasibility and scalability. The PI needs to develop a DEI strategy and show the progress in the next review period or at the end of the project.

- This is a relatively new project. Internships and DEI efforts are not specifically outlined. It is difficult to separate the objectives of this project from the "Continuous Counter Current Chromatography" project led by NREL. It is good to see that the team is already working with industry to enable lignin-based hot-melt adhesives and 3D printing acrylates as potential commercial products. Good progress has been made in the initial verification and lignin deconstruction. The TEA and LCA show significantly reduced energy consumption and higher productivity.

- This is an early-stage project that, if successful, could provide access to a broad range of new molecules useful for either fuel or chemical product applications. The project approach could use more clarification. If the target is an SAF, the need for individual molecular separation is less clear than if the objective is lignin specialty product valorization. Although there is a good strategy to identify and mitigate risks, the risks associated with scale-up may not be adequately captured. For early-stage projects such as this one, I think that articulating the vision for success through commercial deployment has value, even if it can only be conceptual at this stage of technology development. One comment of concern was that the largest CCC unit in existence had a 5-kilogram/day (?) capacity, which does not support that the risks are low. It appears that there are good collaborative efforts with the labs.

- The presented work is very similar to the "Continuous Counter Current Chromatography" work presented by Gregg Beckham. It would be very helpful in judging progress and milestones if it was clear which work was funded by which grant. I would want to see more details on the team's DEI efforts and how they will be incorporated into the rest of the work. It is great that the team is currently talking to adhesive companies who can be offtakers for their lignin products to turn them into adhesives.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their valuable feedback, and we appreciate the positive comments on the progress made to date. In response to specific points raised by the reviewers: There are active DEI efforts undertaken under this project, and they will be highlighted in more detail at the next review. Regarding this work in comparison to the "Continuous Counter Current Chromatography" work presented by Gregg Beckham, the works are highly complementary, and we work diligently to ensure that there is no overlap between our efforts. Specifically, this project applies CCC toward the particular mixtures generated from Lignolix's process for a particular set of commercial targets, which are different from the inputs and outputs of the Separations Consortium's work. These differences in product streams and separation targets lead to distinct sets of technical targets and optimization constraints around which the continuous CCC technology is being developed. Regarding feasibility and scalability, we agree that this is one of the key risks to this separation approach. We would like to note that the existing upper limit demonstrated for CCC throughput is in a batch mode, and that a continuous CCC is expected to have higher productivity. Also, this project is targeting binary separations, which will yield further improvements to CCC productivity compared to the existing limits.

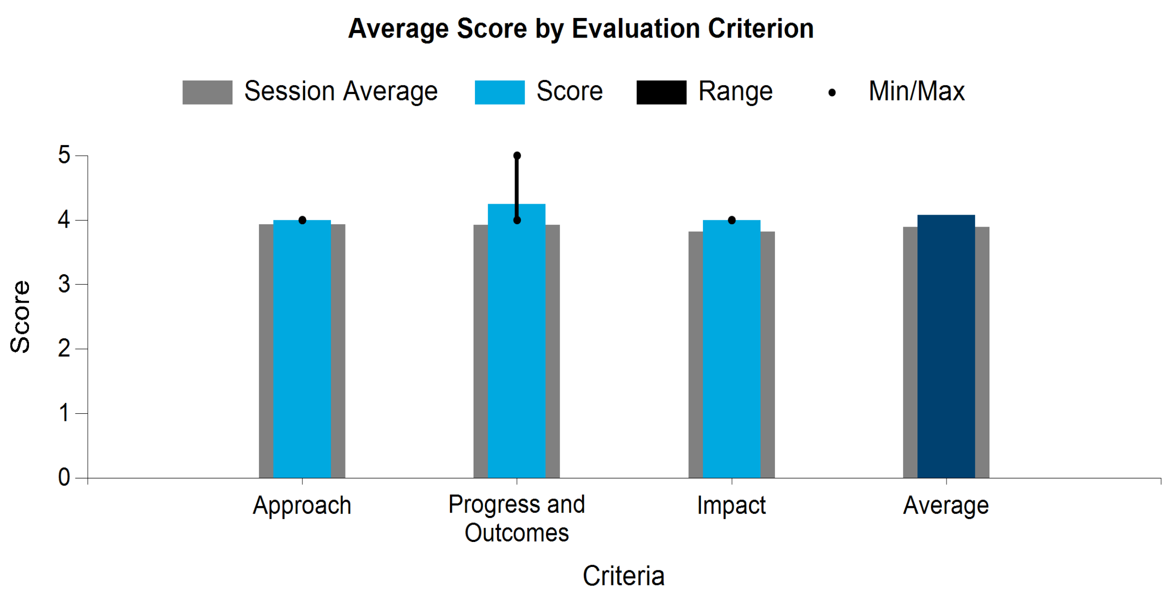
PHYSICAL PROPERTY DATA AND MODELS IN SUPPORT OF BIOPROCESSING SEPARATION TECHNOLOGIES FOR ORGANIC ACIDS SEPARATION

RAPID Manufacturing Institute

WBS:	2.5.1.200
Presenter(s):	Ignasi Palou-Rivera
Project Start Date:	10/01/2021
Planned Project End Date:	04/30/2025
Total Funding:	$5,472,690

PROJECT DESCRIPTION

Cost-effective separations are a key barrier in the scale-up of bioproduct technologies to industrially relevant volumes. Process simulation reduces the cost and risk of scale-up, but models available in current commercial simulators are limited in their ability to accurately predict bioproduct separations. This project will establish a framework for developing highly predictive process models applicable to multicomponent product streams to accelerate the development and commercialization of bioprocessing separations. The work will target the separation of organic acids from multicomponent mixtures, which is typically encountered in bioprocess operations. It will focus on two separation technologies: (1) adsorption and (2) membrane techniques. In both cases, lab-scale thermodynamic and physical property data will be collected, followed by the development of new thermodynamic models; these models will then be incorporated into commercial simulators and used in existing, complete process models. These tasks will be completed by experimental validation with pilot-scale data. The thermodynamic and process models developed in this project will consistently agree with experimental data (lab and pilot) with errors below ±20%. The developed methodologies will be applicable to the separation and recovery of organic acids from aqueous solutions, such as fermentation broth or lignin-rich streams.



COMMENTS

- The project is on track. There is a clear plan on DEI initiatives. This represents a great collaboration among a national lab, a university, and an industry partner. The team successfully collected adsorption lab data (isotherms, kinetics, and column breakthrough) and completed Milestone 2.1.1 on time. It would be great if the team could improve their capability to predict adsorption equilibria for three organic acid systems with prediction errors below ±10%.

- The team has a solid and multifaceted DEI plan. The team collected an impressive amount of adsorption data on three organic acids (and their binary and ternary mixtures) encountered in bioprocess separations. Adsorption thermodynamic modeling was started for single and binary mixtures. How many components will you need to include (and how many will you be able to include in the models) in order to get a useful thermodynamic model of a typical bio-separation? There is communication with simulation software partners, and good progress overall.

- This is an excellent approach to building a methodology that has broad applicability to a range of bioproduct separations and the potential to reduce development costs and cycle times across a range of process technologies. Significant progress has been made in both validating the approach for the work and generating useful data for a number of separations. The program is well managed, organized, and collaborative across the labs, industry, and academia. The risks are low, and the mitigation strategies are well thought out. I would consider placing additional priority on generating useful basic thermodynamic data for bioproducts in general to further support the industrial development of products like SAFs.

- I appreciate the team's work on building a prediction model to cut down the experimental space that a researcher here has to investigate. It is fantastic that the team is looking to make this work publicly available and is engaging with industry players to implement their models. I think that this work should be integrated with the wider BETO portfolio to see if there are synergies between this project and other efforts in the portfolio. I appreciate that the team can expand their model in the future if they have access to computational or experimental data on other targets.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the review panel for their positive comments and constructive input. We are very excited about our initial success and the potential for this team to develop process models for bioprocess separations backed by multicomponent organic acid physical property data as well as thermodynamic data and models. DOE's support for a tightly integrated project between a university, a national laboratory, and an industry partner is greatly appreciated. Reviewer 2 asked a question about how many components need to be included in order to get a useful thermodynamic model of a typical bio-separation. To validate the thermodynamic model as a useful model for a typical bio-separation, up to three components need to be included. The model is being developed for multicomponent systems, and there is no upper limit on the number of components to be included in the models.

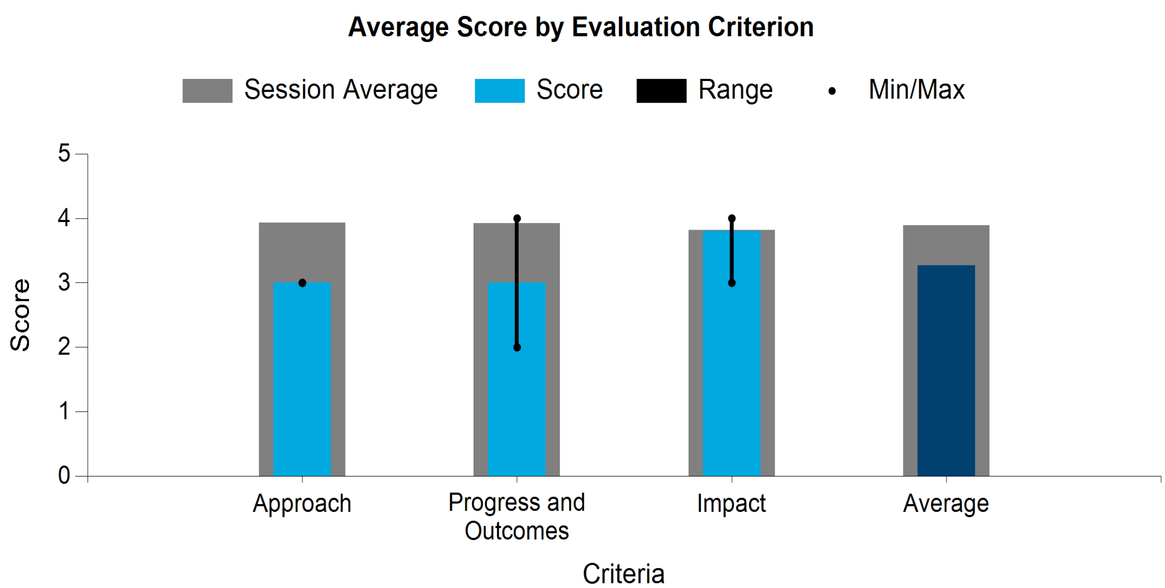
INVERSE BIOPOLYMER DESIGN THROUGH MACHINE LEARNING AND MOLECULAR SIMULATION

National Renewable Energy Laboratory

WBS:	2.5.1.500
Presenter(s):	Brandon Knott
Project Start Date:	10/01/2017
Planned Project End Date:	09/30/2023
Total Funding:	$400,000

PROJECT DESCRIPTION

This work aims to identify PABPs through computational property prediction. Given the exceptionally large biologically available design space, a major goal of this project is to guide the targeted synthesis of polymers and small-molecule materials toward those that have the highest likelihood of performance advantages. This is pursued in collaboration with the "Synthesis and Analysis of PABP" project. High-throughput property prediction enabled by ML and the elucidation of structure-function relationships enabled by molecular simulation facilitate a hypothesis-driven approach for the down-selection of candidate biomolecules to pursue experimentally. We have established bioproduct-relevant data sets, developed high-throughput polymer structure generation, and built end-to-end neural networks to predict various physical properties on the order of a million biopolymers. The ML tool developed here (PolyID) produces accurate property prediction (e.g., predicting glass transition temperature within 20°C) and >20 polyesters and polyamides synthesized by experimental partners further validate the model predictions. Molecular simulation tools (e.g., density functional theory) are also facilitating the discovery of the mechanisms of polymer formation and chemical recyclability. The computational tools actively developed within this project are increasingly being deployed via industry collaborations to industry-relevant problems.



COMMENTS

- There has been some progress in this review period. The project is on track. The milestones have been completed on time, and most milestones have resulted in peer-reviewed publications. The team used neural networks for polymer property prediction (glass transition (Tg), melting temperature (Tm), barrier, and moduli). Discovering suitable polymer materials with PABP for use in certain applications lies in accurately predicting the required properties. The team needs to talk to materials experts in industry to understand the real-life problems. Tg, Tm, barrier, and moduli are important, but these are basic properties and do not provide great information for the targeted applications. The team should predict environmental stress cracking (polycarbonate and polycarbonate/acrylonitrile butadiene styrene [ABS]), thermal conductivity (without fillers), flammability (without fillers), etc. The PI did not present their DEI strategy and progress. They should also extend their studies to the polymer blends property prediction.

- The integration of PickAxe and PolyID has the potential to create and down-select new polymers and small-molecule PABPs from bio sources. The approach will advance the SOA and help guide and narrow synthesis of PABPs. Predicting Tg alone will not predict structure-function relationships of the polymers synthesized, so it remains to be determined whether new polyhydroxyalkanoate (PHA) has other desired properties. Are there other properties you can select as outputs apart from Tg? It looks like there are very good collaborative partners/partnerships with a wide variety of industries. I really like the lower-toxicity plasticizer work, as there is great need for these types of materials. Replacing PET with a novel PHA is going to be difficult to accomplish industrially. Looking at bio-derived sources for PFAS replacements might be interesting, as many states are starting to regulate its use. Is there a DEI plan attached to this project?
- This review is based solely on viewing the slide deck. It appears that this project is much more narrowly conceived than (most) others. The information presented is dense and detailed, but it does not include a number of the evaluation bullet points. Slide 20—the overview quad chart—states that the project has two end-of-project milestones. The first is the computational method that is described. The second is to "predict solubility of PET in ≥25 novel lignin-derived performance-advantaged solvents and benchmark against experimental values." The project appears to be ending in 2023, and I did not see information on this second milestone. Slide 23, which is after the ending slides, *might* be related to this milestone, but it does not appear to have data on solvents. The design of slide 23 makes the information it contains very difficult to understand.
- This project takes an interesting approach to a complex computational problem by trying to use ML to predict the properties of new polymer systems, with the expectation that the development cycle will be sped up by reducing the amount of experimentation required to define polymer properties. There are potential flaws in this approach, as the available data from which to run the ML are very infrequently collected using the same parameters and are often not designed to be fed into large data sets. The risks of poor initial data quality and the potential negative impact on the calculations may not be appropriately mitigated. The team should also consider expanding the range of calculated properties beyond something like the glass transition temperature to more properties that would be useful for technical application, such as mechanical properties. The team should also consider expanding into mixtures; polymer blends are very common, and there could be significant utility for plastics recycling efforts, which frequently deal with mixed component streams.
- The team has mainly been predicting thermal properties for polymers like Tg and Tm. The goal of the project is predicting the solubility of PET in 25 novel performance-advantaged solvents. It is not clear to me how the presented work will reach that milestone before the end of the funding period. I appreciate that the team increased its efforts to partner with industry and presented on its ongoing work with Exxon, Patagonia, Algix, Tempur Sealy, and Kraft.

PI RESPONSE TO REVIEWER COMMENTS

- The project team thanks the reviewers for their time, attention, and thoughtful feedback. The suggestions to expand the number and type of properties predicted by PolyID align with our future plans. Although thermal properties are important for various manufacturing and performance applications, we acknowledge that many other properties are also critical for the industrial deployment of a new polymer. We plan to expand the number and type of properties by seeking out more data as well as developing correlations that may allow for the prediction of more specific, industrially important properties from those with more data available. Toward this goal, we plan to engage materials experts from industry to identify particular properties for application spaces (e.g., thermal conductivity) and polymer production (e.g., melt viscosity). We also appreciate the questions related to our DEI plan. We did not discuss our DEI efforts per BETO's guidance, as our project was established before the current BETO framework around DEI; however, this project is currently undergoing merit review for another 3-year cycle. Therefore, we are actively building these efforts into our plan for the next 3 years. These plans to address DEI include actionable goals for outreach to MSIs, which include recruitment and educational activities aimed at increasing the participation of underrepresented groups in STEM. We are also planning trainings for our current project staff and have ongoing efforts around internship programs that target MSIs and underrepresented groups. In our presentation, we did not delve into our progress on our end-of-project milestone around performance-advantaged solvents, as this is a relatively new effort (starting and stretching throughout the current fiscal year). Our target for performance-advantaged solvents was developed in response to the increasing demand from several experimental BETO and industry-funded projects for the computational screening of solvents for applications in polymer upcycling, separations, and more. In the current fiscal year, we have developed a workflow utilizing quantum mechanical and thermodynamic-based property prediction tools and are on track to convincingly meet this end-of-project milestone around bio-derived solvents for PET. The framework developed for these solubility calculations will be leveraged in future work for the development of performance-advantaged solvents for various applications with partner BETO projects. At the outset of this project, a significant risk was that insufficient data would be available to make sufficiently accurate property predictions to guide the synthesis of PABPs. As we discussed in our presentation, we have compiled a database of ~1,800 polymer chemistries with experimentally determined properties. This has been the basis for training our novel ML framework. We have quantified the error in model predictions (e.g., ~20°C mean absolute error for glass transition temperature), and our experimental PABP partner project synthesized 22 polyesters and polyamides that were experimentally determined to have thermal properties that fell within the prediction range. These mean absolute errors are nontrivial and are likely due to factors such as those noted by the reviewer (and others); however, the predictive capability of the PolyID tool has proven sufficient to be useful toward its end goal: targeting synthesis to more promising PABP candidates. As we move forward into the prediction of more specific, industry-driven properties, as described above, the property prediction errors will be continually quantified, and the sources of error will be determined within the framework of our database and novel domain of validity method. If specific functionalities or property predictions are found to be important to industry, and if they are lacking in our models, we will make concerted efforts to add them to the database to increase the domain of validity and decrease prediction errors.

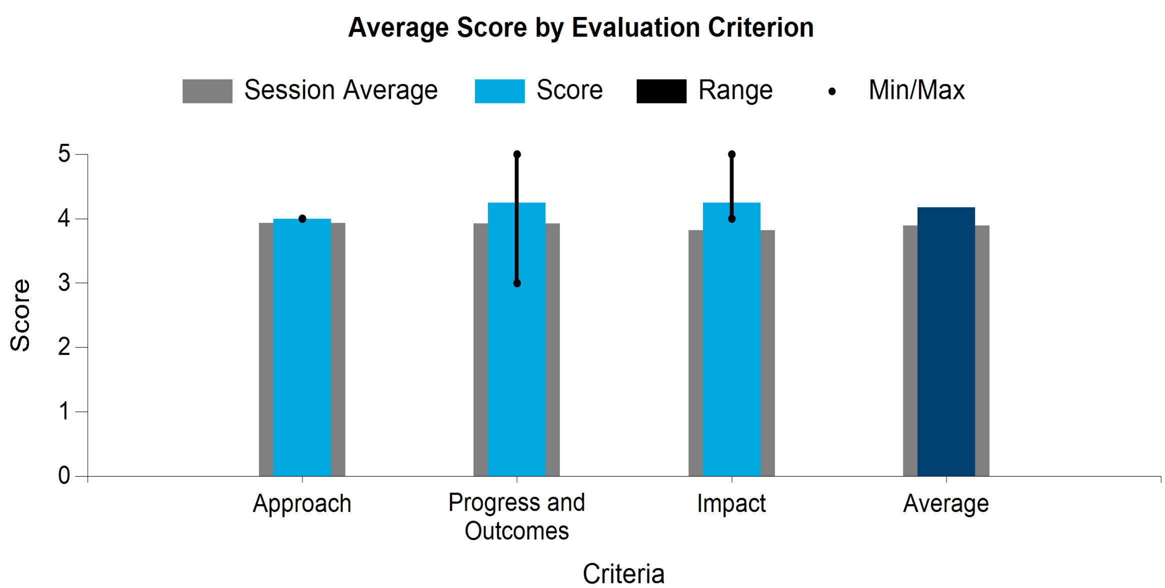
IDENTIFYING PERFORMANCE-ADVANTAGED BIOBASED CHEMICALS UTILIZING BIOPRIVILEGED MOLECULES

Iowa State University

PROJECT DESCRIPTION

WBS:	2.5.1.600
Presenter(s):	Brent Shanks
Project Start Date:	07/01/2020
Planned Project End Date:	09/30/2022
Total Funding:	$3,125,000

Given the lack of structure/function relationships between chemical structure and end-use performance, there is a need to develop a systematic strategy to identify performance-advantaged molecules. We explored the use of bioprivileged molecules as the basis for such a strategy. Two known bioprivileged molecules, triacetic acid lactone and muconic acid, were used as the basis of molecular libraries for the synthesis and screening of novel organic corrosion inhibitors and flame-retardant nylon polymers, respectively. Simultaneously, we worked on developing a computational framework to identify new bioprivileged molecules. We used literature data mining in conjunction with AI to identify promising chemical structures that could be used in conjunction with reaction network generation to suggest potential bioprivileged molecules. A goal of the project was to then use those new molecules to synthesize and screen additional molecules for use as corrosion inhibitors and flame-retardant moieties.



COMMENTS

- There has been great progress in this review period. The project is on track. The presenter gave an excellent presentation. Developing organic corrosion inhibitors and PFAS-free flame retardants for plastics using biomass-derived molecules with improved performance is really important and timely for the end-use applications. It is important to be able to address the flammability issue on the development stage and yet obtain information that pertains, in a well-defined way, to full-scale applications of interest, especially electric vehicles and consumer electronic applications. Although assessing the flammability of plastic materials through ASTM D2863-2013 is out of scope for this project due to the scalability of materials at this point, in future work, it would be great if the PI and team could compare the flammability of the biomass-derived molecules introduced to polyamide 66 (PA66) with limiting oxygen index and UL 94 VO testing to investigate the ignition time, burning time, and time taken to retard the fire. The team should also think about a patent application for their chemistry to reduce the melting temperature of PA66. A reduction in temperature will open the new space to compound natural fibers with PA66, which is extremely challenging due to natural fiber degradation, color change, and odor. The team should also use an artificial neural network-based system to predict ignition time, peak and total heat release, and mass residue after a burning reference and flame-retarded PA66 in a mass-loss-type cone calorimeter using small-scale thermal and flammability test results and structural properties. Flame-retardant PA66 applications are not common for the automotive and consumer electronic industry. Polycarbonate, polycarbonate/ABS, PP, and PET are the most common materials used in thermally challenging areas. The PI did not present their DEI strategy and progress.

- The researchers have identified very good targets for this project, especially in the realm of flame-retardant plastics. In automotive, there is a very urgent need for non-brominated flame retardants for new battery vehicles, so if a safer alternative can be developed from bio sources, it could have a large impact. The target polymers would be in nylon, but even more important is PP for battery covers (new designs) and ABS for electrical components. Brominated coatings are also applied to PET fabrics as a flame retardant, and safer alternatives are desired. The char results look promising, but adding V0 vertical burn tests would provide further confidence that the flame retardants could pass automotive tests. Because there are two parallel objectives—(1) synthesizing novel molecules with improved performance and (2) using data mining and AI to develop a systematic strategy for the identification of new bio-advantaged molecules—there has been significant progress and innovation. There should be engagement with industrial material suppliers from the transportation sector (nylon (BASF), PP (LyondellBasell), and ABS) to gauge their level of interest and to begin to anticipate the cost of synthesis of the molecules proposed.
- This is an innovative approach to identifying PABPs that could solve industrially important technical problems for corrosion inhibition and flame retardancy, both of which require environmentally difficult molecules to function. The computational approach is valuable and has the potential to reduce both the time to market and the cost of development for new bioproducts. This general approach is used broadly for pharmaceutical target molecules to good effect, and this model has been demonstrated here to have potential for industrial bioproduct applications. The future challenge for this approach is that the mechanisms for targeting need to be better elucidated to make this approach fully practical. A pharmaceutical model usually has a target site or metabolic pathway identified, and the retrosynthesis and ML can be tailored to more effectively meet the target. In this project, because the mechanisms for flame retardancy and corrosion inhibition are not well understood, the targeting efficiency is relatively low.
- I appreciate that the team is investigating two properties that are very highly sought after (corrosion resistance and fire resistance) and not very well understood on a structure-action level. The team is closely integrating with Linda Broadbelt's PickAxe effort. Although the team is struggling with cutting down the number of potential molecules to feed into the reaction network to synthesize, and with closing the loop of their discovery platform, the team's data mining efforts have already identified molecules with advantaged properties. I would suggest that the team collaborate with a synthesis-focused team to close the loop of the system. I would suggest that the team further explore industry connections to allow more people to identify bio-derived molecules with superior properties to SOA materials.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the comments of the reviewers as well as their suggestions on how to further the work after the completion of the project. We have been pursuing outreach to industry, but the reviewers have provided some interesting additions to our efforts.

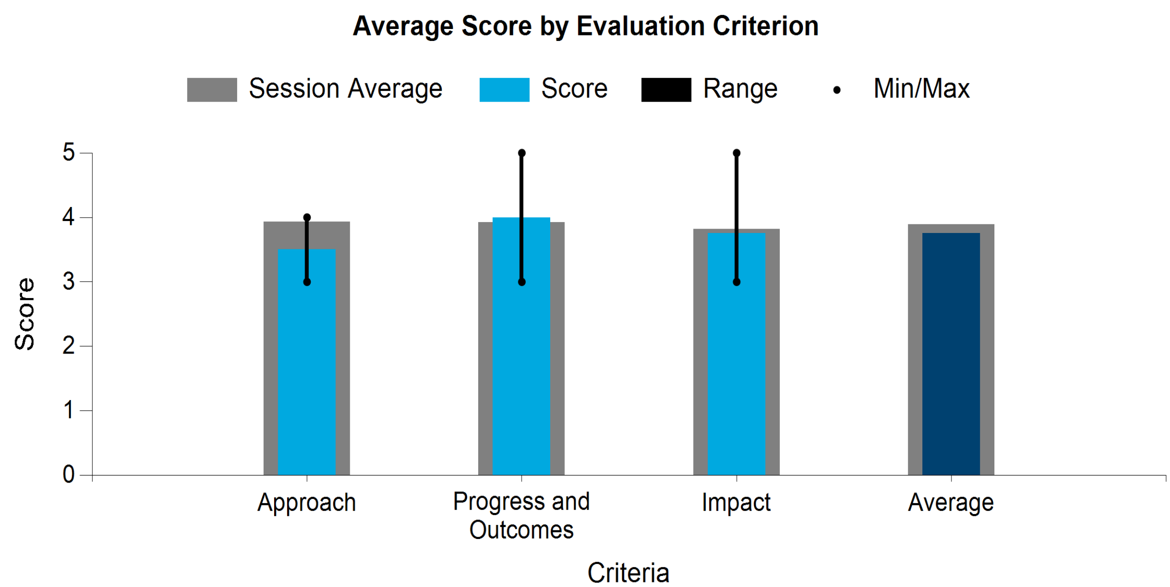
DEGRADABLE BIOCOMPOSITE THERMOPLASTIC POLYURETHANES

University of California San Diego

PROJECT DESCRIPTION

WBS:	AMO.01
Presenter(s):	Jon Pokorski
Project Start Date:	04/01/2021
Planned Project End Date:	03/31/2024
Total Funding:	$2,088,114

The goal of this project is to transform TPUs into a biodegradable composite material that incorporates viable bacterial spores. This would eliminate a significant plastic waste stream that is currently unrecyclable and undegradable and that generates ~1 million tons of waste annually in the United States. Additionally, we aim to improve the functional properties of the TPU, increasing tensile toughness by at least 20%. To do this, we are incorporating evolved bacterial spores into TPU biocomposite materials. The spores act as soft particles and, when well dispersed, will improve toughness. The evolution of the spores will serve two goals: (1) utilizing TPU as a sole carbon source to promote biodegradation upon spore germination and (2) improving tolerance to processing conditions (e.g., extrusion). By the end of the project, we aim to achieve the degradation goals set forth in the DOE BOTTLE FOA. The project aims to develop a simple method to impart biodegradation that will have minimal disruption in product formulation; simply, bacterial spores would be added during extrusion with little to no modification of the production method.



COMMENTS

- Because this presentation was not given, it is unclear what work has or has not been completed based on the information provided. Were "proper nutrients," as described in the notes for slide 3, provided during the biodegradation shown on slide 20? What is the nutrient mix, and how likely is it that a piece of TPU would encounter that mix in a landfill or other environment?

- The concept is both elegant and novel. Taking a current commercial material and rendering it biodegradable via the addition of spores while also enhancing mechanical toughness is particularly attractive. The interaction between different project aspects is strong. The results show excellent progress in terms of improving the heat tolerance of spores, and that addition can improve the mechanical properties of TPU. From the degradation experiments, adding spores does not appear to increase the rate of degradation, but it does appear to change the microbial consortium. Focusing on melt processing is appropriate, as this is representative of what will need to be demonstrated for commercialization. Overall, the team is making excellent progress toward achieving the goals and is focusing on demonstration of the enhanced degradation with the addition of spores. To demonstrate substantial commercial potential, demonstrating that adding spores does indeed enhance degradation is necessary. Having BASF as an engaged partner on the project will help answer these questions and determine the viability of commercialization. If enhanced degradation can be demonstrated, further analysis to understand the degradation products is warranted. Interaction with other projects in the BETO portfolio focused on TPU degradation could have added value here. Are there any regulatory handling risks with a spore-based approach that would need to be assessed if commercialized?

- This early-stage project has made good progress in its evolutionary engineering work to improve the heat tolerance of a particular spore strain that could also use TPU as a sole carbon source. The touted attributes of a spore-embedded polyether urethane (submicron/soft/living/green) represent an interesting concept and could be compatible with applications where spores would not be foreign—e.g., in agriculture (seed coatings or soil nutrient supplements). I encourage the team to work with their industry partners to validate the market concepts proposed for this degradable TPU, to initiate LCA/TEA, and to determine whether there are regulatory hurdles in introducing a product with spores.
- The team did not present in person. Built-in degradation through spores is a creative approach to accelerating the degradation of plastics. Is the discoloration of the plastics due to the spores an issue for applications? How are you going to further test the viability of spores in the plastic over time? What are the targeted applications for these spore-containing plastics? The team should explore industry partnerships to test whether their composites remain viable under the conditions required for these applications.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the Project Peer Review committee for the comments, and we apologize that we were unable to present due to illness.
- As far as we know, there should not be any regulatory hazards with the chosen spores. These are components of over-the-counter pharmaceutical products (probiotics) and are generally regarded as safe.
- The biodegradation studies were carried out in healthy, microbially rich compost. We have performed germination studies in compost extract to verify that the nutrients laden in compost were sufficient to germinate spores and yielded similar results as Luria Bertani media. More recent results indicate that the spores are able to germinate and facilitate degradation in otherwise sterile compost, indicating that composting conditions and the relative health of the compost play a minimal role in degradation.
- Thank you for the comment regarding additional applications. This type of composite material could also find use in agricultural films, and in that domain in general, and it is something we are actively exploring.
- Yes, the spores are responsible for the brown color of the plastics, which could be mitigated with dyes or additional components. Some intended applications are footwear, and the construction of such products could mask the physical appearance of the biocomposites. We are working with BASF to further validate the target applications. Last, we have stored spore-containing materials for more than a year, and they retain the ability for full germination.

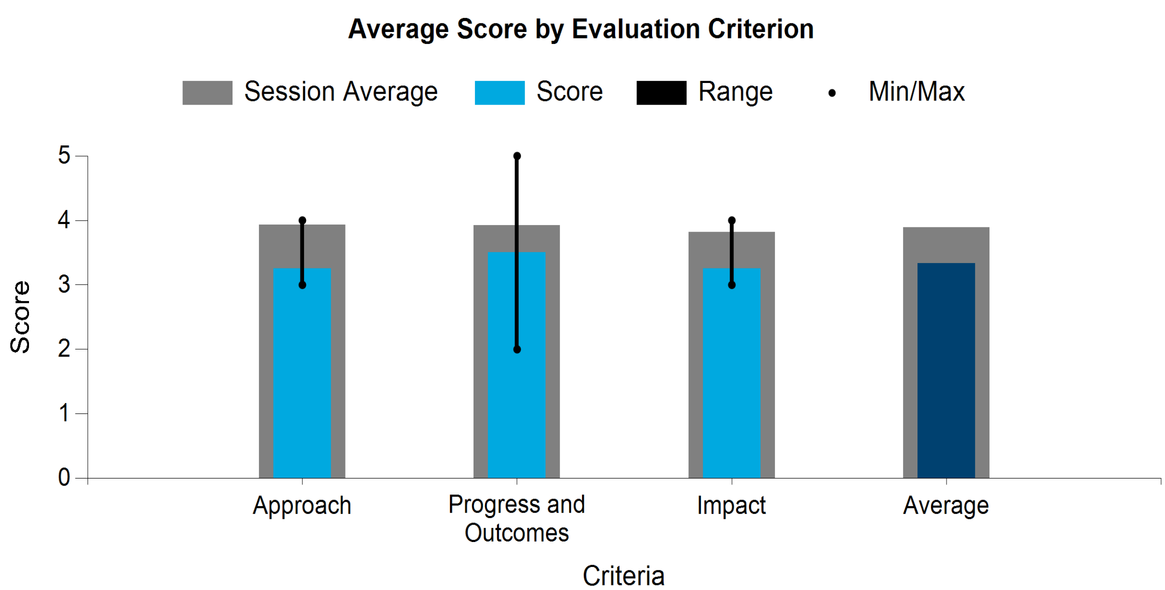
HIGHLY RECYCLABLE THERMOSETS FOR LIGHTWEIGHT COMPOSITES

University of Akron

PROJECT DESCRIPTION

WBS:	AMO.02
Presenter(s):	Junpeng Wang
Project Start Date:	04/01/2021
Planned Project End Date:	05/31/2024
Total Funding:	$2,049,242

The project focuses on the development of recyclable thermoset composites that can be produced from >50 wt % bio-based carbon sources (CO_2 and biomass). We aim to develop novel, highly recyclable thermoset materials, termed vitrimers, that combine the mechanical advantages of thermosets with the recyclability of thermoplastics. At service temperature, vitrimers are rigid like conventional thermoset polymers; at temperatures above the vitrimer transition temperature (Tv), vitrimers flow and behave as viscous liquid thermoplastic polymers. We will (1) prepare thermosets from CO_2-based materials, (2) demonstrate the mechanical recycling of thermosets, (3) demonstrate the chemical depolymerization of thermosets and carbon fiber recovery, and (4) model the cost and carbon footprints of circular composites. It is estimated that the manufacture of the next generation of recyclable CFRP will have huge market growth opportunities in aviation (commercial and military), transport, wind turbines, and compressed gas storage tanks for natural gas vehicles and fuel cell vehicles, among others. This highly collaborative project brings together expertise from the University of Akron, PNNL, and Raytheon Technologies Corporation. The project outcome will have both economic and environmental benefits in alignment with the interests of DOE's BETO and Advanced Manufacturing Office.



COMMENTS

- If I understand the goal(s) here, the timeline is very ambitious. Alas, I did not gain sufficient understanding from the presentation or the subsequent discussion to have a clear grasp on either the beginning (how the materials would be sourced) or the end (how the materials would come apart). I have questions about the economic viability, particularly on the end-of-(first)-life collection. These seem like key aspects if this is intended to be commercially viable.

- The approach here is innovative, targeting a new CO_2-based matrix material that allows recycling to recover the energy-intensive carbon fiber. If successful, it would address the carbon intensity and recycling challenges faced by current carbon fiber PP composites. The management and communication plan is clear. As lightweight, high-strength materials will play a role in decarbonizing transportation, it is important that the high-energy-intensity and recyclability challenges for these materials are addressed. EERE has substantial investment in this space via other offices, such as the Wind Energy Technologies Office and AMMTO—has this project leveraged that wider ecosystem for feedback? My largest concern with the approach is how the focus on unfilled vitrimer recycling and particle size sensitivity will be used to inform the final target, which is composite recycling. The integration between the LCA/TEA and the experimental work is very nice, as is the engagement of Raytheon as an industry partner. If the target will be an alternative to thermoplastic PP/carbon fiber (CF) composites, does the use of the vitrimer substantially change the EOL options, given that PP/CF composites could also be downcycled? The mixture of benchmarking between epoxy/CF and PP/CF should be resolved so the benchmarking of all properties is against a single reference. This project's main benefit resides in the use of CO_2 in the vitrimer synthesis to lower the matrix carbon footprint, as well as the potential for vitrimer systems to be chemically degraded, although that has yet to be demonstrated. Vitrimers have substantially different flow and creep characteristics relative to thermoplastic or thermoset matrix materials, making their introduction technically challenging. If you are not going to exploit the thermal reprocessability of vitrimers for recycling, I wonder if the challenges of introducing them as matrix materials are sufficiently offset if you are going to recover monomers via a depolymerization route. Strong industry engagement is necessary when developing a vision for a path to market at the end of the project. The substantial technical hurdles for introducing a new matrix into the composite space as well as new recycling routes raises doubts about the eventual commercialization of this technology.

- This is a very early-stage project with many works in progress. The team management and meeting structure describe regular task and teamwide meetings—do these include Raytheon and PNNL? It would be very valuable to see details on the TEA/LCA to better understand the expected improvements in carbon footprint, material reuse, and CF recyclability for composites in the automotive/aerospace industries. At this stage, it seems that technical success may be likely; however, at this stage, the team does not appear to have the deep industry engagement in place to have the desired impact and adoption.

- It is great that the team has already completed the LCA for the resin precursor, polycarbonate synthesis, and can use the learnings from the analysis to further develop their technology. In terms of reprocessing the vitrimer to retain mechanical properties, the team will have to further optimize their strategy. The proposed process of ball milling will not work on the carbon fiber-vitrimer composites. The team will have to develop an entirely different reprocessing technology for their composite products. Do you have additional strategies for reprocessing optimization?

PI RESPONSE TO REVIEWER COMMENTS

- Overall, the reviewers have identified several common threads that we plan to prioritize moving forward, and we thank them for their feedback. Now armed with BP2's experimental support, we feel confident in meeting an epoxy baseline. Regarding commercial engagement, we will also more outwardly engage with industry on the application of these materials as automotive composites and wind blades using our composite's performance. This includes engaging with DOE consortia and the National Science Foundation's Innovation Corps, as well as conducting more extensive TEA of the potential routes forward. The process and viability of material recovery was also raised several times. We hope to further develop the mechanical and chemical recycling in BP3 through solvent assistant and injection molded processes. Regarding Reviewer 1's question on opportunities for feedback, we aim to transition the project's goals to be more outward facing, now that material synthesis, characterization, and assessment have been established. To date, we have leveraged feedback from conferences, including the Society for the Advancement of Material and Process Engineering (SAMPE), the American Chemical Society, and the AMMTO REMADE Institute. We aim to solicit feedback from the Institute for Advanced Composites Manufacturing Innovation (IACMI) (DOE) and the American Composites Manufacturers Association in BP3. If there are additional mechanisms or organizations the reviewer would suggest we engage with, we would be grateful for any specific recommendations. We thank Reviewer 1 for their helpful comments regarding (1) recyclability, (2) benchmarking, and (3) commercialization. (1) In terms of recyclability, these materials do exhibit unique EOL options relative to PP, epoxy, and other vitrimers. Specifically, they have all EOL options available: they are mechanically, thermally, and chemically recyclable. Mechanical reprocessability of the vitrimer brings energy advantages relative to epoxy in prepreg storage (no refrigeration is needed, and shelf lives are longer) and in repair of defective parts. As the reviewer indicates, shredding of the composites and compression molding of the downcycled composite is not unique to the vitrimers and is comparable to PP composites. The additional comment regarding creep is an issue with vitrimers we are aware of, and are actively investigating in these materials. We are optimistic that the variation of malic acid/epoxide-CO_2 formulations will result in control over the ratio of dynamic:permanent cross-links and thus the degree of creep; however, this has not yet been demonstrated. Chemical depolymerization of the unfilled materials has since been demonstrated, and we are now investigating the CF filled materials. The TEA indicates that recovering the CF will be the primary economic driver, so our chemical depolymerization priority is the energy-efficient recovery of fibers and their surface integrity. (2) In terms of benchmarking, we aim to meet/exceed an epoxy benchmark. In the original proposal, we targeted an improvement in both the baseline mechanical performance and recyclability; however, exceeding epoxy mechanical properties (an extensively optimized industry standard) was presumptive for a new material, whereas comparison to its mechanical recyclability was moot. Now that our mechanical studies indicate we are within 10% of epoxy tensile strengths, we have analytical data supporting a uniform baseline: epoxy. (3) In terms of commercialization, addressing the technical challenges of new material adoption is an important part of our TEA. We have identified technical challenges with viscosity and cure time, which we continue to develop solutions to, and we anticipate that this will require specific tasks in BP3 to be revised. We also aim to centralize processing changes in the supply chain (i.e., prepreg manufacturing will be considerably altered as a new business, but composite production will not). Regarding recycling commercialization, our TEA and LCA indicate that the highest impact is in the monomer and precursor synthesis. As such, we propose that the precursor manufacturer will be the party that benefits the most from material recovery and recycling. We thank Reviewer 2 for their comment, and we hope our written response provides more clarity. The TEA pricing is based on quotes from suppliers who would serve as material sources, specifically of epoxide/CO_2 polycarbonates (Aramco and Covestro), succinic anhydride (Tate & Lyle), epoxide (Envisions LLC), and CF (Profabrics). All capital equipment and solvents are accounted for. We also agree that the material recovery supply chain and the economic viability of recovery is important and a challenge. We will evaluate whether a precursor synthesis business, prepreg manufacturer, or composite company will best serve as the recipient of secondary feedstocks. This depends on the impacts and costs of resin, CF, and melt-recycling, respectively. We agree with Reviewer 3 and feel that significant progress has been made since the last Project Peer Review. First, yes, Raytheon and PNNL do join our regular meetings, and their participants bring both researcher-level detail and commercial perspectives to the results generated. The TEA has been thoroughly conducted on the current composite manufacturing process and shows that a positive return on investment can be achieved with a reasonable capital investment. The initial cost of the resin is certainly higher than our envisioned target, but we believe this can be significantly improved through our other formulations. Understanding the trade-offs between performance and these TEAs/LCAs for our target composite applications is necessary. As a result, we also agree that deeper industry engagement is needed to meet the performance metrics of the composites (within 10% of epoxy strengths) while maximizing our TEA/LCA viability. Reviewer 4’s comment is very helpful, and we have also reached the same conclusion regarding the reprocessing methods. We plan to focus BP3 on additional processing methods, both of the virgin materials and the reprocessing. Specifically, the TEA of prepreg manufacturing would benefit considerably from injection molding of the vitrimer, which would also translate into chopped secondary composites. Solvent-based methods have also been investigated for reducing the viscosity of the composites during virgin synthesis, and they also improve the depolymerization dispersion. We have found that acetone and propylene carbonate both work well, which we find particularly intriguing as cyclic carbonate is the product of depolymerization.

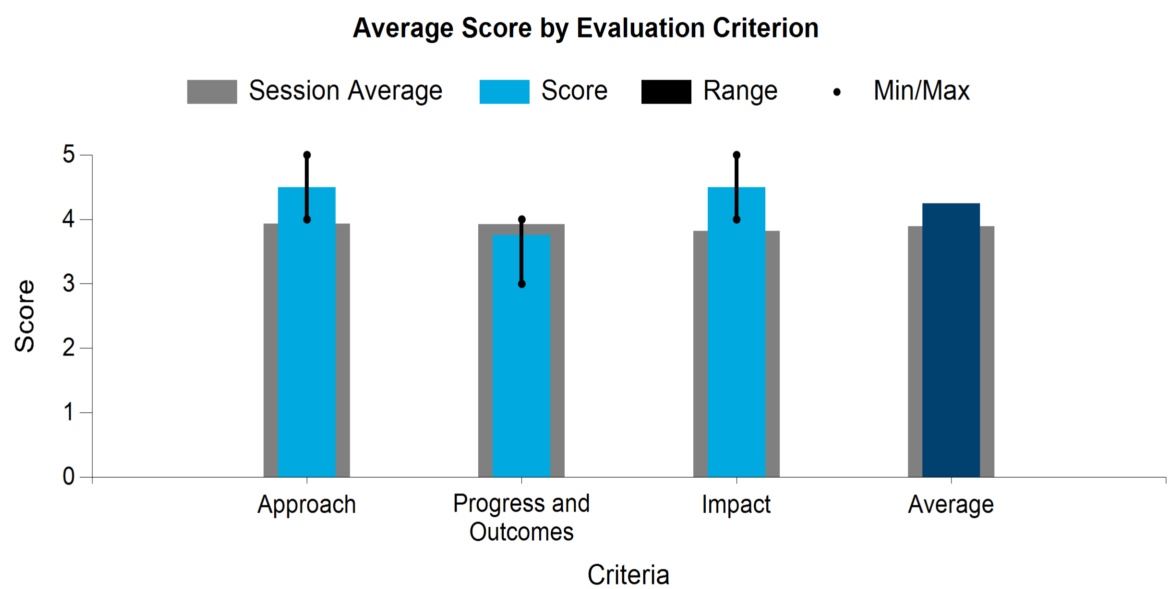
MODULAR CATALYTIC REACTORS FOR SINGLE-USE POLYOLEFIN CONVERSION TO LUBRICATING OILS FROM UPCYCLED PLASTICS (LOUPS)

Iowa State University

WBS:	AMO.03
Presenter(s):	Aaron Sadow
Project Start Date:	05/01/2021
Planned Project End Date:	04/30/2024
Total Funding:	$2,500,000

PROJECT DESCRIPTION

More than 150 million tons of the polyolefin plastics (POs) manufactured each year become waste in landfills and the environment. This PO waste contains the equivalent energy content of ~17% of domestic annual oil consumption. Our team is developing catalytic hydrogenolysis of waste POs into oils for application as lubricants, investigating their properties, and analyzing the economic and environmental implications of this manufacturing route. The project is developing efficient, economic, scalable catalyst preparation and catalytic conversions of POs into LOUPs; studying the tribological properties of the LOUPs; and identifying economic and environmental impacts of this route compared to conventional plastic waste processing and lubricating oil production. Challenges include synthesizing a catalyst that produces comparable or improved reactivity and selectivity compared to that obtained from the small-scale preparation, producing and separating LOUPs from catalyst and residue, and creating molecular structures that lead to high-performance lubricating properties that exceed the optimized conventional manufacturing processes. We have succeeded in finding scalable routes for both catalyst synthesis and LOUP preparation, and TEA and LCA have identified current pressure points that can reduce costs and GHG emissions. LOUP samples show a synergistic improvement in wear scar upon blending and with additives.



COMMENTS

- The approach targets polyolefin waste to lubricant oils, which has the potential to both address the plastic waste issue and reduce the demand for virgin oil for lubricant production. This represents a substantial innovation in that market. This project is a continuation of a Basic Energy Sciences-funded project. The approach is sound, with a clear communication plan between participating entities. The team has been making good progress toward scaling up to larger reactors and expanding to different olefin feedstocks. The parallel LCA/TEA work, along with the experimental activities, is very good, as is the focus on identifying scalable production routes for the catalyst. If the improved lubricant performance remains with real waste feedstocks and commercial additive packages, this would bring an additional technical advantage over just the reduced footprint. A startup company has been spun out from the research effort, increasing the commercialization potential. The clear focus on end application needs, early evaluation to ensure compatibility with additive packages, and engagement with players along the value chain are real strengths of the project, as is the integrated, multidisciplinary project team. Evaluating real PCR waste olefins should be a focus as the project moves toward larger scales to ensure sufficient robustness to potential contaminants and how catalyst lifetimes impact the TEA. There are other efforts targeting polyolefin waste to lubricants—has the team mapped out how their approach compares to other efforts in this space?

- The visual nature of the slides was very helpful in conveying the information. The presentation was fairly thorough in defining terms, which helped me focus on the narrative of the work rather than double-checking units or abbreviations to make sure I understood. If I understand correctly, the process identified so far will work on pre-consumer waste streams where the contents of the materials are predictable, but the catalyst economics will not work for post-consumer waste unless collection is very careful/controlled to produce a consistent stream. I think that doesn't quite match the remit.

- This is a very compelling proposal to convert and upgrade the annual polyolefin waste cost ($60 billion) into a profit of $160 billion for lubricants. The team is leveraging outcomes from a companion Energy Frontier Research Center project built to identify the catalyst $Pt/SrTiO_3$, and it has performed early TEA/LCA with defined boundaries—understanding major GHG contributors (solvents) and developing a risk mitigation strategy. They employ a moderate reaction condition (low pressure, modest temperatures).

- I am very impressed with the progress that the team has made during the funding period. The team is taking the whole system into account when optimizing the TEA/LCA; for example, they are using the reactive heat for process separation. The team has a focus on industry needs and has tested the compatibility of their lubricants with the most commonly used additives. This work has already resulted in a spinoff company called Aeternal that is pursuing the commercialization of polyolefin upcycling to lubricants. Great work!

PI RESPONSE TO REVIEWER COMMENTS

- Reviewer 1 excerpt: Evaluating real PCR waste olefins should be a focus as the project moves toward larger scales to ensure sufficient robustness to potential contaminants and how catalyst lifetimes impact the TEA. There are other efforts targeting polyolefin waste to lubricants—has the team mapped out how their approach compares to other efforts in this space?

- Response: Thanks for the comments. During our last budget period, we are focusing on polyolefin plastic waste from our commercial partners as providers. The primary approach for the chemical upcycling of polyolefin plastic waste involves pyrolysis, which is currently performed at the large pilot scale by a few commercial entities. The most important technical distinction between our process and pyrolysis is the much higher selectivity afforded by low-temperature chemical catalysis.

- Reviewer 2 excerpt: If I understand correctly, the process identified so far will work on pre-consumer waste streams where the contents of the materials are predictable, but the catalyst economics will not work for post-consumer waste unless collection is very careful/controlled to produce a consistent stream. I think that doesn't quite match the remit.

- Response: We appreciate the comment on the clarity of our presentation. Most of our process has focused on polyolefin wastes, currently from post-industrial providers. These are mixed (PEs and PP as films or laminates with adhesives, polyvinyl alcohols, colors, stabilizers, etc.). This waste is high volume, and even though it is not yet consumer-contaminated, it should not be discounted as an easier conversion. Nonetheless, our process has been shown, in some cases, to tolerate additional contaminants. We also think that any sustainable plastic waste management system will require some control along the way—that is, we should not manage all waste as single stream and then separate it, as point-of-source separations can be effective and add efficiency to the life cycle of carbon-based materials.
- Response to additional reviewer comment: We appreciate all the feedback and your time and enthusiasm for this review. Many thanks!

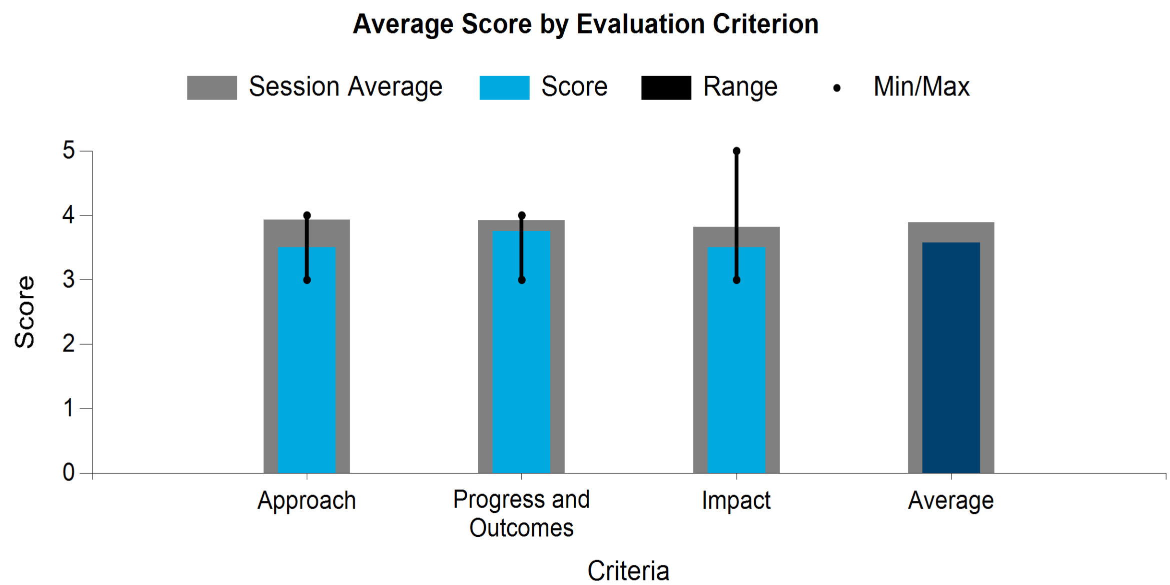
HYBRID CHEMICAL-MECHANICAL SEPARATION AND UPCYCLING OF MIXED PLASTIC WASTE

Case Western University

PROJECT DESCRIPTION

WBS:	AMO.04
Presenter(s):	Joao Maia; Mike Hore
Project Start Date:	06/01/2021
Planned Project End Date:	11/30/2024
Total Funding:	$2,498,539

The main objective of this project is to develop a hybrid mechanical-chemical recycling technology for multilayered and laminated plastics. In particular, we aim to separate and upcycle more than 80% of the two main constituents of such structures, polyolefins and polyesters, for a significantly lower cost and at higher energetic efficiency and much larger throughputs than chemical recycling while maintaining the low-cost and high-volume advantage of mechanical recycling.



COMMENTS

- Please double-check that titles are used equitably and appropriately for all researchers. It was unclear whether that was an artifact of the presenter or the project itself. Accounting for fillers or additives in the materials is one of the core difficulties of working in this space, and it would be reassuring if the presenter/project discussed the risks and mitigations of that aspect directly.

- Leveraging continuous twin screw extrusion combined with the chemical recycling of mixed plastic waste is a very high-risk, high-reward project. If successful, the continuous process and reduced capital costs would increase commercial potential. The technical hurdles are substantial, but the project plan is structured in a way to handle them methodically. The multiscale modeling approach is elegant. The accuracy of predictions must be validated against the experimental results. The project is making good progress along the plan. A key risk that is insufficiently addressed is that real feedstocks will contain contaminants in addition to PET/polyolefins, and these may substantially alter the phase separation behavior or poison the catalysts. The lack of focus on this aspect early in the project is a weakness, and the team should work to include a plan to evaluate these real waste streams earlier in the project, perhaps exploring small-scale mixing experiments while the twin screw extrusion process is being stood up. The team needs to engage with their industry partners to better understand the potential composition of incoming material. Given that gaseous products are proposed to be produced during extrusion, the project team must ensure that the safety aspects of the process are proactively addressed.

- This project has promise because it is agnostic to feedstock, and the capital expenditure projects are 25% of that of SOA pyrolysis. I am intrigued by the hybrid nature of the approach but also by the fact that the substrate is mixed (polyester and polyolefins). I also like the great versatility of this project if it is successful: It may be possible to do drop-in operations and colocate at recycling facilities. The repeated graphic with the split out of the tasks relative to the two feed streams (PET and polyolefins) is very useful—the charts have an adequate description of the tasks and risks; however, the inclusion of a single chart detailing the milestones, tasks, and critical decision points against the projected timeline (in quarters over the budget periods) would be helpful.
- The team is working with model feedstock; if their process is agnostic to feedstock, how can they prove that? The team should focus on proving that their system can work with varied real-world waste streams and sourcing real-life feedstock from local partners. It is great that all three of their industry partners have expressed interest in taking this technology to market.

UPSCALING OF NON-RECYCLABLE PLASTIC WASTE INTO CARBONSMART MONOMERS

LanzaTech

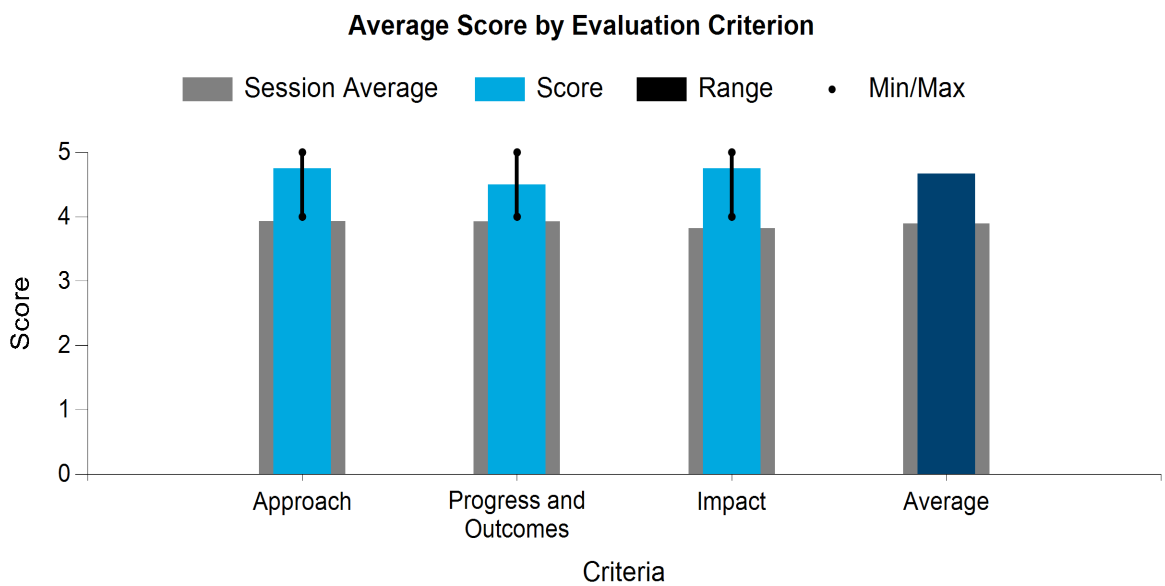
WBS:	AMO.05
Presenter(s):	Sean Simpson; Ching Leang
Project Start Date:	11/01/2021
Planned Project End Date:	03/31/2023
Total Funding:	$1,890,001

PROJECT DESCRIPTION

The project is developing a novel microbial process to produce monoethylene glycol (MEG) directly from nonrecyclable, mixed waste plastic at high yields and efficiencies. MEG is important in the production of PET, a plastic polymer used in common, single-use consumer goods, such as drink bottles, food packaging, and polyester fiber in clothing. Mixed and contaminated waste plastics represent a significant percentage of potentially recyclable MSW residues that are currently landfilled due to a lack of techno-economically viable processes for material recycling/upcycling. LanzaTech is developing technologies to convert these waste plastic residues to MEG, an important chemical in the production of PET. MEG produced from nonrecyclable plastic wastes offers a sustainable, cost-effective alternative to fossil-derived MEG to meet the needs of end users in the chemical and consumer products industries who are seeking to de-fossilize.

Our technical accomplishments are as follows:

- Multipronged engineering approaches have successfully identified pathway bottlenecks and improved MEG production 400 times.
- Enzyme variants were identified via *in vivo* assays.
- Intermediate feeding experiments identified bottlenecks for MEG production.
- InEnTec demonstrated fermentable syngas from multiple MSW feedstocks.



COMMENTS

- The slides were both comprehensive and well laid out. The researchers are skilled, and the microbial work is impressive. If the location of the system boundary for the TEA is the same as the location of the system boundary for the LCA, then neither is sufficient for understanding the way that this would work (or not) in practice. I would recommend clarity on whether metal ingots and vitrified glass slag have market value. The presentation indicated they do, but as those are not as common in plastics analysis, more specifics on that would be useful. The term "recovery" is undefined in this context, at least regulatorily, and can cover a wide range of actions—sort of like "natural" foods.

- This is a well-conceptualized and well-executed project with partnerships along the supply chain (waste collection, gasification, and conversion to MEG). The screening approach appears to be robust, leveraging modeling and high-throughput experimentation. Utilizing both cell-free and *in vivo* screening allowed the project to progress despite the cell-free route proving inconclusive. The project is progressing on time and making appropriate progress to meet the milestones established. The team has successfully increased MEG production 400 times using a combination of approaches that identified different bottlenecks. This is particularly impressive because there is not natural MEG production in microbes. Because the work has proved successful, widening the view to MEG uses is warranted to evaluate the suitability of MEG produced for different end uses (purity, separations needed, etc.). For the LCA, comparing not only cradle to gate for MEG production but also other PET recycling options (e.g., PCR waste -> PET production) would be valuable for understanding the potential of this technology in the PET recycling ecosystem. The potential impact of this technology is high, as bio-MEG can be introduced into the existing supply chain relatively easily.

- This is a very focused project that addressed each key area: management, approach, and outcomes. The team chose a very experienced gasification partner, InEnTec, to provide the substrate or feedstock for their microbial fermentation process to produce MEG. The milestone chart was very clean and clear. The team took a multipronged approach to overcoming the challenges in identifying stable enzyme variants. The increase in MEG titer (500 times) by pathway engineering and enzyme screening is a tremendous achievement in a short time. It would be helpful to know where the current production is relative to MEG rate/titer/yield metrics (not specified in the presentation) that would make the bioprocess economically viable.

- The team is working with industry partners in both waste management and gasification as well as consumer brands. I greatly appreciate the team's effort to engage players on both ends of the supply chain. I appreciate that the team is dedicating a whole team to TEA/LCA to inform their decision making in developing their process. This project is a good example of demonstrating a pathway to TRL 7 while starting with a very early technology by leveraging the know-how of industry partners.

PI RESPONSE TO REVIEWER COMMENTS

- Note: Subject to disclaimers on the associated presentation.

- Comment: This is a well-conceptualized and well-executed project with partnerships along the supply chain (waste collection, gasification, and conversion to MEG). The screening approach appears to be robust, leveraging modeling and high-throughput experimentation. Utilizing both cell-free and *in vivo* screening allowed the project to progress despite the cell-free route proving inconclusive. The project is progressing on time and making appropriate progress to meet the milestones established. The team has successfully increased MEG production 400 times using a combination of approaches that identified different bottlenecks. This is particularly impressive because there is not natural MEG production in microbes. Because the work has proved successful, widening the view to MEG uses is warranted to evaluate the suitability of MEG produced for different end uses (purity, separations needed, etc.). For the LCA, comparing not only cradle to gate for MEG production but also other PET recycling options (e.g., PCR waste -> PET production) would be valuable for understanding the potential of this technology in the PET recycling ecosystem. The potential impact of this technology is high, as bio-MEG can be introduced into the existing supply chain relatively easily.

- Response: We are pleased by the enthusiasm the reviewer expressed about the potential impact of MEG produced using our biocatalyst approach. We are targeting the production of MEG that meets the specifications for PET production, which is one of the highest grades of MEG used in manufacturing and has the largest market. LanzaTech has significant expertise in this area, predicated on the company's experience producing MEG "indirectly" through an ethanol intermediate. In those instances, the MEG produced has been used as a chemical feedstock for polyester textiles that have been used to make consumer apparel. MEG produced directly from gases will be suitable for numerous downstream applications. The LanzaTech vision goes beyond PET recycling/depolymerization. The LanzaTech process represents the opportunity to valorize municipal waste streams containing unsorted, nonrecyclable plastics and other materials. It is estimated that only ~5% of plastic waste is recycled in the United States, primarily due to costs associated with material separation. The LanzaTech process is unencumbered by heterogeneity and offers a means to recover and recycle carbon from plastic waste at much higher rates than offered by pathways that require highly pure (i.e., PET) plastics.
- Comment: The slides were both comprehensive and well laid out. The researchers are skilled, and the microbial work is impressive. If the location of the system boundary for the TEA is the same as the location of the system boundary for the LCA, then neither is sufficient for understanding the way that this would work (or not) in practice. I would recommend clarity on whether metal ingots and vitrified glass slag have market value. The presentation indicated they do, but as those are not as common in plastics analysis, more specifics on that would be useful. The term "recovery" is undefined in this context, at least regulatorily, and can cover a wide range of actions—sort of like "natural" foods.
- Response: LanzaTech appreciates the reviewer's comment. LanzaTech uses TEA and LCA as a tool to quantify the impact of various performance metrics to ensure that the project outcomes will be commercially relevant. In this instance, TEA and LCA are not used for assessing a business case for the technology and process; however, the outcomes of the LanzaTech project are anticipated to inform the development of multiple business case scenarios, including those that may have additional value from multiple products (i.e., vitrified glass slag, ethanol, etc.). This effort will be executed downstream of the DOE project. "Recovery" in this instance specifically refers to carbon recovery. High rates of carbon recovery will reduce the amount of virgin fossil resources required to address the global demand for plastics, which at this time continues to increase.
- Comment: This is a very focused project that addressed each key area: management, approach, and outcomes. The team chose a very experienced gasification partner, InEnTec, to provide the substrate or feedstock for their microbial fermentation process to produce MEG. The milestone chart was very clean and clear. The team took a multipronged approach to overcoming the challenges in identifying stable enzyme variants. The increase in MEG titer (500 times) by pathway engineering and enzyme screening is a tremendous achievement. It would be helpful to know where the current production is relative to MEG rate/titer/yield metrics (not specified in the presentation) that would make the bioprocess economically viable.
- Response: We are grateful for the reviewer's satisfaction with the gasification partner and with the project approach and management overall. We are also grateful to receive the reviewer's acknowledgement of the significant titer achievement. The titer and selectivity-based targets set out in our proposal were based on our preliminary TEA supporting their relevance to commercialization. Because this project is still in the early stages, and we are focusing on identifying and implementing optimal pathways to produce MEG in continuous stirred-tank reactors (CSTRs), we have not begun reporting rate and yield metrics; however, in Year 3 of the project, we will begin pilot-scale

fermentations using our best MEG-producing strains. Pilot-scale performance is a much more accurate representation of strain performance compared to CSTRs. We intend to use rate and yield metrics more when we advance to optimization in pilot-scale fermentation architecture, and we agree with the reviewer's assessment that these will be critical to evaluating the economic viability of the process.

- Comment: The team is working with industry partners in both waste management and gasification as well as consumer brands. I greatly appreciate the team's effort to engage players on both ends of the supply chain. I appreciate that the team is dedicating a whole team to TEA/LCA to inform their decision making in developing their process. This project is a good example of demonstrating a pathway to TRL 7 while starting with a very early technology by leveraging the know-how of industry partners.
- Response: We thank the reviewer for these comments, and we appreciate that we agree about the importance of engaging partners that are involved in various aspects of the commercial process. LanzaTech continues to work directly with customers to ensure that the products made from plastic waste will meet all necessary specifications for varied applications in packaging and fibers.

CIRCULAR ECONOMY OF COMPOSITES ENABLED BY TUFF TECHNOLOGY

University of Delaware

WBS:	AM0.06
Presenter(s):	Joseph Deitzel
Project Start Date:	07/01/2021
Planned Project End Date:	12/31/2024
Total Funding:	$2,499,983

PROJECT DESCRIPTION

Carbon fiber composites (CFCs) exhibit superior properties and, combined with part consolidation, significantly reduce system weight compared to metal approaches. CFCs are utilized in lightweight structures in automotive, aerospace, wind, infrastructure, and many other applications. Growth rates are significant (7% in the United States alone) and are driven by automated processing approaches, lower-cost CF materials, and (in the case of automotive applications) the need to meet government regulation. Raw material costs of continuous CF can range from $20 per kilogram for low-modulus and high-filament-count carbon tow materials (Zoltek, DowAksa) to more than $200 per kilogram for ultrahigh-modulus CFs. In addition, CFCs have high embodied energy (~230 megajoules/kilogram), resulting in a significant energy burden during virgin fiber production. Recycling CFCs has the potential to recapture the material value at a much lower cost, reduce the embodied energy of the CFCs, and provide a pathway to reducing waste. Nevertheless, CFC recycling is in its infancy as an industry in the United States, with the key challenges being (1) the ability to recover both the fiber and polymer content and (2) conversion of the recycled material into high-value CFC without significant property loss, reducing the original embodied energy and cost.

Existing recycling strategies include thermolysis, pyrolysis, and solvolysis, and these have yet to demonstrate a viable process capable of simultaneously producing high-quality fibers while recovering useful chemical functionalities from extracted epoxy resin. The diversity of epoxy resins used in CFCs has led to a variety of new catalytic approaches to depolymerize these binding resins using milder conditions, which would allow for the economic degradation of epoxy resin and the recovery of intact CF. Existing catalytic methods in the academic literature for chemical depolymerization systems generally employ either oxidation or Lewis-acid-catalyzed hydrolysis; however, in all cases, no publicly available sources have attempted to build a TEA-driven process approach to target key limiting factors in transitioning this technology to a continuous unit operation.

Another challenge of the existing recycling technology is the breakdown of the continuous fiber material into recycled, discontinuous chopped or short fiber random and semi-aligned forms, which results in reduced mechanical properties of fabricated composite structures. For example, the tensile strength of Massachusetts Institute of Technology's DEP recycled preforms (156 million pascals with fiber length distribution between 6 and 25 millimeters) molded with polyester is ~20% compared to an equivalent IM7 fiber quasi-isotropic prepreg composite. This is mainly due to the random fiber orientation and low fiber loading of the preform and reduced fiber and adhesion properties of the recycled fibers.

The University of Delaware Center for Composite Materials (UD-CCM) will team up with members of the BOTTLE Consortium, including NREL and Colorado State University (CSU), to address these challenges and develop and demonstrate a novel CFC recycling process. NREL and CSU will develop the fiber/polymer separation and depolymerization process, and UD-CCM will demonstrate CFC processing of the recycled discontinuous fiber content using the Tailorable Universal Feedstock for Forming (TuFF) process, allowing full property translation. The patented (U.S. 10,669,659) fiber alignment process has been developed under a recent 4-year Defense Advanced Research Projects Agency (DARPA) program led by UD-CCM and scaled in a pilot facility at UD-CCM (10,000 pounds/year, 18 inches wide) that converts short fibers to high-performance parts in one facility. The innovation has been selected by the American Composites

Manufacturers Association as the 2019 winner for the “Infinite Possibility for Market Growth” Award for Composites Excellence for its potential for greatest impact to new and emerging markets.

The objectives of this program are to combine (1) an innovative short fiber alignment process developed by UD-CCM with (2) a new recycling approach to separate fiber and polymer content of CFCs innovated by NREL and (3) a novel recyclable polymer material (CSU) to (4) demonstrate the closed-loop recycling of high-performance CFC to implement a sustainable CFC manufacturing approach for the first time. The program will demonstrate the feasibility of manufacturing highly aligned short fiber composites at our industry partner sites with high fiber volume fraction (>50%) and mechanical properties that are two- to threefold higher than current recycling methods. If successful, the proposed approach will allow true composite recycling with associated energy reduction (75%) and carbon utilization (>85%) over multiple component life cycles without significant loss of performance.

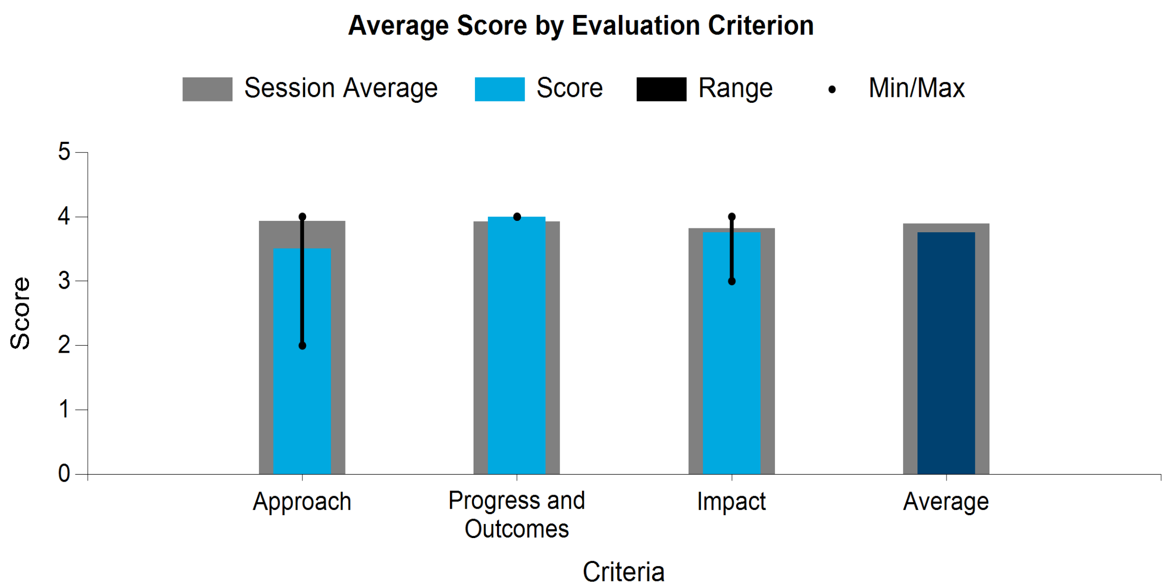
By combining the unique talents of NREL in catalysis, process engineering, solids handling, and TEA and LCA with the University of Delaware’s expertise in short fiber aligning technology, the polymer engineering breadth of CSU, and the expertise of our industry partners, this proposal will provide a unique opportunity to tackle the grand challenge of CFC recycling and will meet/exceed the stretch goals of this FOA (70% energy savings and 85% carbon utilization). We will engage our industry members (Arkema, Axiom, Composites Automation) to provide waste CFC, support material production, evaluate our recycling process, and transition opportunities to commercial material forms and applications.

Accomplishments in the program to date include:

- Established baseline epoxy/T700 composite properties
- Conducted initial demonstration of single-iteration recycling for vacuum-assisted resin transfer molding process processed Elium/T700 part achieving ~100% translation of tensile modulus and 64% translation of tensile strength in the recycled part compared to the virgin T700/Elium TuFF composite
- Measured baseline interfacial shear strength for Elium thermoplastic and T700 with Elium compatible FOE sizing
- Successfully fabricated high fiber volume fraction (~50%) Elium T700 TuFF panels
- Successfully fabricated, for the first time, Epoxy/TuFF prepreg materials using commercial equipment (Axiom)
- Translated conventional heating data to sand bath reactors for thermoplastic recycling reactions. Ordered new reactors to further this preliminary work with cross-linked thermosets. These reactors arrived in January 2023, so they will be used to test higher-temperature reactions for thermosets in Quarter 2 of FY 2023.
- Finished optimizing thermoset swelling conditions in both acetic acid and N-Cyclohexyl-2-pyrrolidone as solvent
- Characterized two cross-linked epoxies received from Axiom and generated two partially cross-linked thermosets to mimic the thermal properties of these commercial materials
- Based on the results of the model epoxy compound studies, we have down-selected to a base-mediated epoxy recycling scheme as the focus for future work.
- Evaluated monoethanolamine and methylene valerolactone (MVL) monomers as candidates for recyclable resins. Monoethanolamine was a key candidate at first but suffered from low polymerizability at room temperature and exhibited low Tg. MVL was selected to address the polymerizability. Upon

further study, poly-MVL showed enhanced thermal properties and recyclability (~99% monomer recovery for 1-gram samples).

- Adjusted the initially reported small-scale synthetic pathway for MVL based on the initial TEA to bring sustainability and economic feasibility to the forefront of the large-scale synthesis (>100-gram quantities)
- Shipped 10 grams of poly-MVL to the University of Delaware for initial studies and will soon send 30 grams of MVL monomer for further studies
- Began TEA of the large-scale synthesis, polymerization, and recycling (currently in progress via collaborators at NREL).



COMMENTS

- This is a highly ambitious project that addresses multiple sustainability challenges for CF composites: (1) EOL recovery of fibers from current epoxy/CF composites, (2) demonstration that the TuFF process can use recycled fibers, (3) development of recyclable matrix materials with lower carbon footprints, and (4) demonstration of monomer recovery from new matrix materials. This vision would allow the recovery and reuse of high-embedded-energy CF from current materials and transform them into more circular composite systems for extended material lifetime of the CF components. Given the highly ambitious nature of the project, the approach is logical, with risks mitigated by a layered approach. The communication within the project and to the wider community was not explained. Is there an advantage to connecting with ongoing activities via IACMI, for example? Despite the delay with starting due to subcontracting, the project appears to be making good progress toward the defined milestones and go/no-go decision points. The project has strong links across the value chain of partners that will be needed to bring the innovation to market, which is a strength, with a strong emphasis on evaluating whether the TuFF material can be integrated into existing prepreg processes. These are nice to see given the early TRL of the activities. If successful in recovering CF for multiple life cycles, this project has the potential for large impact due to the high embedded energy in the fiber components. The project has potential for impact even if all activities are not fully successful (e.g., the value of CF recovery and reuse, even if novel matrix development is not achieved). If successful, demonstrating the compatibility of TuFF with CF recycling would strengthen the case for the commercialization of a potentially revolutionary composite processing technology. Addressing the high embedded energy of CF composites—which have a role to play in lightweighting and clean energy technology by enabling the use of recycled short fibers—has wider decarbonization impacts.

- I was unable to determine where the team is in the timeline (slide 9 is opaque to an outsider) and whether the unknowns are resolvable in the proposed timeline. The presenter did not shape the presentation to match the time allocated. This made it difficult to assess. Streamlining the presentation would help strengthen the clarity of the narrative to make it more effective. Combining the ~7 slides with pinch points and a timeline into one clear slide would have been great. Although some visuals are helpful and text-heavy slides can get in the way of communication, this slide deck has many visuals that are not doing the work to justify their inclusion. The red and green text in the slides was helpful to me to illustrate benchmarks and comparison; I recommend using a tool such as https://www.color-blindness.com/coblis-color-blindness-simulator/ (there are others, this is not an endorsement of any particular tool) to make sure that this color distinction is viewable by all potential viewers.

- This project leverages a DARPA-funded TuFF manufacturing facility and merges several key technologies to design readily deconstructable and recyclable CFC. The demonstrated TuFF process is central to the proposition in this project. The recycling by design landed on MVL as the better monomer candidate to produce a resin matrix that is both recyclable and has the desired physical properties. I did not understand the rationale for using model small molecules and polymers for the catalyzed degradation instead of one of the new recyclable resins. Is there insufficient quantity? Please explain the task priority: It is stated that working to overcome surface residuals and appropriate length sorting of fibers is critical, as these factors negatively impair performance, yet the tasks for BP3 do not reflect this. Will this impair/impact the go/no-go for BP2, where 95% retention of property(ies) for recovered composites must be achieved (to date at 60% for tensile strength)?

- I cannot understand what the TuFF process is or how it works from the presentation and additional questions after the session. I appreciate that the team has three industry partners already. I would encourage the team to share samples with these industry partners as well as with their academic partners.

PI RESPONSE TO REVIEWER COMMENTS

- I would like to thank the reviewers for their attention and comments on our presentation. I will try to respond concisely to the questions raised by each reviewer, and I invite those interested in further discussion to reach out to me directly at jdeitzel@udel.edu.

- Response to Reviewer 1: We thank Reviewer 1 for their kind comments. With respect to the question about communication within the group: We have regular monthly meetings for the materials development group (UD-CCM, CSU, NREL) and the processing group (UD-CCM, Composites Automation, Arkema, and Axiom) to discuss progress on various aspects of the project. We chose to divide this into two separate meetings to better manage discussions. Additional meetings between individual members are scheduled as needed to follow up on specific questions about chemistry, processing, etc. With respect to outreach to the larger community, members of the group engage in the usual academic avenues of participating in technical conferences and peer-reviewed publications. Examples of technical conferences include the Composites and Advanced Materials Expo, JEC, SAMPE, and the Frontiers in Biorefining Conference. Members of UD-CCM and Composites Automation also participate in the monthly meetings for the SAMPE recycling working group. We are, of course, open to and actively seeking further opportunities to engage with other parts of the wider recycling community.

- Response to Reviewer 2: We thank the reviewer for their comments and suggestions for streamlining future presentations. As pointed out by the first reviewer, this program is ambitious and has multiple research thrusts aimed at addressing different aspects of the composite recycling problem, which makes summarizing the program in a 20-minute time slot challenging. Moving forward, we will endeavor to present follow-on progress in a more concise manner. We also very much appreciate the suggestion of tools that can be used for making future presentations more accessible to viewers who are colorblind.

- Response to Reviewer 3: We thank the reviewer for their questions. As we discussed in the introduction slides of the presentation, we are pursuing several different research thrusts to address the key challenges associated with recycling composite systems. The first challenge is how we convert recycled fibers, which are almost always found in a discontinuous (chopped) form, into composites with properties comparable to those made with virgin, continuous CF. We address this with the TuFF process, which takes an aqueous bath slurry of discontinuous fibers and creates a preform of highly aligned short fibers that can be infused with a resin matrix and consolidated into high-performance composites. The second challenge is recycling the resin component of the composite. Here, we are pursuing parallel paths. Path 1 looks at the catalytic breakdown of the matrix for epoxy-based composites in order to recover the fiber and monomer. This is of great interest because epoxy composites comprise the majority of composites used today. In this research, NREL first developed model linear epoxy-amine molecules to be used to evaluate various base and acid catalyst candidates. This enabled exact analysis of both starting materials and depolymerization byproducts using standard chromatography and spectroscopy techniques that would not be possible with cross-linked thermosets. Using this approach, we identified an optimal catalytic depolymerization route, using base catalysts in this instance, which demonstrated the recovery of ~60% BPA monomer. Current work has begun applying this approach to cross-linked epoxy systems. Path 2 looks at the novel class of recyclable-by-design polymers, which have the advantage of a more efficient path to monomer depolymerization. For this class of materials, our baseline is the commercial Elium resin made by Arkema. For this class of material, Elium will be the baseline used to demonstrate multiple iterations of recycling because of its availability in terms of quantity. In parallel, we are also evaluating bio-derived versions of the recyclable-by-design resins being developed by Colorado State, which have the advantage of greater thermal stability (higher Tg) and more efficient depolymerization (>95% monomer recovery, compared to ~70%–80% for Elium). These materials, however, are available in relatively small quantities; thus, they are considered exploratory in nature, with a focus on determining their baseline mechanical properties and their ability to be processed into composites on a small scale. The third challenge is the need to clean the fiber surfaces of residue left over from the depolymerization process. At the outset of the program, it was understood that there could be a need to revitalize the surface chemistry of the recycled fibers to promote good resin adhesion, and strategies to address that issue are in place (ozone treatment of the surface, followed by vapor deposition of adhesion promoters); however, what we did not anticipate at the program's start was the sensitivity of the TuFF process to the presence of residual byproducts of the depolymerization process on the fiber surface. As a result, a major focus of the research at the end of BP2 and into BP3 will be to look at how to (1) optimize the depolymerization process for all matrix candidates (epoxy, Elium, RgB resins) to minimize residue and (2) develop low-cost, non-energy-intensive strategies to clean the recycled fiber surfaces in order to get optimal dispersion in the TuFF slurry. This will be the key to maximizing the full translation of strength in the recycled fiber TuFF composites (which has already been demonstrated for both chopped virgin CFs and waste CFs from weaving and prepregging processes that have not been exposed to a resin matrix). Finally, it is important to note that the demonstrated 100% translation of modulus and 60% translation of tensile strength for the recycled TuFF composite exceeds the published values for composites made from recycled short fibers by a large margin. We believe that we understand the mechanisms (adhesion of filaments into small fiber bundles due to the residue from depolymerization byproducts), and, as previously stated, a major focus of BP3 will be looking at ways to limit the formation of the residue as well as potential methods for removing it from the fiber surface.
- Response to Reviewer 4: The TuFF process takes an aqueous slurry of short fibers and turns them into a sheet of highly aligned fibers that can be stacked into thicker preforms and infused with resin to make composite parts with mechanical properties equal to that of traditional continuous fiber composites. A

short video describing the process in greater detail can be viewed here: https://www.youtube.com/watch?v=xKhPywwhjao. Regarding the question of sharing the TuFF material with our industry partners, that is a key aspect of the program. Composites Automation holds the sole license for the TuFF process and is the one making the material to be used in the project. They are working together with UD-CCM, Axiom Materials, and Arkema to demonstrate the feasibility of making TuFF-based prepreg materials with both epoxy and Elium resins. TuFF material has already been provided to Axiom, and we have demonstrated that TuFF/epoxy prepreg can be made using a standard commercial film impregnation process. Currently, Axiom is working with Arkema to explore potential approaches to achieving the same success with the Elium resin.

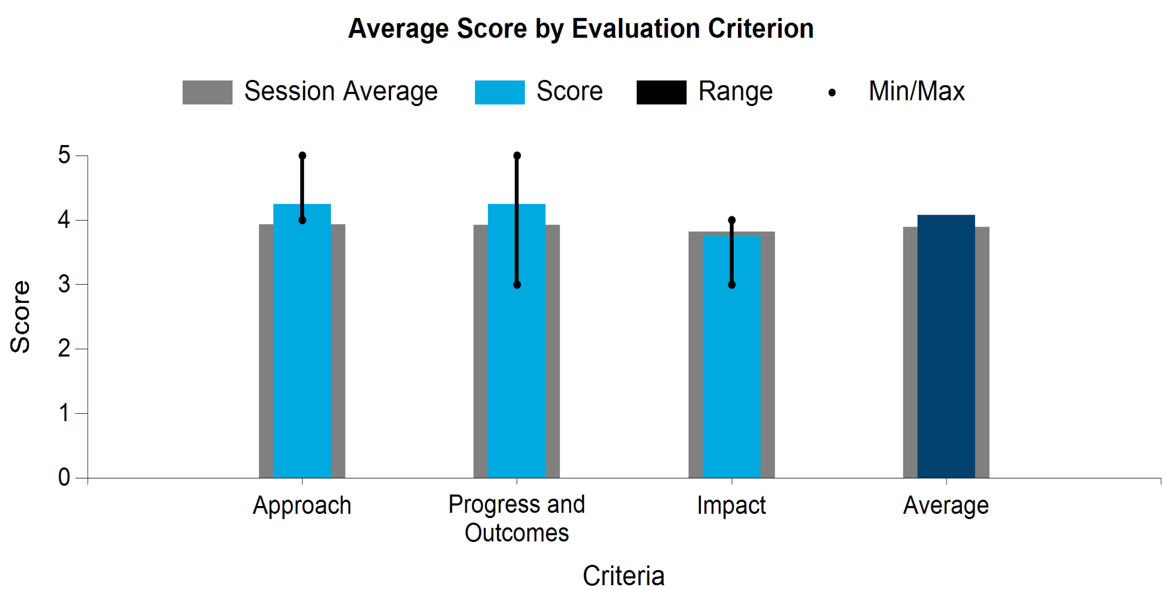
RECYCLABLE AND BIODEGRADABLE MANUFACTURING AND PROCESSING OF PLASTICS AND POLYMERS BASED ON RENEWABLE BRANCHED CAPROLACTONES

University of Minnesota

PROJECT DESCRIPTION

WBS:	AMO.07
Presenter(s):	Paul Dauenhauer
Project Start Date:	06/01/2021
Planned Project End Date:	05/31/2024
Total Funding:	$2,499,997

A chemical process is proposed for parallel closed loops of renewable polymers based on alkyl-caprolactone monomers, allowing for a broad range of materials and applications while also providing flexibility in material EOL options without long-term waste. A "lignin first" approach converts lignin (derived from trees and grasses) to aromatic monomers using the existing Massachusetts Institute of Technology and NREL reductive catalytic fractionation process. These alkylated aromatic monomers then undergo tandem reduction to cyclic ketones and Baeyer–Villiger oxidation to alkyl-caprolactones for use in multiple classes of polymeric materials. These polymers can biodegrade to carbon dioxide and water and are eventually converted back to lignin or other biomass via photosynthesis (loop #1). Alternatively, chemical processes convert the polymers back to their base monomers (loop #2). The entire project aims to design a complete process from biomass to monomers to PUs and polyesters as well as the recycling technology to convert the polymers back to the monomers.



COMMENTS

- Please double-check that the correct spelling is used for all researchers' names; this sort of detail would reflect a collaboration that is open to correction, which is important in making use of the talents of all participants. The forthrightness of the presenter in admitting the many unknowns, both personal (on parts of the project led by others) and broad (aspects of the work that are not complete) was good. The first set of unknowns does seem to indicate a weakness in internal communication. I would recommend making sure that the visuals in the presentation are interpretable to viewers and thus justify their inclusion. The process flow diagram on slide 10, for example, needs to be redesigned for this format if it is critical to understanding the narrative of the presentation. At present, it takes up space without informing.

- This project is an early TRL proof of concept for transforming a bio-based monomer to polymer to recycling via monomer recovery; however, some risks are mitigated by basing the concept on an existing lignin reductive catalytic fractionation process previously funded by DOE at NREL, as well as early TEA/LCA with a focus on meeting the target price for the monomer of interest. The project is well structured with a clear connection between the different technical tasks and work streams. The continual sharing of reaction conditions to ensure integration between processes is particularly strong. It is useful that BASF is participating so that feedback on potential applications can be identified for the resulting polymers as well as for process engineering. While the biomass monomer development is very strong and the potential for degradable polymers is good, the chemical recycling route is more uncertain, as it would require substantial changes in the recycling infrastructure as well as the collection of the material at EOL. For an early TRL activity, this project has a very good focus on ensuring a route to commercial viability with potential to commercialize the monomer even if the polymer development does not become successful.
- The management structure is good—there is clear alignment of task responsibilities among institutions and individual PIs. The team has demonstrated good oxidation outcomes (yields and selectivity) to lactone (with peroxide) synthesis from biomass precursor, and with tin octanoate catalyst, they have demonstrated excellent polymer conversions (> 95%) and depolymerization.
- The team included a reaction chart that shows which university/industry partner is responsible for which steps (slide 8). It would be helpful if other projects that divide different reaction steps between institutes could include an equivalent chart. I appreciate that the team started their TEA/LCA before going into the experimental parts. In terms of carbon recyclability, the team has been able to reach 90% conversion in a glass vial. In translating to a continuous process, the team has not been able to reproduce these yields yet. I appreciate that the team is figuring out mitigation strategies to reproduce these yields in a scalable process. The team did not include a quad chart in their presentation; these are very useful to judge their progress.

A CLOSED LOOP UPCYCLING OF SINGLE-USE PLASTIC FILMS TO BIODEGRADABLE POLYMERS

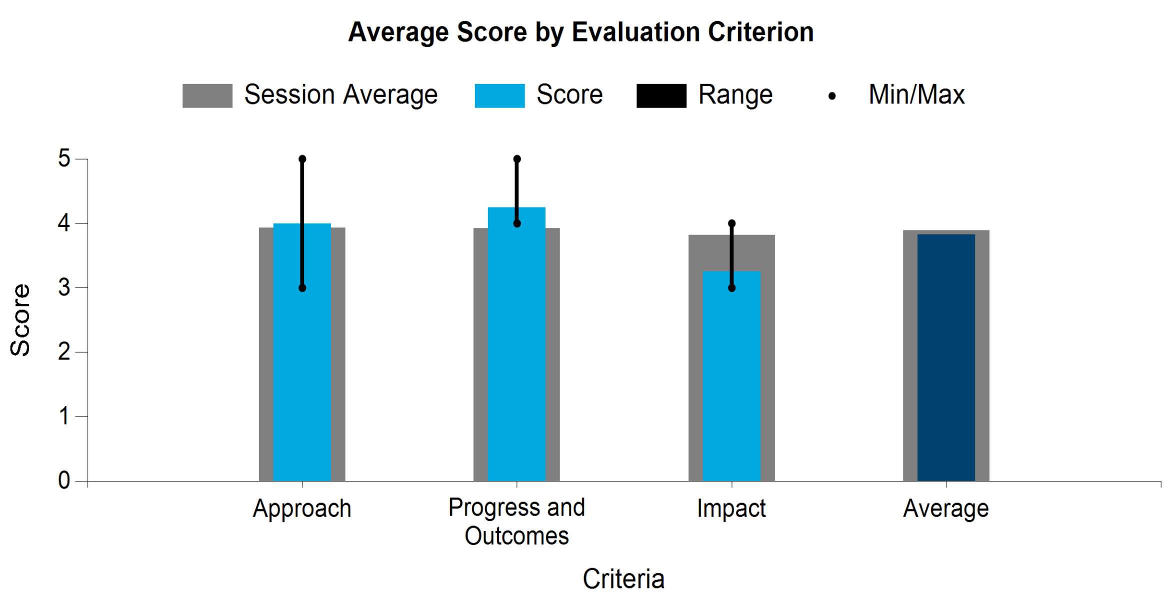
Iowa State University

PROJECT DESCRIPTION

WBS:	AM0.08
Presenter(s):	Xianglan Bai
Project Start Date:	06/01/2022
Planned Project End Date:	05/31/2025
Total Funding:	$2,500,000

The goal of this proposed project is to develop a novel plasma-biological hybrid technology to upcycle mixed single-use flexible plastic film (SUPF) wastes into biodegradable PHAs using a circular carbon approach. The detailed objectives to achieve this goal include: (1) characterize SUPFs containing mixed waste streams from MRFs to understand plastic feedstock variability; (2) innovate the industry protocol for film recycling to obtain decontaminated SUPFs primarily comprising polyolefins; (3) use low-temperature plasma and CO_2 to produce a fermentable intermediate liquid from the decontaminated SUPF wastes; (4) biosynthesize PHAs from the SUPF-derived intermediates to increase conversion efficiency and improve PHA recovery; and (5) employ TEA and LCA modeling to determine process economics and environmental impacts of the proposed technology.

Successful completion of the project will enable an innovative plasma and biological hybrid process to convert waste plastic film to biodegradable polymers with reduced energy inputs, carbon emissions, and production costs. An economically viable plastic-wastes-to-PHAs process leveraging waste CO_2 as a carbon source will advance and innovate the incumbent SOA technologies for plastic recycling/upcycling and PHA production. The project will interest stakeholders in various sectors, such as waste management industries, polymer manufacturers, polymer users, and renewable energy industries. The research outcome of the project will also advance scientific understanding and deliver new knowledge in multidisciplinary fields. Overall, upcycling plastic wastes meant for landfills into low-cost biodegradable plastics via a circulated carbon approach provides a straightforward solution to the challenging problems caused by the increased production of petroleum-based plastics and their disposal, utilizing waste CO_2 at the point source.



COMMENTS

- The slide deck is clear and comprehensive. The benchmark comparison with petroleum is helpful, but it needs clearer labeling to indicate which is which on the slide. LCA boundaries matter for this plasma pyrolysis technology; resolution of the presorting of input materials is needed to accurately assess/ understand how practical it might be. The problem statement includes this aspect in the risks identified, and the description of the project team's collaboration was impressive. There is no arrow indicating contaminants on slide 5, and it does not appear to be included in the TEA/LCA on slide 14.
- The project management structure and communication are appropriate and clear. The integration of TEA to identify risks is a strength. The DEI plan is described and adequate, although moving forward, ensuring that all the diverse team experiences equal inclusion should be a focus. The goal is to convert PCR polyolefin waste into oils that can be metabolized by microbes to produce PHA. The novelty of this project is in the catalysis of the waste plastic to oils and demonstrating that oils from real waste streams can be successfully converted to PHA. As such, a continued focus on utilizing real waste streams is essential. It is great that the LCA/TEA began early in the project, but the waste handling and pretreatment steps must also be included in these. Industry partners are identified, but it is not clear how engaged they are in the project. The vision of utilizing the CO_2 from the biosynthesis in the plasma process may have implications for siting commercial systems, e.g., may require colocation. The team should consider whether it makes sense to site the waste-to-oil installation closer to waste collection sites and transport the oil to the biosynthesis facility or colocate both. A patent is pending by Iowa State, but what is the plan to pursue commercialization beyond that if the results are successful? More actively engaging potential partners for commercialization would increase the potential for impact.
- There was transparency about DEI and assumptions for the LCA and TEA. The key value is using single-use plastic as feedstock. In this early-stage project, the first step—deconstruction to make oxidized intermediate liquids—is promising, and the team has promising results. I am skeptical about whether fermentation can produce PHAs at commercial efficiency and have an economic impact. The team should engage with a partner(s) in a detailed market analysis to determine the economic value of the types of polyalkanoates that are proposed.
- I appreciate that the team is working with three MRFs to source their feedstock waste. I appreciate that the team is including TEA/LCA at this early stage of the project. The team is working with their industry partner, QEG, for bio-based PHAs and expert advice on commercially ready products. I would encourage the team to strengthen this partnership and try to exchange materials with their partners during this project.

PI RESPONSE TO REVIEWER COMMENTS

- Response to Reviewer 1: The TEA assumes a SUPF price ($30/tonne) that includes waste handling and pretreatment expenses. Waste plastics are usually available for a tipping fee of 10–$50/tonne (https://www.epa.gov/sites/default/files/2015-12/documents/historic_tipping_fees_and_commodity_values_02062015_508.pdf). This SUPF price represents a handling and pretreatment cost of $40–$80/tonne. The LCA and future TEA will include a more detailed representation of the supply chain steps from waste collection to the conversion facility. One of our future tasks is conducting a supply chain analysis to identify potential siting locations colocated with CO_2 sources. Some material resource facilities have both a CO_2 source from organic waste combustion and a plastic stream. QEG is a commercial company working on the anaerobic fermentation of organic waste to produce biofuels. QEG will work with the team on the PHA fermentation and purification and evaluate its commercialization potential for scale-up. Quasar's facility has a CO_2 byproduct (>97% purity; the residue is mainly methane) after methane is recovered for renewable natural gas. The QEG facility is generally built close to waste handling facilities. There is potential to build new refinery facilities next to QEG digesters.

- Response to Reviewer 2: The system boundary for the initial LCA begins with waste collection and ends with the PHAs and hydrocarbon production. Presorting is included in the waste collection step. Information on the presorting data and contaminants will be collected from this project. The contaminants are typically handled through sedimentation ponds and are often reused within the facility. The water is sent to the municipal water treatment plant when it becomes too dirty.

- Response to Reviewer 3: QEG is working with the research team to evaluate the commercialization potential of the PHA fermentation process. We are expecting to increase the PHA yields in the PHA fermentation process. Our commercial strategy is to co-ferment plastic wastes derived from oxidized intermediate liquids with VFAs produced from AAD to produce PHAs. We will evaluate the economic feasibility of this option. At the same time, we are working on applying PHAs for higher-value products in another project.

- Response to Reviewer 4: The project team has been working closely with QEG by holding biweekly subtask group meetings and monthly team meetings to discuss project progress and develop industry-relevant strategies for PHA synthesis/extraction. Physical material exchanges are also planned.

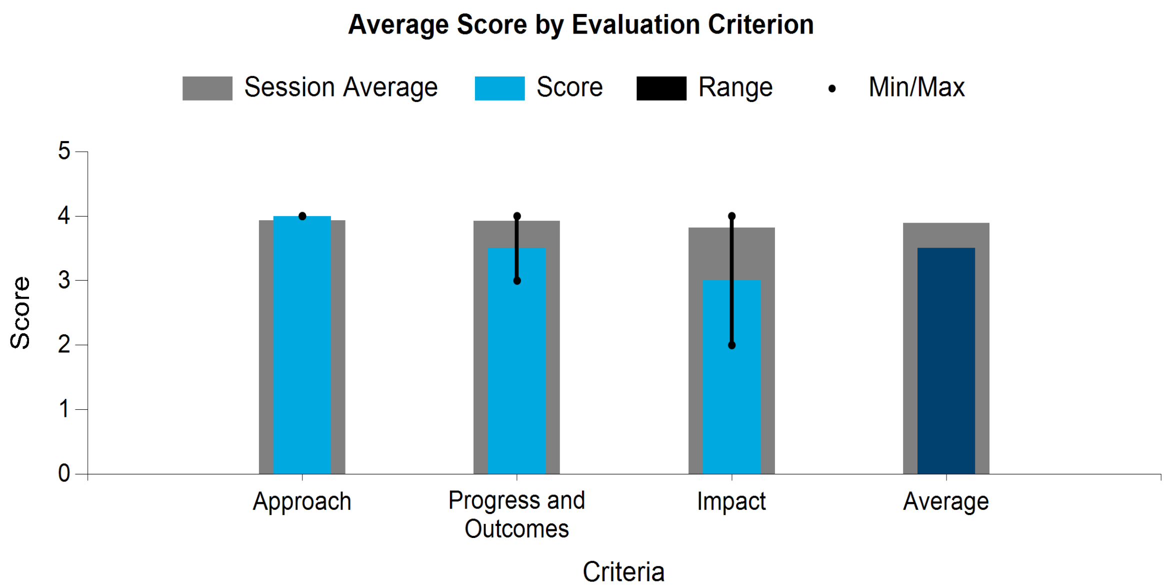
INTEGRATED CHEMOLYTIC DELAMINATION AND PLASMA CARBONIZATION FOR THE UPCYCLING OF SINGLE-USE MULTI-LAYER PLASTIC FILMS

University of Massachusetts Lowell

WBS:	AMO.09
Presenter(s):	Hsi-Wu Wong
Project Start Date:	07/01/2022
Planned Project End Date:	06/30/2025
Total Funding:	$1,600,276

PROJECT DESCRIPTION

We are developing an integrated chemolytic delamination–plasma carbonization process to upcycle single-use, multilayer waste plastic films with heterogeneous compositions into high-value chemicals, carbon materials, and hydrogen. The main objective is to develop a process that is capable of (1) treating a wide range of different compositions, (2) producing high-value products, (3) using environmentally benign solvents, and (4) scaling modularly for small-scale, distributed manufacturing. In addition, the project aims to develop a more diverse, equitable, and inclusive workforce for the sustainability sector by supporting and engaging underrepresented students in STEM and underserved communities in Massachusetts. Major project accomplishments to date include (1) identification and testing of two safer solvents for film delamination, (2) design and assembly of a plasma carbonization reactor, and (3) an apparent kinetic model for noncatalytic delamination.



COMMENTS

- More explanation of how the chemical variety in the layered input will be handled, or, given the early stage of the work, an explanation of the plan to develop a strategy for this would have provided more confidence in the team's ability to achieve the intended results. The attention to worker safety is positive. More explanation of the plan for identifying input material was needed. Does the team have a sense of the type or range of films currently in the pre-consumer or post-consumer waste streams that is their target and whether that segment or range can be obtained in a form that aligns with the intended process(es)? The project team has defined their work more narrowly than I understand the remit to be.

To convey the intended information, slide 17 would need to be redesigned, both for scale/visibility and for content. The DEI plan was concrete, specific, and well described, which was distinctly superior to other presentations.

- This is an ambitious project targeting novel delamination, PET decomposition, and plasma carbonization to convert multilayer films to PET monomers, hydrogen, and carbon products. As such, it carries multiple technical challenges to be overcome. The team has identified risks and has a mitigation plan in place. The viability of the project will depend on the potential market for the variety of different products envisioned (PET monomers, H_2, carbon), and starting to think about potential commercialization routes as technological progress is made would increase the potential for impact. Additionally, considering how to incorporate real waste streams to understand the potential challenges that may arise beyond the system studied currently (contamination, wider range of compositions)—leveraging the connection with Dow and other projects in the space—would be useful. The bar for commercialization appears to be high. It appears that entirely new installations are envisioned; thus, the siting and integration into supply chains deserves consideration. As the two stages of the process (delamination/PET decomposition) and plasma can be decoupled, the team is strongly encouraged to engage with others in this space to evaluate whether the delamination step is necessary, given the high activity around different PET deconstruction chemistries and options. There was a strong DEI plan as part of the project, with outreach to a variety of different communities, including special lectures for learning-disabled students. The team is congratulated on their approach here, going beyond recruiting a diverse range of early-stage researchers. Although Dow has been active in providing advice about the selection of model test materials, identifying partners who could move commercialization forward if successful should remain on the team's radar.

- The team has just begun project work, but their goals are very clear—there are quantitative metrics, and they are very aligned with BETO goals. The team has provided one of the more detailed and active DEI plans. It is too premature to assess the impact, but the team has engaged industry partners, and this input shapes the probability that the technology products are at least commercially relevant.

- I appreciate that the team is incorporating their TEA/LCA to guide the development of their solvent and chemolysis and treats the development of TEA/LCA and their reclamation system as an interactive process. I appreciate the team's pragmatic approach to tackling waste of different compositions. The plan is to remove the PET and carbonize the material that cannot be separated out. I would want to see the team treat films of different compositions and move on to treating mixtures of films of unknown composition.

PI RESPONSE TO REVIEWER COMMENTS

- The project team is grateful for the reviewers' thoughtful comments. We have summarized the primary topics that reviewers have raised, and our responses are below.

- Treatment of real waste streams of variable or unknown composition: The two-layer commercial-grade film under study in the project thus far consists of a layer of aluminum-containing PE and a layer of PET, bonded by an adhesive layer of PU. The film was selected on the recommendation of our Dow collaborators due to its simplicity. The baseline performance of the chemolytic delamination and plasma carbonization processes can easily be evaluated and established for comparison, yet it is still a widely available commercial-grade film. We do plan to treat other real-world waste films with more complex compositions in the near future, as documented in our statement of project objectives, starting in Quarter 8 for Task 2 and Quarter 6 for Task 3. The effects of solid contamination and the ability to use melt filtration to remove such contamination will also be investigated in collaboration with our Dow collaborators. Because up to 40% of the manufactured multilayer films are discarded during the packaging fabrication processes, our initial focus will be on the pre-consumer waste streams; however, post-consumer waste films with more heterogeneous compositions (e.g., food waste) will also be studied if time permits.

- The necessity of delamination: The project team has started investigating and developing a one-step chemolytic delamination process using glycolysis. Our preliminary results showed that the model two-layer Uline film described above was partially delaminated under mild conditions (150°C, 1 hour), with the possibility of the PET layer being simultaneously decomposed into small products. The identification and quantification of the glycolysis products are underway and will be shared with the DOE team soon. The results will inform whether a one-step chemolytic delamination process or a two-step chemolytic delamination process is more feasible and economically viable.

- Commercialization pathways and connecting with potential partners: In addition to considering the trade-offs between a one-step and a two-step chemolytic delamination process, the project team is also looking into the pros and cons of a plasma carbonization process (with target products of hydrogen and carbon materials) versus a plasma-gasification process (with target products of hydrogen and carbon monoxide, i.e., synthesis gas). The process flowcharts of all these scenarios have been sketched (and shared with the DOE team during monthly progress meetings, as opposed to slide 17 presented during the Project Peer Review). The establishment of the mass and energy balance bounds of critical operations is underway. Once these bounds are established, the process flowcharts of different scenarios will be sent for TEA and LCA. We would also like to clarify that our industry partner, Dow, is not only actively engaged in providing suggestions of feedstock selection but also playing a critical role in guiding the selection of the most attractive commercialization pathways and potential products for our proposed technology.

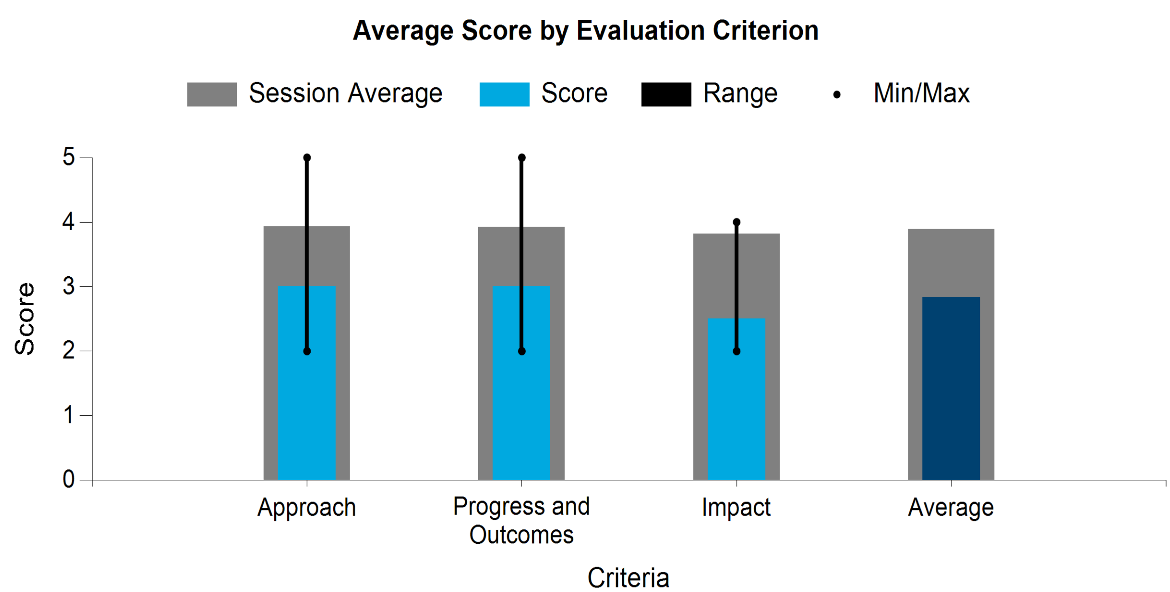
CATALYTIC DECONSTRUCTION OF PLASMA TREATED SINGLE-USE PLASTICS TO VALUE-ADDED CHEMICALS AND NOVEL MATERIALS

North Carolina A&T

WBS:	AM0.10
Presenter(s):	Debasish Kuila
Project Start Date:	08/01/2022
Planned Project End Date:	07/31/2025
Total Funding:	$2,499,994

PROJECT DESCRIPTION

The objective of this project is to advance a combination of nonthermal plasma (NTP) treatment of waste polyolefins and subsequent catalytic deconstruction to selectively make C2–C4 olefins; benzene, toluene, xylene (BTX); and oxygenated intermediates (target products) at lower energy consumption than virgin plastics. The objectives include: (1) evaluating NTP pretreatment of PE and PP and characterizing polymer modification and functionalization via scanning electron microscope, Raman, Fourier-transform infrared, and X-ray photoelectron spectroscopy techniques; (2) establishing a mechanism for depolymerization and oxidation pathways using reactive dynamics simulations; (3) developing novel catalyst compositions and structures to achieve >40% selectivity to C2–C4 olefins via the thermal catalytic deconstruction of plasma-treated plastics; (4) achieving >70% carbon utilization of target products via the catalytic deconstruction of plasma-treated polyolefins; (5) demonstrating up to 50% energy reduction in target products (C2–C4 olefins, BTX aromatics, and oxygenated intermediates); and (6) demonstrating feasibility via TEA/LCA. The expected outcomes and deliverables are as follows: (1) a lab-scale prototype of a combined NTP and upcycling process using waste polyolefins demonstrating >70% carbon utilization of target products and >40% selectivity to C2–C4 olefins with 50% energy reduction; (2) a technical report detailing the plasma conditions, catalyst compositions and operating conditions, performance of the lab-scale system, and spectra of the high-value products and byproducts; and (3) TEA and LCA with a development plan for scale-up and a commercial process. Finally, these objectives and deliverables will be advanced under a framework that motivates the improved inclusion of underrepresented groups in STEM through mentorship and investigator engagement in equity and inclusion training.



COMMENTS

- I would suggest updating the slide deck for future presentations to clarify what activities are being evaluated and included in the team's analysis and what is meant by "renewable energy." The work of preparing waste materials that are ready to use is in the flow drawing but not in the to-do list. Excluding the LCA of the input materials significantly affects the ability to evaluate the proposed and accomplished outcomes. The benchmark table in slide 4 is helpful, but the scale of the information on this slide renders much of it invisible. Consider redesigning this, possibly into multiple slides where each has one point. A plan for tuning the project for target olefins would be reassuring. Slide 13 probably contains really useful information. "Key performance parameters to be tracked through the lifetime of the project" and benchmarks' "yield slate" are both potentially informative for a reviewer (like me); however, the slide is confusing, and I was unable to identify those items.
- This project was the most difficult for me to understand, both in terms of the approach and progress. As such, I am concerned that even if the project is technically successful, communicating about it to those who could move the technology forward to commercialization will become a barrier. This should be a point of attention for the project team. Given the size of the DOE investment ($2.5 million), the desired outcome of moving from TRL 2 to only TRL 3 is substantially less than other, smaller projects in the portfolio. Because the project was delayed in starting, there has been limited progress, and as such, it is appropriate for this beginning state. Because one of the benefits envisioned is the ability to use green electricity rather than thermal cracking, it is worth noting that the electrification of crackers is planned at the commercial scale in Europe, so there are potential other routes to providing a similar benefit. Given the range of partners involved, ensuring clear communication between different work streams will be important. Whereas the carbon utilization is compared to pyrolysis, the energy metric is baselined against fossil olefins. To judge the commercial potential of this process, carbon utilization, energy, and cost should be benchmarked against a pyrolysis recycling route, as that is what it would be competing with in the market.
- This project is in a very early stage—just beyond the conceptualization stage. Perhaps this accounts for the fairly diffuse project milestone statement in the quad chart. As such, I can recommend that the team develop a more detailed valorization plan. The transition in technology readiness is not very ambitious for the project's lifetime and leads to concern about how transformative and impactful the technology will be.
- The researchers were not able to effectively communicate their plans for the future development of their work. The preliminary data does not show production of their desired targets. I would implore the team to put their future development plan down in writing, demonstrating how to get to these targets in higher selectivity using their plasma treatment. I appreciate that the team will use actual plastic waste in BP2.

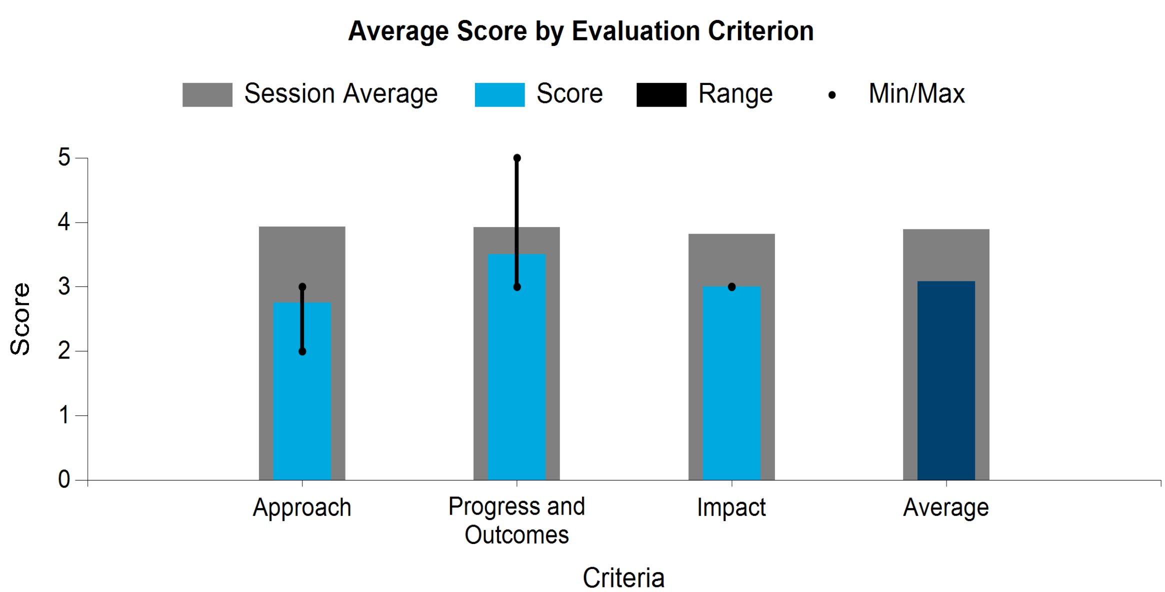
PROCESS INTENSIFIED MODULAR UPCYCLING OF PLASTIC FILMS TO MONOMERS BY MICROWAVE CATALYSIS

West Virginia University

WBS:	AMO.11
Presenter(s):	Yuxin Wang
Project Start Date:	07/01/2022
Planned Project End Date:	06/30/2025
Total Funding:	$1,500,001

PROJECT DESCRIPTION

The overall objective of the project is to develop a plastic film upcycling technology that is economically feasible, has lower GHG emissions, and achieves efficient conversion of the embodied energy of plastics to value-added monomers. Compared to a conversional ethane or naphtha cracking process for ethylene production, the proposed technology can achieve 55%–66% energy savings, 50%–63% GHG reduction, 57%–76% post-use carbon management, and 69%–75% cost savings. The technology is based on microwave-specific effects on the heterogeneous catalytic conversion of plastic films to monomers. The use of microwaves enables the depolymerization of plastic films both kinetically and energetically favorable at lower temperatures with high selectivity. The project will be accomplished by exploiting microwave-initiated interfacial chemistry in the selective cracking of C-C bonds in plastic films. The project will focus on the development of microwave-susceptible catalysts, microwave reactor design, and process optimization. Specifically, the scope of the project consists of designing and building a continuous feeding microwave reactor for process scale-up as well as conducting TEA and LCA to evaluate economic, energy, and environmental benefits. Kinetic parameters of the optimized catalysts will be determined based on which reactor and process designs for the pilot- and commercial-scale microwave catalytic upcycling system are developed.



COMMENTS

- Slide 2 has a cycle diagram that nicely outlines the ins and outs of the process, although the subsequent parts of the presentation do not account for the non-carbon fraction of the waste stream that would be coming in. The benchmark slide is also well done. There was insufficient information on the risks and mitigation factors. The DEI plan seems underdeveloped compared to the timeline and the other projects at this stage.

- This project targets the catalytic decomposition of waste polyolefins to BTX and olefins via microwave catalysis. This route would have a lower energy requirement and a higher yield than current alternative recycling routes (pyrolysis, gasification, hydrogenolysis); however, there are two key technical hurdles. One relates to the design of a continuous microwave reactor handling solid/high viscous feedstocks. The second is the need to recover and recycle the very high catalyst loadings needed because the catalyst also controls the heat transfer in the system. As real waste streams will contain both contaminants that may poison the catalysis and nonorganic content (pigments, fillers), continual recycling of the catalyst will either lead to accumulation of ash in the system or require separation from the catalyst. To understand if these challenges can be overcome, real waste materials should be incorporated early in the project. A DEI plan exists but is rather limited in ambition, as it just focuses on recruiting underrepresented researchers. The team is encouraged to monitor the inclusion that the team members experience in the project.

- The team is leveraging an existing Advanced Research Projects Agency–Energy project to inform the design of the microwave reactor. Because this is a fairly basic research project, I would like to see more details in the plan to examine catalyst and reaction conditions (lower temperature). It would also be helpful to have the economic analyses define a desirable product mixture target (e.g., % BTX) that achieves the most desirable economics. Currently, the demonstration or proof-of-concept system deploys a high catalyst load. The key for chart 12 for the gas composition is confusing; both the pink and blue are designated as C2–C4, so it is not easy to interpret what the compositional change is between the thermal and microwave processes.

- I appreciate that the team is building a preliminary TEA/LCA in BP1 and is then expanding on it in BP2. I would like to see if the team can increase selectivity by its choice of catalyst as well as using a feedstock that is closer to real-world waste. In terms of collaboration with industry, I would love to see the team reach out to industry partners to use their products as feedstocks for resin production as well as sourcing waste to use in their process.

PI RESPONSE TO REVIEWER COMMENTS

- Many thanks to the review panel for their time and comments. Through this project, we strive to develop a SOA microwave catalysis technology to decompose plastic polyolefin films to valuable monomers. The catalysts and continuous microwave reactor are the two main challenges in this project. To mitigate these risks, a microwave-susceptible catalyst will be developed and fully evaluated to optimize the activity and selectivity to the target monomers. Meanwhile, the kinetic parameters (reaction temperature, ramping rate, catalyst/plastic ratio, etc.) will also be fully studied. Moreover, as part of the real-world waste feedstock and continuous feeding process, catalyst poisoning and recovery will be studied. To mitigate the risk of catalyst deactivation by contaminants in waste plastics, we plan to develop a catalyst regeneration protocol. Meanwhile, we will develop low-cost catalysts that can be purged with ash at EOL. In addition to collecting real-world plastic for laboratory continuous reactor processing, we have reached out to a single-use plastic recycling company for commercial-scale processing information, which will facilitate the design of a larger continuous flow reactor. Further, the TEA/LCA models will be developed to analyze the economic, energy, and environmental benefits of the developed technology with real-world plastic as feedstock based on laboratory results and industry information. As in the beginning stage (Quarter 1), DEI is still in development; however, all team members are working on it, and we expect the whole team to foster more DEI at all levels. In addition to recruiting underrepresented researchers, we will also monitor how inclusive the team members' experience is. Outreach activities are also planned; these include volunteering in initiatives that educate K–12 youth on STEM principles and/or the importance of plastic recycling/circularity, and disseminating information about plastic waste and recycling in local communities.

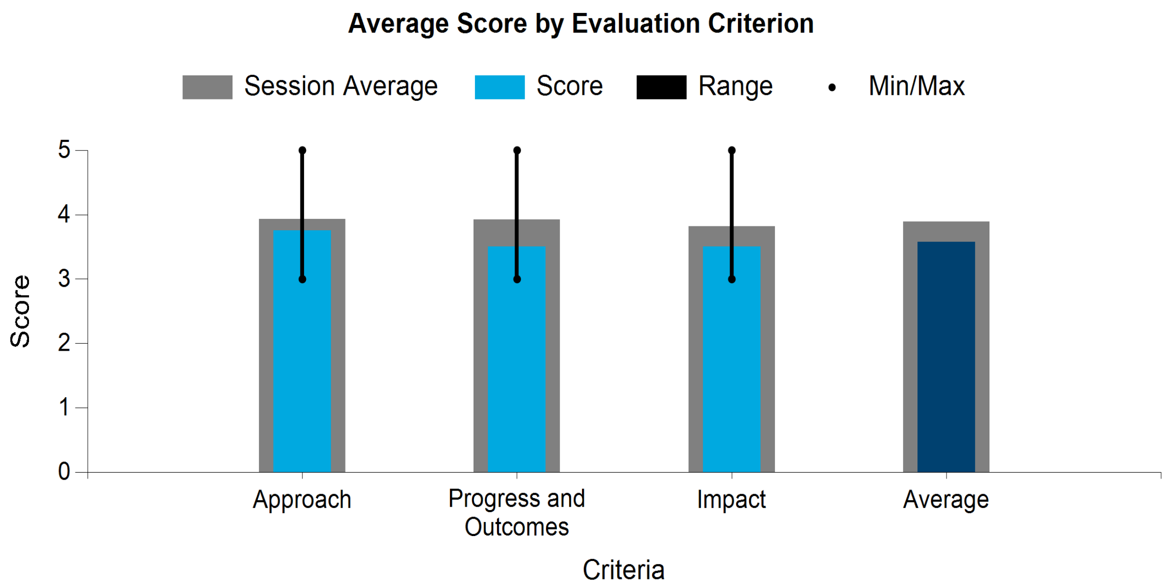
ALL-POLYESTER MULTILAYER PLASTICS (ALL-POLYESTER MLPS): A REDESIGN FOR INHERENTLY RECYCLABLE PLASTICS

Michigan State University

WBS:	AMO.12
Presenter(s):	Muhammad Rabnawaz
Project Start Date:	06/01/2022
Planned Project End Date:	04/30/2025
Total Funding:	$1,705,811

PROJECT DESCRIPTION

Due to their adaptability and affordability, more than 100 million tons/year of flexible and rigid multilayer plastics (MLPs) are produced worldwide, accounting for >30% of all plastics produced; however, MLPs possess complex structures comprising up to 12 layers of various materials with different physical, mechanical, and chemical properties. This complexity limits the recyclability of MLPs and impedes the development of EOL solutions. The overarching goals of this project include: (1) producing "all-polyester MLPs" that offer packaging performance (sealing, barrier, mechanical, etc.) that matches or exceeds those of commercial 5–12-layer MLPs; and (2) providing multiple EOL solutions (e.g., chemical and mechanical recycling) for all-polyester MLPs.



COMMENTS

- Please check the slides against a colorblindness tool. Despite having only the slides to review (no oral presentation), I am able to follow the narrative of the presentation and understand where the project is and where it is going. This is excellent communication.

- This project focuses on the development of an all-polyester multilayer film for food packaging applications. As such, it is envisioned that the films can either be mechanically or chemically recycled with high carbon recovery. A strength of this project is the active involvement of Amcor to provide input on processing and property requirements. As such, this project has a wider view on performance metrics than many of the other projects presented. This is a strength of this work. There is a DEI plan included, and it is good that the team is not just focusing on completing an activity but on following the impact of the outreach. The project is at an early stage (month 8) but is on track for meeting the milestones identified. Incorporating TEA/LCA as early as possible to help steer development choices is recommended. Because chemical recycling is an envisioned EOL option, engaging with other projects focused on the chemical recycling of polyesters early on is strongly encouraged. As the LCA has not been completed and the composition of the materials is not shown, it is very difficult to judge the potential environmental impacts of the candidate materials at this stage of the project.

- This is a very intriguing proposal to create an all-polyester multilayer film; I would have liked to have heard the presentation. The team has engaged a good industry partner; Amcor is an industry leader in providing film packaging for a broad variety of consumer and specialized applications. The DEI plan has specifics, and the team has good engagement activities with underrepresented students. The technical approach description could be significantly strengthened (or more helpful to the reviewer) if, instead of providing sweeping performance metrics for the all-polyester multilayer film, it showed discrete tables that aligned the performance of each candidate polyester functional replacement (polyester 1, polyester 2, and polyester 3) against the specifications for each of the three layers (structural, barrier, and sealant) that each will replace. Other elements that would be helpful in the project description include (1) describing what the technical risks are and how you plan to mitigate them; (2) tailoring the desired barrier properties to a particular application (the needs are different across various applications/industries)—what is the first target for the prototype you are developing?; (3) developing a testing strategy for multilayer stability; and (4) addressing other issues—e.g., sterilization and regulatory considerations.
- I would encourage the team to perform a TEA and LCA early in the development cycle of this multilayered product. If possible, I would encourage the team to have industry partners test their multilayer films. As this will be in contact with food, the team will need to ensure that their multilayered product is food safe and passes all regulations. As this is a product that is supposed to be a widely available technology (recycling), I would encourage the team to *not* support exclusive licenses to the technology.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to express our appreciation to the reviewers for taking the time to participate in BETO's 2023 Project Peer Review of this project and for their thoughtful and excellent analysis and constructive feedback on this project. In response to the valuable feedback from our reviewers, we are keen to incorporate their insights into our future work. One recommendation was to include TEA and LCA in the early stages of our project to guide our development choices. We anticipate that our initial TEA and LCA will be ready by or before month 12 of this project (currently, we are in the 10th month of this project). We will also start early on the chemical recycling portion of our project, focusing on polyesters at Michigan State University. We will be supported in this endeavor by the advice and expertise of PNNL. We will also create discrete tables where we will align the performance of each candidate polyester functional replacement against the specification (structural, barrier, and sealant). Managing potential risks is a crucial part of our process. Therefore, our project team consistently discusses potential technical risks and brainstorms mitigation strategies during our regular project meetings. As recommended, the project team will finalize the initial target application(s) for the first multilayer polyester prototype early on. Further, we will work with our industry partner on the stability of the multilayer, sterilization, and regulatory considerations as well as on the testing of all necessary properties of the multilayer films by industry. Finally, following the recommendation, we will work closely with our Michigan State University technology team to develop a nonexclusive licensing strategy for this technology.

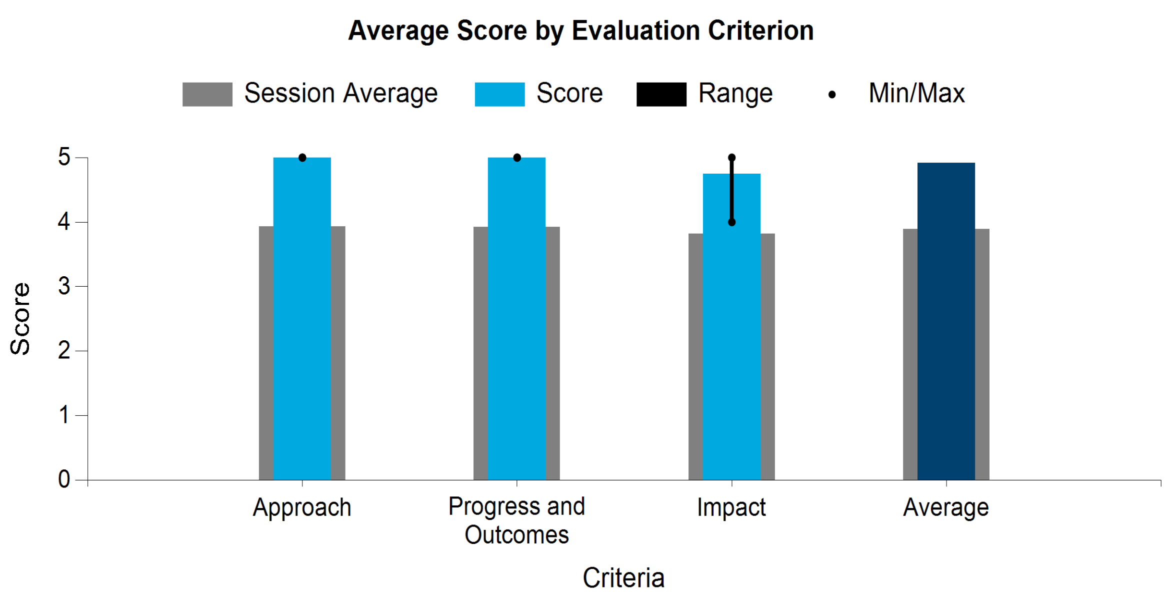
INTRODUCTION AND BOTTLE OVERVIEW

BOTTLE Consortium

PROJECT DESCRIPTION

WBS:	BOTTLE1
Presenter(s):	Gregg Beckham; Megan Krysiak; Michelle Reed
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$250,000

The BOTTLE Consortium aims to develop robust processes to upcycle existing waste plastics and develop new plastics that are recyclable by design—both of which are in direct alignment with DOE's Strategy for Plastics Innovation. We accomplish our work in the BOTTLE Consortium through an organizational framework that includes three primary research tasks (Deconstruction, Upcycling, and Redesign), which are supported by three crosscutting tasks (Analysis, Characterization, and Modeling). BOTTLE also has tasks focused on industry engagement and DEI. This presentation will review the approach and management structure of BOTTLE, the importance of analysis-guided research, and the key metrics for carbon, economic, energy, and GHG emissions. In the FY 2021–FY 2023 period, BOTTLE has drafted and enacted a comprehensive DEI plan, assembled a world-class technical advisory board to provide constructive feedback on our performance, had our first in-person all-hands meeting in summer 2022, and onboarded and off-boarded research activities based on active project management and analysis. From an impact perspective, BOTTLE researchers have published more than 40 peer-reviewed manuscripts (many in leading journals), submitted >30 patent applications, and initiated six funds-in industry partnerships.



COMMENTS

- This was a polished presentation that covered the bullet points in each review question.
- Overall, the BOTTLE Consortium approach and management structure are extremely well thought out, well executed, and well aligned with DOE and BETO priorities and strategic goals. Particularly impactful is the integration of analysis into the projects early on, as well as the yearly portfolio review, which has resulted in decisions to stop activities and focus on more promising routes. The active engagement of the technical advisory board should be continued and fostered, with composition

reevaluated as the BOTTLE portfolio shifts and as projects move up in TRL. The communication structure is clear, and there are multiple routes being leveraged for internal and external collaboration. As BOTTLE expands, active evaluation of the communication structure is encouraged to ensure it is still effective. The DEI plan is under development, and several supporting activities have already been accomplished. With continued attention, this area is on a good trajectory. One aspect of the value chain that is not currently strongly represented is the recovery of plastic waste that would flow into the proposed processes. Whether this should be encompassed within BOTTLE or a different DOE activity, it is important to include so that the technologies developed have a viable supply chain and are developed to handle realistic feedstock forms, compositions, and contaminants. As their activities are moving toward TRL >2, BOTTLE should develop a strategy here to ensure that the commercialization of the technologies has the desired impact. BOTTLE has the opportunity to be a thought leader in driving sustainable plastic innovation forward. BOTTLE serves as a convenor of actors along the value chain to not only develop new technical routes but also to nucleate actors behind the most promising pathways to help build the critical mass needed for deployment and drive system change.

- Projects nested in the BOTTLE Consortium are advantaged by the technical resources in this integrated structure of five national labs, five academic institutions, and industry partners linked by CRADAs. BOTTLE meets and excels in all review criteria. It is very hard to find a better-structured program with a clear, cohesive structure and exceedingly capable leadership. The meeting structure seems to be sharing data and resources efficiently and regularly with internal members and also with external audiences, as the team has created a functional, live website to push out current articles. The risk/mitigation strategy is solid, and BOTTLE is swift to sunset projects that are not on a trajectory to meet targets. The DEI plan is thoughtful and proactive. BOTTLE has demonstrated a strong commitment to moving projects toward development and commercialization with a much-strengthened engagement with industry. Several actions reveal that the consortium leadership team seriously responded to suggestions from the 2021 Project Peer Review. These inputs will inform their asks in the 2023 renewal application, which will expand their reach to bring on institutions/experts with large-scale polymer processing capabilities. The consortium is aware of at least one gap—polymer processing—that would enhance its agility in moving its targets, and this will likely be addressed in the 2023 renewal proposal.
- The team leader seems to have very open communication internally, which is also evident in their very cohesive presentation. The lead is aware of risks and mitigations in individual sub-efforts. It is great that the team conducts portfolio analysis to decide what to accelerate, discontinue, or continue. These decisions are usually made within a group; the group members take on a new project, and this does not impact funding for each individual group. I wonder how this project will develop in the future. Is the team going to return to early-stage research and get more hard problems from industry to solve, or is the team going to push the research further down the TRL pipeline? There are advantages and disadvantages to both approaches. If the team wants to continue into higher TRLs, I believe they will have to bring additional teams into the consortium that are specialized in processing and scale-up.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the review panel for their positive feedback. We also sincerely appreciate the constructive input, and we will act upon these suggestions. In terms of the "plastics waste recovery" value chain, this is excellent feedback, and we agree that this is a critical element of the supply chain to ultimately enable a circular plastics economy. We have previously worked with other BETO-funded and DOE-funded efforts to examine plastic waste mass flows in the United States on a geographical basis (e.g., https://doi.org/10.1016/j.resconrec.2022.106363). Moreover, AMMTO funds efforts in various analysis-driven plastic supply chain modeling efforts that are complementary to BOTTLE's mission (e.g., see https://doi.org/10.1111/jiec.13423). Last, and especially as we intend to advance a few key deconstruction technologies up the TRL, we are also working with industry partners to source realistic plastic waste. The reviewers identified polymer processing as a current gap, and, during the Q&A, we discussed monomer synthesis and manufacturing R&D at a larger scale as another gap. Both gaps will be addressed directly as we move into the proposed renewal phase for the FY 2024–FY 2026 project cycle. The comments regarding how to balance early-stage research relative to pushing promising technologies up the TRL ladder is excellent, and we are carefully considering what the balance of these activities should be going forward. We mostly view the balance as a funnel, where multiple promising early-stage technologies should be evaluated in parallel, and only select technologies should be selected, guided by both technical promise/feasibility and analysis, to be advanced in TRL. Moreover, as we advance technologies along the TRL ladder, we will also actively pursue additional funding mechanisms, including industrial funding, to support and eventually off-board scale-up to industry partners and other support mechanisms. Doing this will allow us to balance our resources to maintain a "full pipeline" of early-stage, promising innovation and a select number of technologies that BOTTLE can advance to TRL 4–5 before transferring them to other support mechanisms.

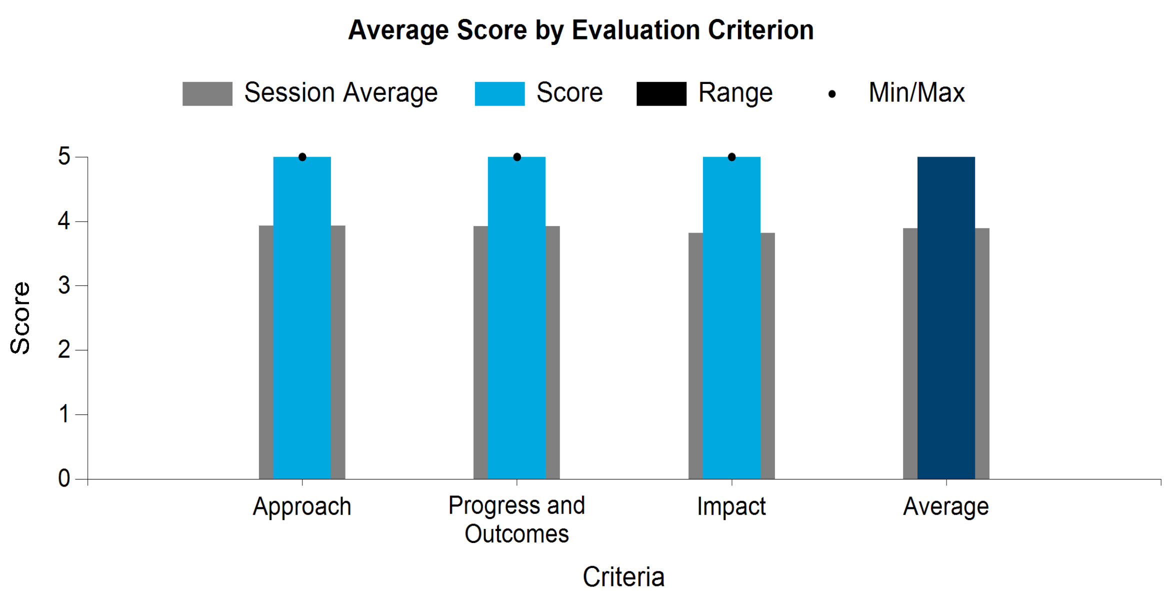
ANALYSIS

BOTTLE Consortium

PROJECT DESCRIPTION

WBS:	BOTTLE2
Presenter(s):	Jason DesVeaux; Michelle Reed; Taylor Uekert
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$400,000

The use of analysis is foundational to BOTTLE. In particular, we conduct TEA, LCA, and supply chain modeling for each new BOTTLE innovation, ranging from new deconstruction and upcycling technologies to redesigned polymers. These critical analysis tools are used in parallel with laboratory research to ensure that BOTTLE technologies can ultimately meet our key metrics. The BOTTLE team used analysis early in the current 3-year project cycle to identify research priorities from a scale, energy, and economics perspective (https://doi.org/10.1016/j.joule.2020.12.027), and recently we presented a comprehensive framework for comparing new circularity-focused approaches to linear, incumbent practices (https://doi.org/10.1146/annurev-chembioeng-100521-085846). This presentation will also review case studies in analysis for closed-loop PET recycling across a range of recycling methods, baseline studies that we have conducted for plastics pyrolysis and gasification as another comparator for BOTTLE technologies, and a comprehensive study of existing closed-loop recycling technologies from a full suite of environmental impacts and feedstock quality metrics. We have undertaken studies of circular polymers being developed in the Redesign task, and we will present an exemplary case for a bio-based acrylic polymer that can replace polymethyl methacrylate. Overall, analysis is critical to enable the BOTTLE Consortium to focus on impactful, realistic technologies.



COMMENTS

- Even if all the projects are not using the same LCA, it would be helpful for each to illustrate what is included in the analysis of what they are doing. For some, it appeared that it only included carbon footprint, which, while important, does not reflect the full range of impacts that plastic may have. It would benefit from including analysis of plastic additives, for example. The existence of this analysis effort is very reassuring for the overall effort.

- The analysis component of BOTTLE is one of its strengths and should be commended. By publishing transparent, consistent comparisons of different routes, it has the potential to influence both industry decisions as well as policy ones. As such, it is important that these analyses are periodically updated as more data become available or as improvements are made. It was particularly gratifying to hear that the analysis publications have resulted in industry reaching out to explore publishing high-quality LCA of their pilot or commercial processes. For increased impact, as the analysis activities identify actionable opportunities to decrease the impacts of different routes, it would be useful to collect these across the portfolio to identify which process improvements will have the greatest crosscutting benefits. The early and frequent engagement between experimental efforts and analysis should continue, as this is key to maximizing decarbonization potential at speed. The outreach efforts to socialize tools such as materials flow through industry at the American Physical Society short course are encouraging for widening the life cycle thinking within the polymer development community. Gathering feedback from industry and academia on how to make the analysis outcomes, tools, and data should be intentional to maximize impact. The interactive graphic with links to publications is a nice start, but more may be needed to make the results optimally useful for the community.

- This project provides a very sound and disciplined analysis approach that is consistently and uniformly applied to each program. The project fosters a transparent commitment to open-source practices and published a framework for plastics analysis in 2022. The case examples are powerful; these include the upfront sensitivity analyses that enabled a credible, specific target for the research focus (e.g., cheaper feedstock to achieve price parity of recycled (r-TPA) versus virgin (v-TPA) to accomplish a more impactful process. The application of this analysis framework has achieved the desired impact of enabling the deployment of technological routes with a higher commercialization potential.

- I think this project is absolutely fantastic. The team's TEA and LCA results are used in other parts of the consortium to inform go/no-go decisions. If possible, I would love other BETO projects to build on this very thorough analysis as well. I would use this analysis as a benchmark for everybody else's economic and sustainability analysis.

PI RESPONSE TO REVIEWER COMMENTS

- We are delighted to see that the review panel found the Analysis task to be a strength of the BOTTLE Consortium. We agree with the comment regarding updates to the analyses as new data and insights become available. We are indeed doing this now for PET enzymatic hydrolysis and waste plastics gasification, for instance. The idea about crosscutting benefits across analysis cases is good—we will consider how to do this carefully. We will continue to expand the functionality of the analysis-focused part of the BOTTLE website. Another reviewer remarked on the fact that we are not using the same LCA—we note that this confusion is an artifact of the short nature of the presentations. We have a self-consistent LCA approach across the BOTTLE Consortium, but due to time constraints, we were unable to show all the details. Further, we are actively working on incorporating additional impact categories—especially those focused on plastic additives, microplastics, and social effects—as more data become available. Overall, we were delighted to receive such a positive reception of the Analysis task from the review panel.

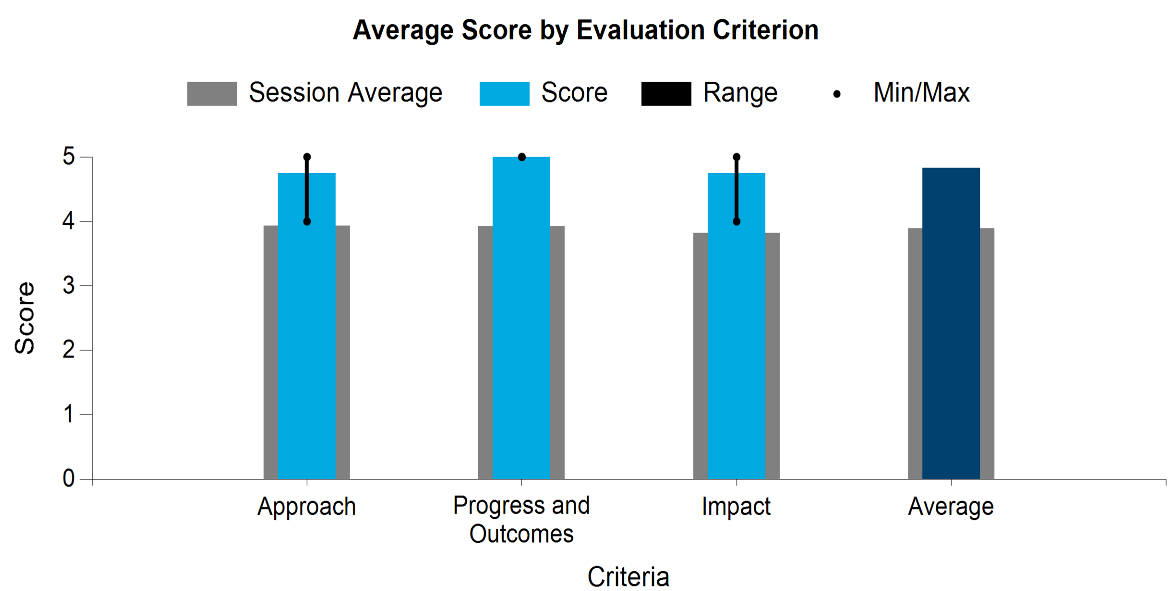
DECONSTRUCTION

BOTTLE Consortium

PROJECT DESCRIPTION

WBS:	BOTTLE3
Presenter(s):	Michelle Reed; Taraka Dale; Yuriy Roman-Leshkov
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,737,500

The Deconstruction task is pursuing the chemo-catalytic and biocatalytic depolymerization of today's plastics into molecular building blocks that can either undergo closed-loop recycling or valorization to higher-value products. For the FY 2021–FY 2023 project cycle, Deconstruction is the largest task in the BOTTLE Consortium due to the urgency of developing new recycling strategies for plastics that are not sufficiently recycled (or recycled at all) today. This two-part presentation will first focus on the development of chemo-catalytic methods to convert mixed polyolefin waste into small-molecule hydrocarbons, oxidative deconstruction of mixed plastic waste to oxygenates that can be converted microbially to a single product (in collaboration with the Upcycling task), and a catalytic glycolysis strategy for PET closed-loop recycling. The second part of this presentation will focus on innovations in enzymatic PET recycling through the development of process-advantaged enzymes that are specific to crystalline PET substrates and are able to operate at ~65°C and low pH. Exploratory efforts are also underway to use enzymes to depolymerize nylon and PUs. Together, the Deconstruction task in the BOTTLE Consortium has developed a suite of innovative technologies to depolymerize many commodity polymers, and we are using analysis now to determine the most impactful paths forward that warrant further scale-up and process integration.



COMMENTS

- This was very thoroughly explained and covered each evaluation bullet point. I appreciated that the first section highlighted additives to plastics as a major risk and had a mitigation strategy: controlled studies with known additives. I would have appreciated more explanation of what is meant by autoxidation. Oxidative funneling tolerates additives—are they getting included or released?

- The approach of starting with a wide range of technologies (hydrogenolysis, oxidation, glycolysis, photoelectrochemical, enzymatic) addressing key polymer classes of polyolefins and PET is appropriate. The down-selection to focus on the most promising options guided by analysis should be applauded. The results of these early TRL deconstruction efforts have excellent potential for innovation. Particularly promising is the autoxidation funneling route, which has the potential to allow the conversion of compositions used currently into more circular or benign systems. Particularly exciting are the preliminary results on the oxidative funneling of polyvinyl chloride systems. If successful, this opens a route to transform the materials of today to those of the future. The creation of a spinoff company, Tereform, based on this work is encouraging for future commercialization. The enzymatic degradation work is very well done, with a solid experimental approach. Compared to the other routes explored, it has less potential for impact. A narrowing focus will allow BOTTLE to achieve a higher impact potential. The hydrogenolysis deconstruction targeting lubricant oil would be worth benchmarking against the LOUPs project, which is targeting the same waste stream and application area.

- Deconstruction is at the heart of this technology area. The team deselected the photochemical and electrochemical approaches and diverted resources to more promising areas. The principals employ an excellent mix of model/mechanistic and engineering analyses to optimize. A nice outcome for all this work is a platform with select targets and a choice of the best feedstock and process to achieve GHG, yields, etc. The promising work with the autoxidation of mixed plastic waste streams has resulted in a spinoff company, Tereform. The crystalline PETase enzyme discovery work has the potential to be a useful preprocessing step for PET with a lower energy demand.

- It is very exciting that the team found a first enzyme that is preferential for crystalline PET. How does the very early work of Taraka Dale tie in with the rest of the BOTTLE group? Can you funnel these early TRL technologies through faster because you have all this expertise under one umbrella?

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the positive feedback on the Deconstruction task. In terms of the enzymatic hydrolysis work, we agree that this has a more limited scope relative to the other deconstruction technologies presented, and we will carefully consider this input going forward, toward maximum impact. In terms of how this fits in with the rest of the BOTTLE team, PET closed-loop recycling technologies—including enzymatic hydrolysis, glycolysis, and methanolysis—are all of keen interest to the BOTTLE Consortium, so enzymatic hydrolysis fits in under the umbrella of closed-loop PET recycling processes. For the comment regarding the oxidative funneling process tolerating additives: We did not have sufficient time to explain this in detail, but we note that organic additives are very likely oxidized in a similar manner to the polymers present in the systems. We are currently conducting further analytical chemistry work to this end to track the fate of additives in this process and others. On the point about moving these early TRL technologies faster because of the complementary expertise in BOTTLE: That is certainly our intention. We really appreciate the positive comments and the constructive feedback for the Deconstruction task.

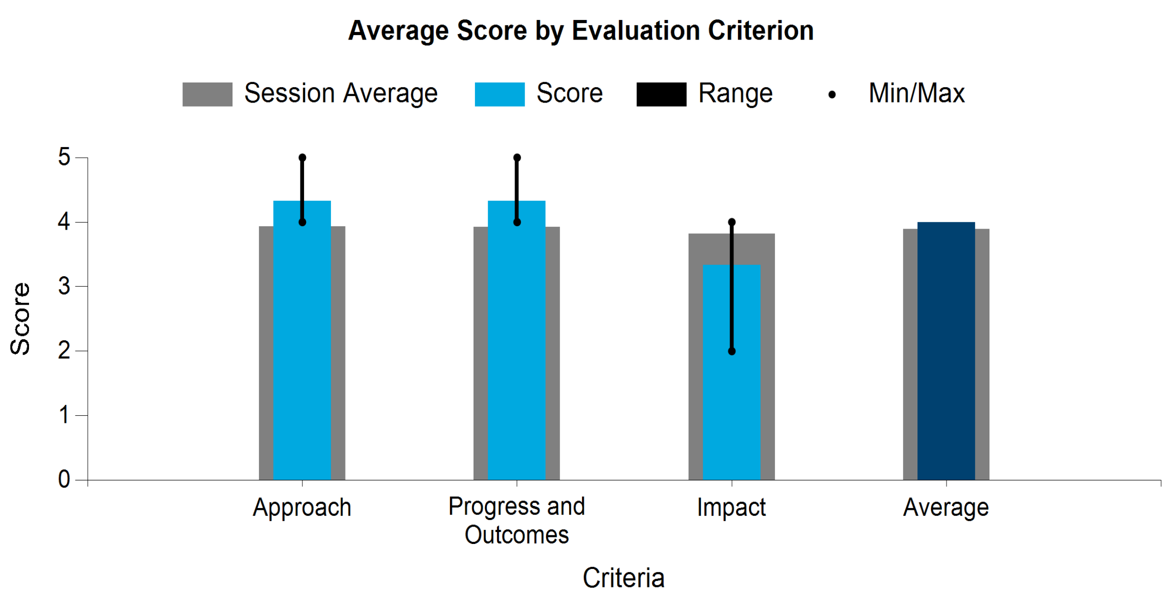
UPCYCLING

BOTTLE Consortium

WBS:	BOTTLE4
Presenter(s):	Adam Guss; Michelle Reed
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$800,000

PROJECT DESCRIPTION

BOTTLE's Upcycling task aims to convert intermediates derived from the deconstruction of today's plastics into molecular building blocks that can be converted into recyclable-by-design polymers with the Redesign task. Accordingly, the Upcycling task is a critical "bridging" task in BOTTLE. Efforts in the Upcycling task focus specifically on: (1) the discovery and engineering of new metabolic pathways and enzymes to convert intermediates from mixed waste plastics to central carbon metabolism; (2) metabolic engineering to convert mixed oxygenates into single compounds; and (3) the consolidated bioprocessing of PET, wherein a microbe secretes a PET hydrolase enzyme and converts the depolymerization products to value-added compounds in a single step. This work has led to the "biological funneling" of oxygenates from PET, polyethylene, and polystyrene into tunable bioproducts. The pathway discovery work has led to the discovery of pathways for PET co-monomers, including isophthalic acid, among others, which are now being engineered into production strains. For the consolidated bioprocessing of PET, we have successfully engineered a thermophilic bacterium to secrete thermo-tolerant PET hydrolases and consume both TPA and ethylene glycol, which are key steps toward enabling this concept. Overall, the Upcycling task is enabling the conversion of mixed plastics into PABPs and recyclable-by-design monomers through cutting-edge science.



COMMENTS

- Interesting question: If microbes break down waste plastic and poop out useful materials for making new plastic, does that mean the waste plastic is transformed into bioplastic by the participation of the microbes? That seems to be what this presentation is saying. This highlights the need for commonly shared definitions.

- The project could benefit from TEA to determine whether it is on target and sensitivity analyses to determine which factors to focus on to achieve the highest benefit. I am concerned about the practicality of a pure biocatalysis route to upcycling; it may not achieve practical production rates. The investigators should engage with industry to focus the upcycling scheme on reasonable metrics.

- This is a very integrated project that touches many other aspects of the consortium. I appreciate that the team is using products from the oxidative funneling process. I am excited to see the team scale up their production of monomers.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the feedback on the Upcycling task. Whether a waste-based plastic can be considered a bioplastic is debatable, and we did not mean to convey that. Instead, the use of a microbial conversion process here enables funneling mixed-plastic-waste-derived intermediates into a single product, and bio-based substrates could also undergo similar transformations. We apologize for any confusion caused here. We are conducting TEA now on multiple upcycling pathways that involve biological transformations, and we will be able to report these analyses in the next Project Peer Review and in the peer-reviewed literature in the meantime, especially toward the synthesis of new monomers for recyclable-by-design/circular polymers.

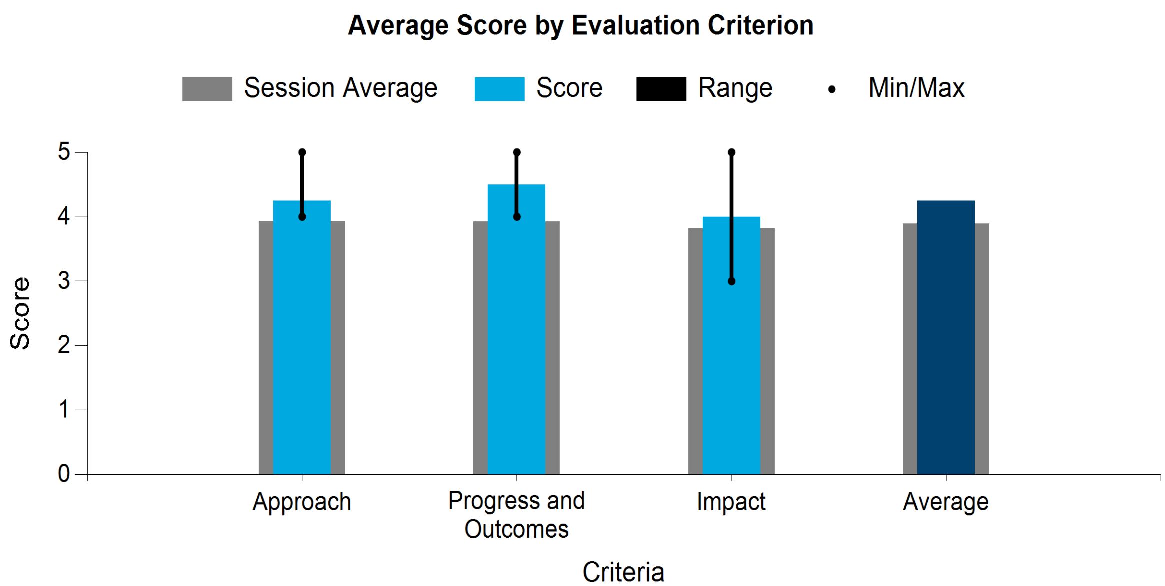
REDESIGN AND MODELING

BOTTLE Consortium

PROJECT DESCRIPTION

WBS:	BOTTLE5
Presenter(s):	Eugene Chen; Linda Broadbelt; Michelle Reed
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$895,000

The Redesign task in BOTTLE focuses on the synthesis of polymers that can be recyclable by design, sourced from waste-based or bio-based feedstocks, and can replace linear plastics. In close collaboration with the Redesign task, the Modeling task primarily focuses on predicting pathways (PickAxe) that can be used to efficiently manufacture building blocks, either biologically, chemically, or through hybrid approaches, coupled to an ML tool (PolyID) that can predict key properties of recyclable-by-design polymers before experimental work is initiated. These tasks have made multiple exciting innovations since FY 2021, including the development of key design principles for circular polymers; the demonstration of a bio-based, circular replacement for polymethyl methacrylate; and innovations in the “hybrid monomer” concept for polyester, nylon, and polyolefin replacements. Moreover, the Redesign task has greatly advanced the ability for PHAs to be chemically synthesized, enabling much greater control and tunability. This now includes the ability to be melt-processable to produce recyclable, bio-based alternatives to polyolefins. The Modeling task is directly addressing the cost of new monomers for these redesigned polymers through pathway predictions as well as supporting other BOTTLE efforts in deconstruction and upcycling. Going forward, the portfolio of new polymers from the Redesign and Modeling tasks will be a major focus area for the BOTTLE Consortium.



COMMENTS

- What is the thread connecting the graphs in the second half of this presentation? What is the story? The connections of the second half were not clear.

- The approach of the recyclable-by-design polymers guided by modeling is sound. Particularly strong is the integration and use of modeling to down-select what systems should be pursued from the huge potential design space; however, further model development is needed to move to a wider range of relevant properties, particularly those that will be strongly influenced by microstructure and crystallinity. An initial screening based on chain composition makes sense, but working more on developing chain chemistry–structure–property relationships and the influence of processing should be considered. Strong interaction with industry partners on the key property requirements for targeted applications (beyond just mechanical or barrier properties) should be considered, particularly as they relate to processing. As projects move toward higher TRL, a much more nuanced discussion around how performance is defined will be needed to identify areas of course. The planned activities around monomer scale-up to ensure sufficient volumes for evaluation will be critical and should be expanded moving forward. Because the early results are so impressive, starting initial TEA/LCA to help guide monomer and polymer selection is important.

- Programs like this recyclable-by-design program have benefited from early industrial guidance with realistic property targets for each major polymer class. The presentation on the bio-acrylics production of the monomer and its properties was compelling. I like that the team is building on the concept of "hybrid monomers"—e.g., 4,6-nylon and the two lactones (caprolactone and butyrolactone)—to generate polymer products that have the desired mix of recyclability and performance attributes. The outputs of performance, processability, and recyclability exceed the incumbents, and this approach highlights several good monomer targets. I like that the team has developed approaches to predict crystallization, glass transition, and melting temperature (Tc, Tg, and Tm, respectively). I appreciate developing the Monte Carlo framework.
- I am very impressed by the team's partnership with Amazon and that their materials are being used in industrial projects. I appreciate that PickAxe is freely available, and the number of PickAxe uses would be an interesting metric to track.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you to the review panel for their positive input on the Redesign and Modeling tasks. We fully agree that additional metrics for predicting beneficial polymer properties are crucial, and as noted in the presentation, we are working actively to that end, including with industry input. We agree that monomer synthesis at larger scales alongside TEA and LCA will be critical in the redesign efforts. We apologize if the threads connecting the first and second parts of this presentation were not clear—the Redesign and Modeling tasks work very closely together, so we thought it would be beneficial to present them back-to-back. We share the reviewers' excitement about the future of circular polymers and the ability to predict their properties and the most efficient monomer synthesis pathways. We look forward to sharing the results to these ends in the next Project Peer Review.

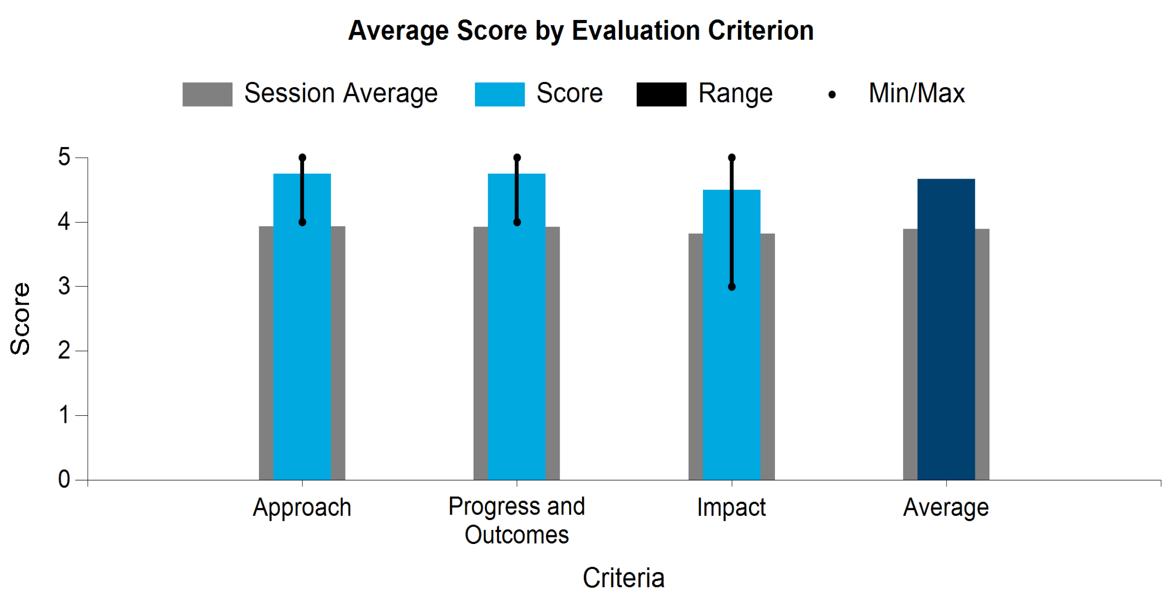
CHARACTERIZATION

BOTTLE Consortium

PROJECT DESCRIPTION

WBS:	BOTTLE6
Presenter(s):	Christopher Tassone; Meltem Urgun Demirtas; Michelle Reed
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$767,500

We use the synchrotron capabilities of the Stanford Linear Accelerator to characterize chemical and biological catalysts reacting with polymers with *in situ* and *operando* techniques with the Deconstruction task. This effort has developed multiple new approaches for *in situ* and *operando* measurements. These critical measurements directly inform reactor design and scale-up activities. In collaboration with the Redesign task, the Characterization task is applying both advanced scattering and spectroscopic measurements as well as conducting critical EOL measurements using ASTM-based methodologies. These key activities directly inform both polymer processability at scale and potential degradability if redesigned polymers leak into the environment. For EOL studies, we are developing new capabilities in the scale-down of biodegradation tests alongside strategies to determine the fate of redesigned polymers in realistic environments. Moreover, the Characterization task reported a framework for analyzing polymer deconstruction approaches to promote scientific reproducibility in the community (https://doi.org/10.1038/s41929-021-00648-4). We will soon report a comprehensive characterization of commercial plastics for the research community to understand the potential of additives and contaminants to affect deconstruction and upcycling approaches.



COMMENTS

- The science was solid and very interesting and gets full marks for what it is. The connections beyond interesting science (potential for use, scale-up, and commercialization) were not made clear within the presentation.

- The characterization efforts are well integrated into the projects and activities, which is a strength. Continued interaction to ensure a low barrier to interfacing as well as thoughtful decisions about when fast feedback versus deep dives are needed should be continued. Particularly nice is the characterization development allowing monitoring *in situ* in relevant conditions. Using such approaches to help identify or improve the robustness of catalysts to conditions and contaminants seems particularly important to ensure that approaches can be deployed. Integrating the EOL (degradation testing) results that monitor impacts beyond CO_2 to include methane monitoring with LCA is critical for matching systems/applications where recycling or degradation are most appropriate. Additionally, I advise the team to consider mapping inherently dissipative applications (paint wear, seed coatings) with biodegradable materials while prioritizing recyclability for applications with the best potential for material recovery and reprocessing. The work on monitoring degradation beyond CO_2 production has impact beyond just BOTTLE projects, and the dissemination of the methodologies and insights gained will benefit the entire field of biodegradable polymer development and mitigate potential unintended consequences, depending on the degradation products formed.

- The team is allocating appropriate resources (for both in-depth characterization and rapid high-throughput screening) to create reactors to mimic realistic conditions for assessing the deconstruction mechanisms. I applaud the commitment to scaling down existing ASTM test methods. Is it also possible to consider conceiving accelerated tests for internal guidance while not abandoning these long-term ASTM test measurements for promising candidates? The discovery work to elucidate the "plastisphere" microbiome is noteworthy. This will be very useful knowledge and will be a great asset for the biodegradation research community.
- It is fantastic that the characterization team is physically exchanging samples with all the other parts of the consortium and has worked with all the other groups in BOTTLE. It would be interesting to see if the team could assist other parts of the BETO portfolio that are producing plastics as well. In addition, all teams working on modeling and computation could benefit from having consistent data sets on different plastics. Are there standard operating procedures for characterization that have worked well within BOTTLE that could apply to other projects as well (for example, "Inverse Biopolymer Design Through ML and Molecular Simulation")?

PI RESPONSE TO REVIEWER COMMENTS

- Thank you to the review panel for their input on the Characterization task. In terms of "connections beyond interesting science," the work from the Characterization task overall was highlighted in multiple examples of direct impact to improve deconstruction-, upcycling-, and redesign-relevant processes and materials—indeed, these impacts were embedded in those three presentations as well (indicated by the characterization icon on the slides). These impacts have a direct impact on the potential for use, scale-up, and commercialization. The comment regarding scaled-down and accelerated testing mechanisms versus maintaining the existing ASTM methods is excellent, and we agree that we need to maintain the industry-accepted methods while also innovating for higher throughput. In terms of working with other parts of the BETO portfolio, many of the same researchers in the BOTTLE Consortium work on multiple projects resulting from FOAs, in the PABP project portfolio, and with academic collaborators (all this work is often in the same laboratory with the same equipment). Thus, there are already existing mechanisms for this transfer of knowledge, expertise, and data. We will also look to both formalize this information exchange and expand it as we can.

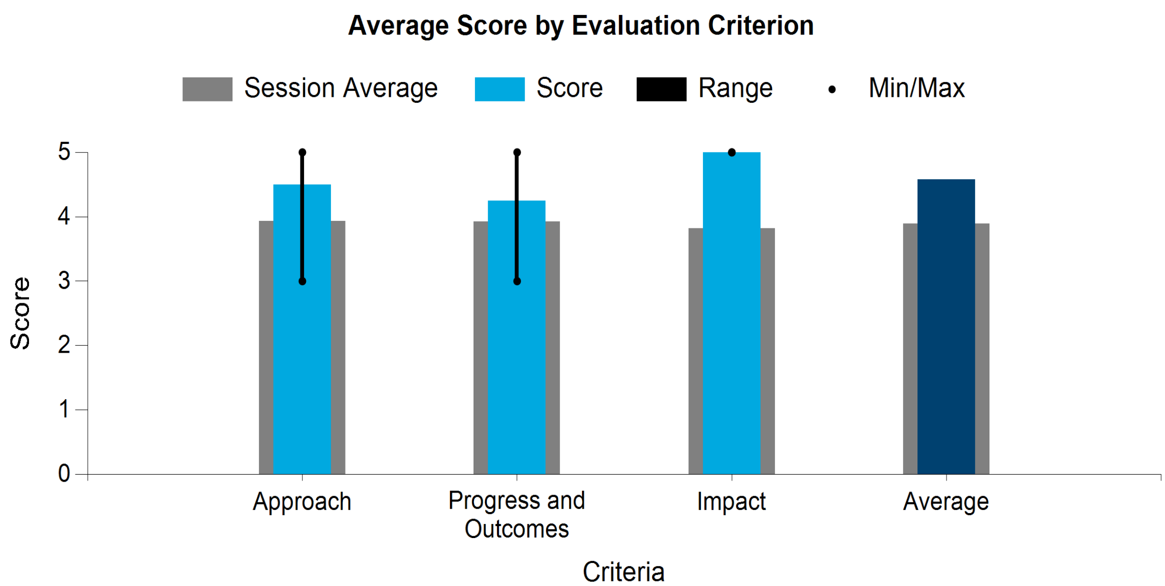
INDUSTRY PROJECTS AND ENGAGEMENT

BOTTLE Consortium

PROJECT DESCRIPTION

WBS:	BOTTLE7
Presenter(s):	Kat Knauer; Michelle Reed
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$150,000

One of BOTTLE's primary goals is to work with industry to catalyze new technologies toward our overall vision and mission using a centralized industry engagement plan. This plan aims to (1) solve real-world problems in plastics upcycling via targeted, company-funded projects; (2) promote industry engagement via streamlined access to BOTTLE partners and technologies; and (3) collaborate with companies to scale and deploy BOTTLE technologies into the economy. Our approach follows a five-stage model: prospecting, initial engagement, knowledge sharing, proposal and contracting, and opportunity won. Since FY 2021, BOTTLE has onboarded a full-time chief technology officer to spearhead industry engagement and lead industrially funded research projects. To date, BOTTLE has engaged with >150 companies, executed six industrial funds-in CRADAs, successfully completed two industry projects, extended two CRADAs with follow-on funds, and submitted more than 30 patent applications. Industry projects span the Deconstruction, Upcycling, and Redesign tasks; harness the capabilities of the crosscutting tasks; and take advantage of the broad IP portfolio developed through DOE funding. BOTTLE partners have an inventory of innovations that can inform the design of industry-specific collaborative projects with the highest probability of producing novel IP. Engaging with a diverse set of companies has also directly informed our R&D portfolio toward maximizing the impact and utility of BOTTLE innovations.



COMMENTS

- This is very effective at answering the impact question, so it gets full marks for what it is, but the presentation does not relate well to the other rating questions.
- Overall, BOTTLE's approach to industry engagement appears highly successful. Streamlining contracts upfront, making information easily accessible via the website, and proactively addressing staffing challenges is working. The approach of targeting consumer-facing brands with sustainability pledges is

generating interest and engagement, and the belief that the brands can drive other supply chain actors to be involved should be monitored as the CRADA projects progress. Given the early-stage research at BOTTLE as well as the massive system shifts needed to deploy at scale to meet BETO targets, it is worthwhile to explore how BOTTLE can act as a convening mechanism to achieve precompetitive development with a critical mass of industry partners to create the scale needed for system shifts.

- The new chief technology officer has gotten off the ground running and is wisely using resource dollars by allocating CRADAs for established entities that invest their own dollars and reserving FOAs for investment with smaller and midsize companies that likely lack deep research organizations. It seems like a savvy and reasonable move to create market pull by building relationships with recognizable brand companies with the expectation of moving beyond these brands in the near future and deepening relationships with the polymer supply chain companies. The engagement pathway is very reasonable, with realistic estimates of negotiation times (lengthier than desirable) and obstacles to sharing knowledge by potential companies. I anticipate that if there are more successes, the current barriers will be lower—there will be a built-in community with advocacy/advertising that will promote the value of a BOTTLE alliance and accelerate opportunities.

- I believe the centralized business development position is fantastic and should be implemented in the other projects of this size as well. Kat being the central contact point for these companies helps speed up contact as well as getting to meaningful contracts. I think having a publicly available CRADA form on the website is fantastic. In terms of licensing, I strongly believe that government-funded research into recyclability should not result in exclusive licenses. The technology should be used widely and without barriers to have the strongest impact. I am very impressed that there have been two startups that have spun out of BOTTLE.

PI RESPONSE TO REVIEWER COMMENTS

- We were thrilled to see the positive reception for BOTTLE's industry engagement model, which we also think is working quite well thus far. Regarding monitoring the shift from brand owners to more upstream supply chain actors: This is an excellent point, and fortunately we have started to see the onset of this transition, with BOTTLE acting as a "nucleation point" for multiple supply chain partners. We believe we will be able to report on this transition more concretely and quantitatively in the next Project Peer Review. Regarding the comment on the "impact question … but the presentation does not relate well to the other rating questions"—we apologize for any confusion. We attempted to highlight the progress and outcomes as well as the approach explicitly in the slides. Regarding the comment on IP licensing ("I strongly believe that government-funded research into recyclability should not result in exclusive licenses. The technology should be used widely and without barriers to have the strongest impact."): National labs and universities developing recycling inventions with DOE funding must balance broad (nonexclusive) access with the need to provide returns (through exclusive licenses) to industry players who have to invest significant sums of money to bring these inventions to market. Industry partners have provided consistent feedback that they will not invest in technologies that are nonexclusively available to their competitors. Universities and national labs have robust protections in place to ensure broad impact of DOE-funded technology through license agreements, including performance requirements and clawback provisions, to ensure the technology is diligently commercialized for strong impact.

OVERVIEW, PROJECT MANAGEMENT AND INTEGRATION, AND DEI

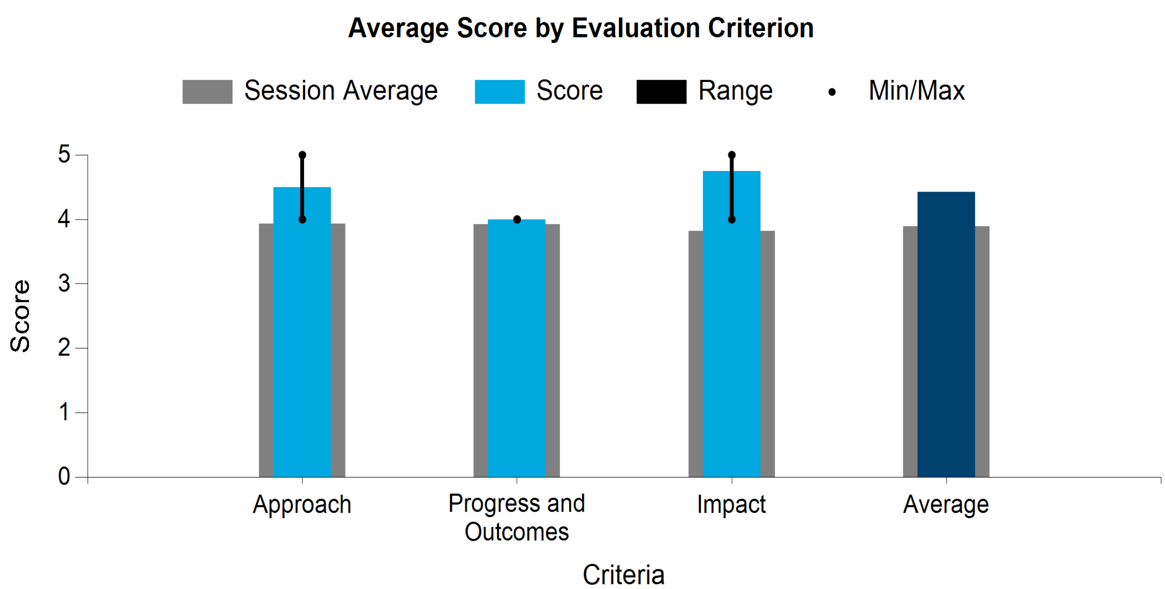
Separations Consortium

WBS:	SEP1.0
Presenter(s):	Lauren Valentino
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$390,000

PROJECT DESCRIPTION

Separations often account for the largest energy, economic, and environmental footprint in chemical processes, including bioprocessing. The Bioprocessing Separations Consortium brings together teams from six national laboratories to address these key challenges by advancing energy-, cost-, and carbon-efficient separations to support the decarbonization of transportation and industry. The consortium is organized into four tasks: (1) Project Management and Integration, (2) Core Experimental Projects, (3) Analysis and Computation, and (4) DEI.

The Project Management and Integration task provides technical guidance, facilitates communication among teams, tracks progress and impacts of the consortium, and guides the go/no-go decision process. This task also manages external communications, particularly with the advisory board, which provides feedback to help the consortium maintain an industrially relevant focus. A key outcome of the Project Management and Integration task is shaping the consortium's multiyear research portfolio by identifying BETO- and industry-relevant separation challenges, assessing consortium capabilities, and considering potential economic and environmental improvements. Finally, the DEI task focuses on fostering a welcoming, diverse, and inclusive environment within the consortium as well as supporting future workforce development for the biofuels and bioproducts industry.



COMMENTS

- The project is on track. The presenter gave an excellent overview of bioprocessing separations and consortia. There were clear objectives and emphasis areas for 2023. I need clarification on the IP rights for all participants. The selection of the IAB is critical, and the PI's engagement with the IAB should be strengthened. It was great to see the integration of TEA, LCA, and computation at the early stage of the project. The approach to DEI looks very strong. Is there any way to target an audience of high school students from under-resourced communities and/or within traditionally underrepresented groups?

- The Separations Consortium as a whole will advance the SOA with regard to bioprocessing. Improving the efficiency of separations specific to bio-based processes is critical for advancing the establishment of materials for transportation (fuel) and other industrial applications, including new materials. A broad range of separation technologies are being developed within the consortium. Management of the projects was standardized across the portfolio with monthly consortium meetings, biweekly TEA/LCA meetings, biannual meetings with the IAB, strong DEI initiatives, and both a laboratory executive board and an advisory board. Advisory board members come from a mix of deep technical expertise and business backgrounds and viewpoints. Implementation strategies for the technologies are less defined. It might be good to have clearly defined off-boarding objectives for commercialization so that once projects are off-boarded, new ideas can begin to be investigated. Off-boarding should be viewed as the ultimate success. Communication and collaboration among the various labs and efforts seemed to be top-notch—it appears that the LCA, TEA, and computational studies are having a significant impact on determining how the projects are executed, which is impressive. Additionally, the consortium has shown flexibility in that some projects have been rescoped to optimize the chances of success. A robust DEI plan, including the Bioenergy Bridge to Career Program with a community college focus, will increase exposure to bioenergy careers and encourage seeking candidates from underserved communities. Overall, the projects looked to be progressing on schedule. For some projects, it may be too early to have a clear connection to commercialization, but all projects had at least some contact with industry collaborators. Some projects may have too many industry voices and should consider down-selecting the number of partners at some point to provide focus.

- Separations are one of the most challenging aspects of bioproduct manufacturing, from both a technical and commercialization perspective. This is because the costs associated with separations can determine whether a bioproduct will achieve market acceptance, whether as a fuel or as a chemical. This program has identified that energy- and water-intensive processes will not allow for the successful reduction of carbon intensity for bioproducts and has identified innovative project areas that will advance the SOA. The consortium is well organized and well designed and appears to foster good cooperative work between the various laboratories. Potential areas for improvement are, first, industry collaboration. The IAB appears to meet regularly and provide good advice on the industrial application of the program efforts, but specific collaborative work with industry partners seems to be limited. A more focused effort on bringing industry collaborators on board to participate in projects would enhance the technical strength of the projects and help to ensure their relevance to practical problems. Including TEA and LCA at early stages is welcome and is an excellent way to provide metrics for assessing the value of technological developments; however, both analyses will necessarily evolve as the technology develops further through scale-up and implementation, so they should not be viewed as static scores. The sensitivity analyses being performed should help mitigate the risk of an overly optimistic early-stage analysis that does not reflect the realities as a project progresses toward implementation.

- It is fantastic that TEA/LCA is essential in focusing this project's efforts and guiding development and that the consortium meets on a monthly basis to ensure that everyone is aligned on tasks and milestones. An overall comment on the consortium: I believe that this group is at a point where the technologies are ready for the next steps in commercialization. I would suggest that the team put additional effort into business development—the BOTTLE Consortium created a business development position to centralize conversations with industry partners and licensing. I would suggest creating general templates for your CRADAs and making them available to your researchers as well as potential new partners via your website. I appreciate that the team is collaborating with other BETO portfolio efforts and industry partners. I believe that the IP on these projects should be centrally handled as well so that the researchers are not stuck with negotiating with several technology licensing offices.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to express our appreciation for the thoughtful, valuable, and supportive feedback provided in the reviews. Regarding IP and business development, IP rights for any work done by the consortium are managed in accordance with the prime contract between DOE and the respective Federally Funded Research and Development Centers in the consortium. Collaborative projects may be established by any consortium laboratory and an external collaborator through a CRADA, which includes IP management. The consortium is committed to the ongoing development and availability of general CRADA templates; this includes revisiting our current CRADA development package. We aim to make the template readily available on our website. We also appreciate the reviewer's feedback on business development, but we would like to respectfully clarify that the consortium's primary focus is on technology development. Regarding the high number of industry collaborators for some projects, we believe that multiple industry partnerships bring diverse perspectives that can enhance the applicability of our projects; however, the reviewer's point about balancing collaboration with clear direction is valid. As projects evolve, we will consider strategically down-selecting the project collaborators, considering the expertise and value that each partner brings to ensure that critical perspectives are not lost in the process. We absolutely agree that the selection of the advisory board is critical because the board serves as a link between the national laboratories and industry, providing valuable guidance, expertise, and industry perspectives to researchers. Although not presented in detail due to time limitations, in 2023, we initiated an effort to update our advisory board. This selection process targeted individuals who can actively contribute to the consortium's goals and provide meaningful guidance to researchers. As of May 2023, the advisory board includes representation from the following entities: Amyris, ADM, BioMADE, AMMTO, Genomatica, Honeywell UOP, ICM Inc., New Culture, Propharma, Siemens, and Virent Inc. As noted during the presentation, the consortium meets with the advisory board twice per year and asks that board members provide advice, review results and progress in comparison with work plans, and provide feedback on the prioritization of research projects (experimental and analytical). In addition to our biannual meetings, in June 2022, we invited the board's feedback on the consortium's 3-year plan to BETO. In July 2021, we hosted a listening day to engage stakeholders on challenges and opportunities in bioprocessing separations. The consortium will continue these regular interactions with the advisory board. Regarding the target audience for our educational workshop, we have chosen to focus on community college students for a few reasons. First, we aim to provide targeted support and resources to facilitate a smoother transition from 2-year programs to 4-year institutions or the workforce. Second, community college students are a better audience for our content. Having completed a high school education, they have a foundational understanding of scientific principles and are better equipped to engage with the content. Finally, with their greater focus on entering the workforce, we seek to provide these students with specific knowledge, networking opportunities, and career guidance in the bioenergy field to enhance their employability.

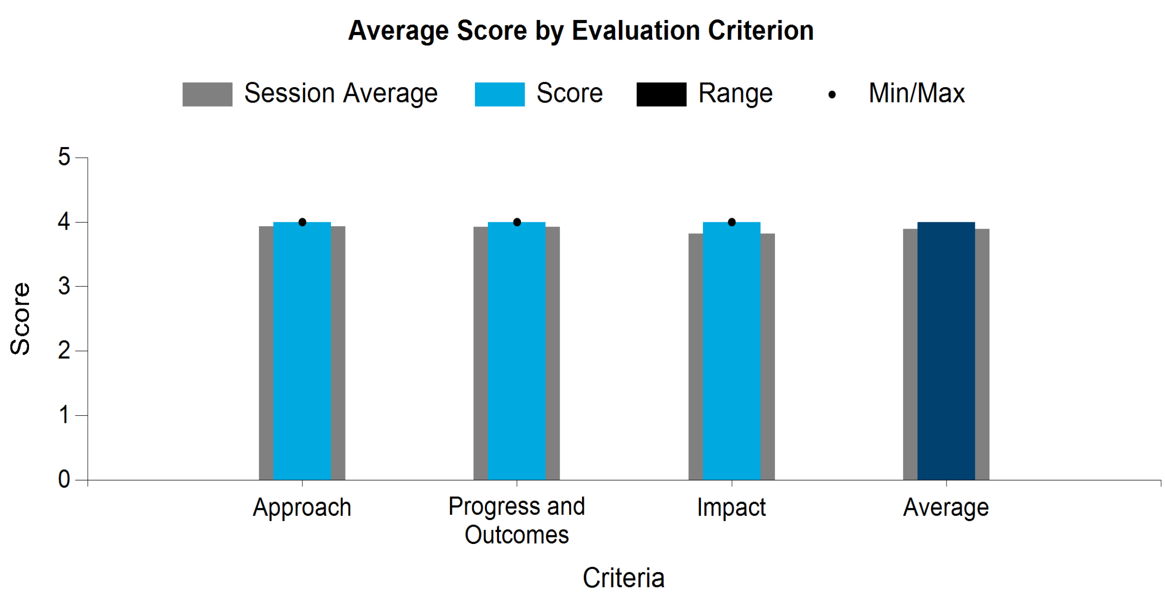
ADSORPTION BASED ISPR FOR ABF PRODUCTS

Separations Consortium

PROJECT DESCRIPTION

WBS:	SEP2.1
Presenter(s):	Gregg Beckham
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$500,000

This task focuses on the development of adsorption-based ISPR integrated with simulated moving bed chromatography for the recovery and purification of carboxylate products that are relevant to BETO. ISPR has been pursued previously in the Separations Consortium to recover carboxylic acids near or below their pKa values with liquid-liquid extraction coupled with downstream distillation; however, there are many acid products in the BETO portfolio that require neutralization well above their pKa values wherein ISPR could still be a major benefit to the bioprocess performance, including muconic acid, beta-KA, 3-hydroxypropionic acid, itaconic acid, butyric acid, and others. In this task, we are combining dynamic filtration with a rotating ceramic disk, resin capacity measurements, tailored resin synthesis, and simulated moving bed chromatography into an ISPR system that can be used to recover BETO-relevant carboxylates from bioreactor cultivations. We are working across process scales and using computational modeling where applicable alongside TEA and LCA to understand major cost, energy, and GHG emissions drivers. The impact of this project will be a bench-scale integrated approach to recovering carboxylate products *in situ*, which will reduce the waste generation from biological carboxylate production processes and improve the productivities of biological systems.



COMMENTS

- The project is on track. The team is developing an ISPR system for the recovery of muconic acid, aconitic acid, 3-hydroxypropionic acid, and beta-KA. Is there any feedback from the IAB on the approach and scalability of this ISPR system? The team needs a strong and detailed DEI plan.

- The success of this project depends on a high level of collaboration with other BETO projects, and it looks as if this is happening. The project started in October 2022, so it is still quite early. Risks and mitigation strategies are sufficiently defined. Is this equipment inherently difficult to keep up and maintain? It would be good to get industry feedback on this. The Quarter 2 milestone of collecting data on the uptake of various acids on the resins was achieved. Industry partners can help refine the project objectives and provide information on their relevance. The slide on nanostructured adsorbents is quite interesting, and it can help tailor the filtration of specific acids. The DEI plan with five interns (are they from underrepresented groups?) and participation in the Bioprocessing Separations Consortium is sufficient for the DEI objective.

- This new project area has the potential to provide an innovative set of technical solutions to the separation problems that reduce the rate of adoption of new bioproducts. The approach aimed at reducing the number of unit operations in the downstream processing of bioproduct manufacture is well thought out and has the potential to significantly advance the SOA in the topic area. Collaborations among the laboratories appear to be well managed and well considered. The progress is impressive given the recent start date of the project. The primary technical risk is that the metrics for the final product qualification are not universally understood. Purity requirements are defined by the end-use application, so assessing the performance of the quality of a separation process may not capture the specific requirements of the end use. This could be improved with more industry involvement for specific project areas that would allow for input on performance requirements. The scope of the project is broad, with many different separation techniques and targets. The use of proxies at this stage is necessary, but the team needs to ensure that translatability across target molecules is maintained. For example, data generated for lactic acid may not be universally applicable when the target molecule changes.

- I appreciate that the team is targeting scales of 10 milliliters all the way up to 100 liters. I greatly appreciate that the team is working with other BETO projects and industry partners to select high-impact targets to focus on. It is very impressive that the team has three CRADAs, one with each industry partner. I would want to see continued collaboration with industry partners in picking high-value targets.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive feedback. We are committed to supporting a sustainable bioeconomy through advancing the recruitment, development, and retention of a diverse and talented workforce. In addition to participating in each lab's DEI plan, including individuals from underrepresented groups in our research team, and providing student internships, the consortium is supporting future workforce development in bioenergy technology fields by creating the Bioenergy Bridge to Career Program. This was presented in the overview presentation for the entire Separations Consortium. We emphasize that the project overall has an exceptionally strong DEI plan. Our equipment is not difficult to maintain, but we wanted to make the point that we have dedicated staff who are experts in its use and upkeep. We find that having dedicated staff to maintain specialized equipment makes the collection, quality, and efficiency of data more consistent, and we were merely attempting to convey that we have been able to staff the project with dedicated experts to focus solely on this effort for maximum impact. In terms of purity requirements, we are working with the PABP projects and industry partners to understand the purity requirements, e.g., for the condensation polymerization of diacid products. We acknowledge the enthusiasm of the reviewers for industry engagement, and we will continue to emphasize this in our R&D activities. The consortium also meets with our advisory board twice per year to gather feedback on the potential commercial viability of all consortium technologies, and we will continue to integrate this into our approach.

CO-OPTIMIZATION OF SCALABLE MEMBRANE SEPARATION PROCESSES AND MATERIALS

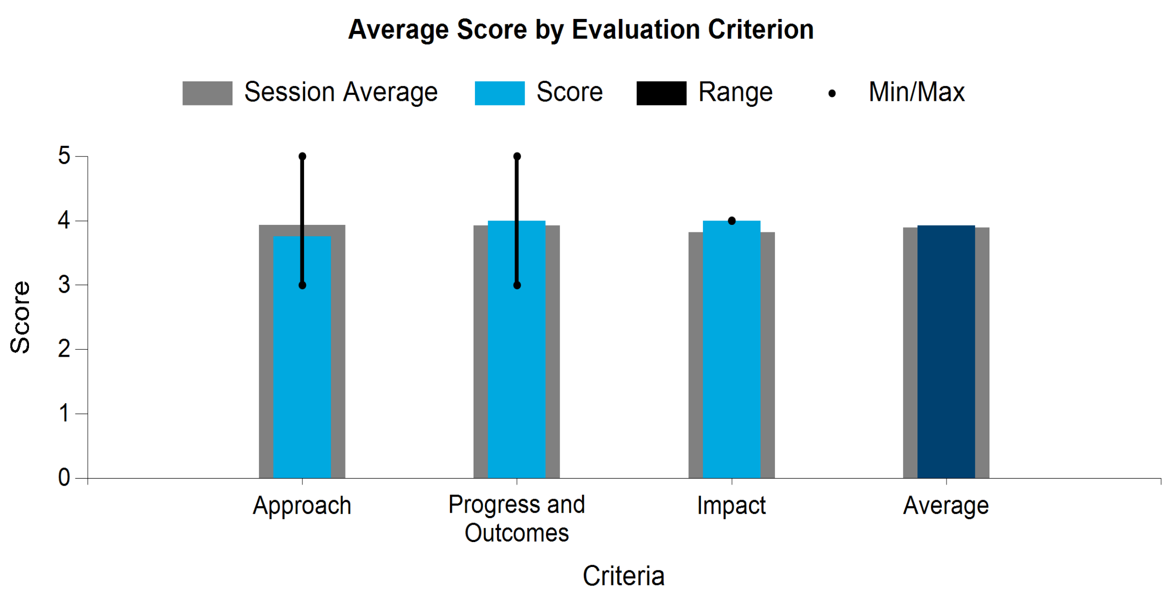
Separations Consortium

WBS:	SEP2.2
Presenter(s):	Meltem Urgun Demirtas
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$385,000

PROJECT DESCRIPTION

Membranes can reduce the energy, carbon, and space intensity of traditional separation processes (i.e., distillation and other thermal-based processes) for organic solvents. Specifically, organic solvent nanofiltration (OSN) and organic solvent reverse osmosis (OSRO) are pressure-driven technologies that require less energy than a phase change; however, owing to similar chemistries and properties among commercially available nanofiltration and reverse osmosis membranes (the majority of which are designed for aqueous-based separations), these thin-film composite membranes are highly susceptible to organic solvent degradation, limited permeance of hydrocarbons, and operational problems, including fouling. This task will focus on simultaneous membrane material and process development, targeting a TRL of 4, for OSN/OSRO. Industry input highlighted the need for high-flux membranes with sharp separation cutoffs. At the same time, manufacturing methods must be based on scalable synthesis reactions. In addition to the characterization of commercially available and surface-modified membrane materials, this task will address gaps related to process engineering and scale-up, with the overall goal of transitioning membrane technology into more challenging separation environments.

By project end, this task will demonstrate scalable membrane surface modification techniques and evaluate membrane performance at the pilot scale. Argonne National Laboratory's roll-to-roll facility will be used to scale up the surface-modified membranes. The membranes will be evaluated in a pilot-scale (140 cm^2) membrane unit using real bio-oil and biocrude samples.



COMMENTS

- There has been great progress in this review period. The project is on track. The team engaged membrane manufacturers, technology developers, and end users; integrated TEA and LCA; and demonstrated scalable surface modification techniques using Argonne's roll-to-roll facility. The coating of parts was not clearly described in the presentation. There was a clear plan on DEI initiatives. The team should continue to work with their industry partners, especially on the TEA and LCA sections at the beginning of their journey.

- The team met with a number of relevant companies to refine the scope of the project—this is great. There is a very strong DEI component for the project, including a diverse team, outreach activities, two interns/years from underrepresented groups, preferred vendor and procurement from disadvantaged-owned businesses, and Bridge to Career program participation. The project is just getting underway but holds promise in replacing high-energy distillation with OSN/OSRO. Current challenges are the lack of material strength and performance stability and fouling. The project leaders intend to improve these issues with surface modifications of the membranes for performance and durability. The team has already acquired commercial membranes, set up bench-testing units, and discussed LCA/TEA pathways with the analysis team. The method has the potential to make an impact in bioprocessing separation.

- This early-stage project has a valid technical approach to solve complex separation problems with an innovative plan. It was not clear where the new membrane technologies will be targeted and how that targeting should inform the overall technical effort. The risks associated with scale-up and operability seem to be addressed, but without better target information, it is difficult to assess the mitigation strategy. The project seems to be more focused on membrane fabrication than on the separation problem, which may reflect the TRL of the project more than the technical approach. The project's starting TRL is listed as 3, with a target of advancing the TRL to 4. It appears that the starting TRL may be earlier. It is critical to have an accurate TRL in order to assess progress.

- The team could reach out to Via Separations (https://viaseparations.com/technology/), a membrane-based startup out of the Massachusetts Institute of Technology that has done extensive research into what industrial streams exist and are currently not separated by membranes. I would encourage the team to test the stability of their novel systems at the temperatures at which they will run in the industrial system. A lot of polymeric-based membranes fail at these elevated temperatures and have limited operating lifetimes. If possible, I would suggest that the team build a model where potential partners with separation problems can see which one of the team's membranes would be useful.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for taking the time to review our work. We appreciate their supportive comments on our DEI and industry engagement efforts. We greatly appreciate this recognition and encouragement of our technical plan, as well as the recommendation of the separation membrane company, Via Separations. To clarify, the focus of this project is to address both membrane material development and process engineering innovations. By addressing both aspects simultaneously, we aim to achieve synergistic improvements that can lead to enhanced performance, efficiency, and cost-effectiveness. As acknowledged by the reviewers, this is a very early-stage project. Initial efforts in Year 1 are focused on conducting experiments to evaluate the SOA in OSN applications. This systematic assessment, along with a literature review, will identify the challenges, research gaps, and potential solutions for organic solvent separation using existing commercial membranes, and it will guide the team's selection of the best technical solutions for modifying and/or functionalizing the commercially available membranes to enhance their performance. Meanwhile, the team will also explore emerging alternative membrane materials and designs that can surpass the commercial membranes. For example, a membrane with an ultrathin hydrophobic polyamide skin layer will achieve significantly higher permeance and selectivity. Regarding the targeted applications, we have reached out to industry to identify specific applications where membrane technologies can provide significant benefits. We identified OSN as a result of this industry outreach. We are actively working to characterize the SOA membrane materials and will continue to engage with industry experts as performance results become available to further narrow the specific application within the biorefinery. We also recognize that different applications may have unique requirements, including operating temperature. Our current membrane test cell can be operated up to 121°C, so our team is prepared to conduct experiments at elevated temperatures if needed. In addition, the team has experience in fabricating polymeric materials that can withstand higher operation temperatures (e.g., up to 300°C). We will leverage this knowledge for our customized membrane development within this project.

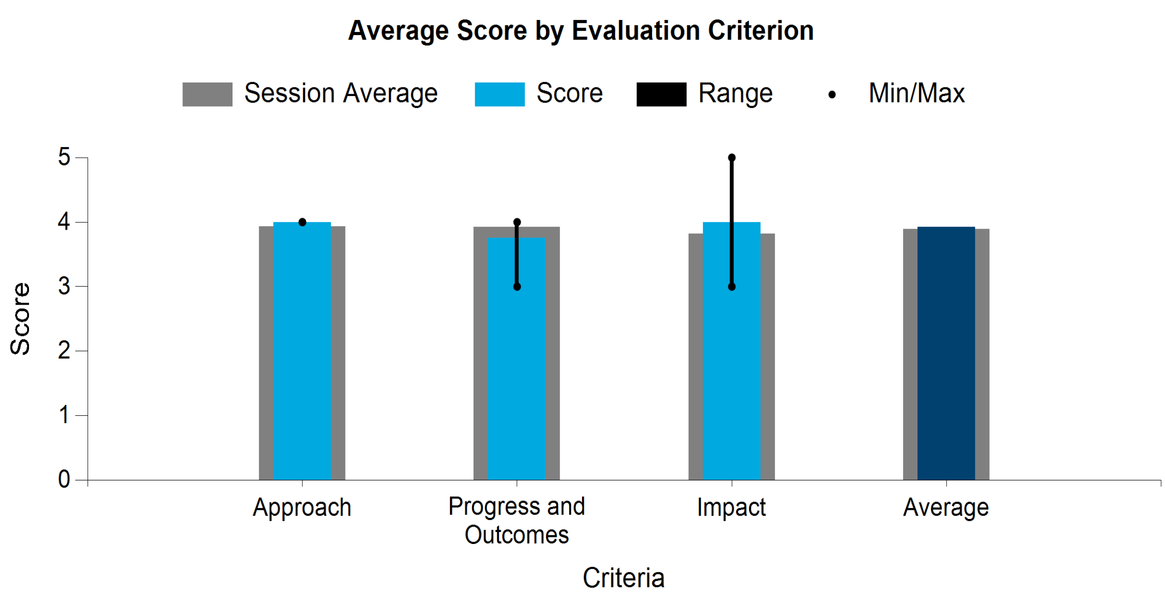
CONTINUOUS COUNTER CURRENT CHROMATOGRAPHY

Separations Consortium

WBS:	SEP2.3
Presenter(s):	Gregg Beckham
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$650,000

PROJECT DESCRIPTION

This task in the Separations Consortium focuses on the development of CCC, which is an advanced liquid-liquid chromatography method. Today, CCC is primarily practiced in batch mode operation, but continuous operation will be required for at-scale deployment in a biorefinery setting. In this task, we are developing a continuous CCC process in collaboration with a company that builds CCC units. This work will be demonstrated on the biorefining challenge of lignin valorization. Specifically, we demonstrate the use of continuous CCC for both monomer-monomer and monomer-oligomer separations in multiple lignin streams of relevance to the biorefining industry. Breakthroughs in this area would be useful for BETO goals in both SAF and biochemicals production, including directly contributing to BETO's 2030 lignin valorization goal. Our approach includes developing new computational modeling approaches to optimize both batch and continuous CCC processes, conducting experimental work to determine optimal solvent systems for multiple lignin streams sourced from BETO-funded projects and industry collaborators, and using TEA and LCA to identify the most impactful areas to ultimately enable this approach in the biorefinery. This task overall will enable high-resolution, multicomponent, continuous separations at scale, demonstrated on a grand challenge biorefining problem.



COMMENTS

- The team focused on lignin monomer-monomer and monomer-oligomer separations with continuous CCC up to the kilogram scale. There has been some progress in this review period. The project is on track. There is great collaboration among NREL, Dynamic Extractions, and Lignolix. I am not sure that this continuous CCC has the potential to create wider and more significant impact. The team should seriously think about feasibility and scalability. The PI needs to develop a DEI strategy and show the progress in the next review period or at the end of the project.

- It is early in the project—the project was initiated October 2022. There is a good DEI plan with five undergraduate internships (hopefully some going to underrepresented groups) and participation in Separations Consortium DEI activities. The risk mitigation plan is good for the project, including hiring a technician for CCC maintenance (keep an eye out for ways to reduce processing maintenance for scale equipment). There is a solid technical approach and risk mitigation. Progress has been made in identifying lignin streams for testing, computational modeling for process optimization, and defining solvents for extractions. Thus far, predictions from the model match experimental profiles. The team is working closely with an industry partner that is interested in enabling continuous CCC, which will increase the odds for eventual commercialization.

- This is an early-stage project that, if successful, could provide access to a broad range of new molecules useful for either fuel or chemical product applications. The project approach is sound and makes good use of computational methods to reduce risk and facilitate more rapid development. Although there is a good strategy to identify and mitigate risks, the risks associated with scale-up may not be adequately captured. For early-stage projects such as this one, I think that articulating the vision for success through commercial deployment has value, even if it can only be conceptual at this stage of the technology development. In this case, there has been a great deal of progress on the basic separation, but a clear statement of what this process might look like at a full-scale biorefinery would have value for understanding and assessing the approach. The project shows good collaboration with both lab and industry partners.

- I appreciate that the team is collaborating with Dynamic Extractions to develop a continuous CCC process. I appreciate that the team is using real-world lignin oils from its partnering BETO projects.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer feedback. All project teams within the consortium are engaging in the following DEI activities: (1) including individuals from underrepresented groups in STEM as researchers, (2) leveraging ongoing programs at each national laboratory to provide student internships, and (3) participating in diversity-focused education and outreach programs. The project team will join researchers and educators from across the consortium laboratories to educate and support the next generation of bioenergy students and researchers through the Bioenergy Bridge to Career Program. This DEI plan was presented by the Separations Consortium PI on behalf of the entire consortium in the overview presentation. In terms of the feasibility of CCC, we stress that this is an early-stage technology, as was mentioned in the presentation. For a frame of reference, a similar method to CCC, centrifugal partitioning chromatography, is now being scaled industrially (but it typically delivers lower product yields and purities than CCC, which is why we are not using that approach). In line with the high-risk, high-reward R&D that is currently at low TRL, to our knowledge, no other separation method available today enables facile separations of multiple target compounds outside of hydrocarbon separations through distillation, which is not appropriate for most biomolecules due to their high oxygen content. A similar reviewer comment was made that the “risks associated with scale-up may not be adequately captured”—this is one of the main reasons we are working with an industry partner through a CRADA on this project. This ensures that we have a direct line of sight to scale up for CCC when we are able to make the system continuous in nature. We will also soon publish a detailed process model of CCC integrated into a full-scale biorefinery to show a clearer picture of how this could fit into an overall process.

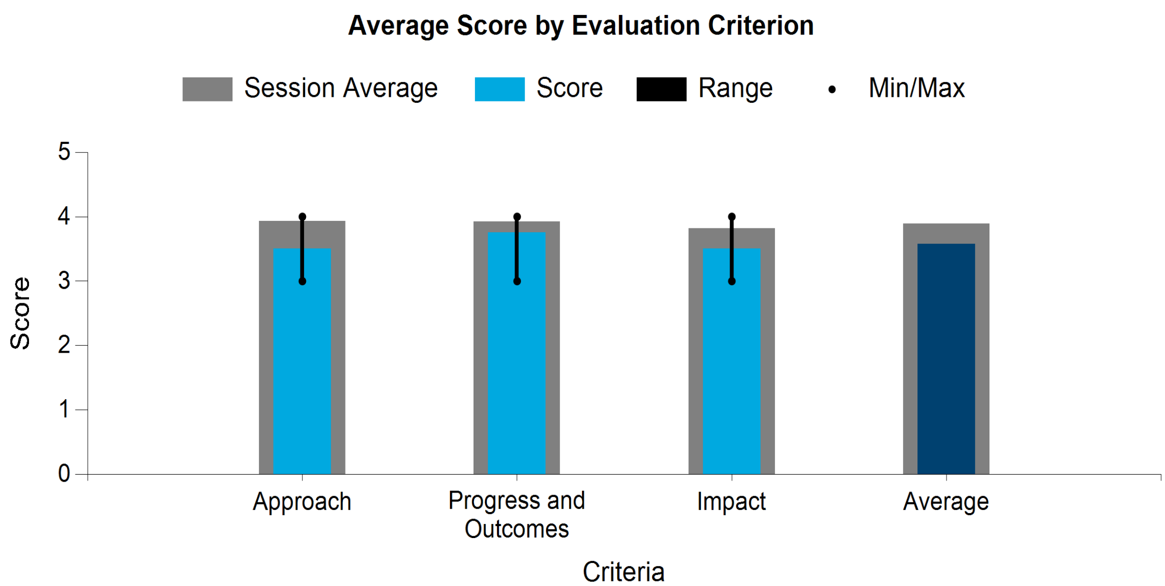
DIOL SEPARATIONS

Separations Consortium

WBS:	SEP2.4
Presenter(s):	Ramesh Bhave; Syed Islam
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$400,000

PROJECT DESCRIPTION

2,3-butanediol (BDO) is gaining attention in the global market as an intermediate product for several applications, such as liquid fuel. It can be produced through fermentation in low concentrations (<10 wt %). A common commercial separation/concentration technology for BDO involves evaporation and multistage distillation, both of which are energy-intensive. The goal of this work is to develop low-cost and energy-efficient separation technologies—supported by TEA, LCA, and computational modeling—to recover BDO from fermentation broth. To achieve this goal, we are developing a membrane-assisted liquid-liquid extraction-based process to separate BDO from fermentation broth. The membrane contactor provides a high surface area for intimate interfacial contact of the aqueous and organic phases. It is a single-step continuous process. Its modular design allows for linear scale-up. Further, it offers several other advantages, including low chemical usage, low waste generation, low energy consumption, and low capital and operating cost. Moreover, it prevents emulsion formation. Organic solvent oleyl alcohol and 1-Hexanol have been identified as the potential solvents to extract BDO with a yield of >95% from an aqueous stream. A porous hydrophobic membrane was selected based on pore size, wettability, and chemical compatibility. Preliminary data showed that the membrane contactor can separate BDO from an aqueous solution using hexanol in a continuous mode of operation.



COMMENTS

- The team explored three new approaches prior to selecting an approach for experimental development. The project is on track, and it seems that the team successfully changed their direction. Quantum and classical mechanics will help the screening and identification of proper solvent candidates. The team identified porous hydrophobic polypropylene hollow fibers as a membrane contactor to separate BDO from aqueous media using hexanol. The PI did not present their DEI strategy and progress.

- No DEI plan was provided. The project aims to separate BDO from fermentation broth with high efficiency and low energy impact. The project started in October 2022, so it is very early. The project has successfully changed direction in response to previous reviewer comments. The risks of general BDO separations were outlined, but risks and mitigation plans for the new process were not specifically outlined in the presentation. The team has achieved progress in identifying two potential solvents, hexanol and oleyl alcohol, through modeling. Are other solvent candidates being considered? It was unclear how the team settled on those two solvents. PP hollow fibers were selected as the microporous membrane, but I am wondering if polyvinylidene difluoride (PVDF) fibers should also be tried because of their increased chemical resistance and thermal stability. The project is on target to achieve its goals. The team should increase their engagement with industry partners within the next year.

- This project has made significant progress since the change in approach developed after the last Project Peer Review. The redirection and improved focus have resulted in what appears to be an initial demonstration of a practical, cost-effective means of separating 2,3-BDO from a dilute fermentation broth mixture, a technical problem that has resisted solution. Validation by an industry partner would improve the impact of the project and better demonstrate that the technical achievements illustrated to date have merit. The technology appears to have a valid pathway to scale-up and makes good use of computational methods to mitigate risk and speed up the development cycle in the solvent selection. More work needs to be done on the solvent recovery portion of the project, but the technical risks associated with that element of the project are low.

- I appreciate that the team is realizing the suggestions from the computational team to use hexane for the separations. It is always great to see computational models making suggestions that can have a real-world impact. The team should work closely with feedstock partners and offtake partners to ensure that their approach is relevant to industry, and they should check their assumptions in the TEA/LCA.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The team explored three new approaches prior to selecting an approach for experimental development. The project is on track, and it seems that the team successfully changed their direction. Quantum and classical mechanics will help the screening and identification of proper solvent candidates. The team identified porous hydrophobic polypropylene hollow fibers as a membrane contactor to separate BDO from aqueous media using hexanol. The PI did not present their DEI strategy and progress.

- Response: The PIs thank the reviewer for the positive comments on the technical achievement. Regarding DEI, the consortium is supporting future workforce development in the bioenergy technology field by hosting the Bioenergy Bridge to Career Program. Researchers from across the consortium laboratories, including this project team, will participate in educating the next generation of bioenergy students and researchers. This was presented in the overview presentation for the entire Separations Consortium. We also strive to include individuals from underrepresented groups in our research team and provide student internships. To that end, we have made an offer for a postdoctoral research associate position to a woman scientist to promote the diversity and inclusion of underrepresented groups in STEM. Additionally, we are planning to host an intern from a local community college (e.g., Pellissippi State Community College).

- Comments: No DEI plan was provided. The project aims to separate BDO from fermentation broth with high efficiency and low energy impact. The project started in October 2022, so it is very early. The project has successfully changed direction in response to previous reviewer comments. The risks of general BDO separations were outlined, but risks and mitigation plans for the new process were not specifically outlined in the presentation. The team has achieved progress in identifying two potential solvents, hexanol and oleyl alcohol, through modeling. Are other solvent candidates being considered? It was unclear how the team settled on those two solvents. PP hollow fibers were selected as the microporous membrane, but I am wondering if polyvinylidene difluoride (PVDF) fibers should also be tried because of their increased chemical resistance and thermal stability. The project is on target to achieve its goals. The team should increase their engagement with industry partners within the next year.

- Response: The PIs thank the reviewer for the positive comments on the technical achievement. In terms of risk mitigation: One of the risks of the proposed process is the identification of a hollow fiber contactor with appropriate properties, such as wettability and pore size. We have successfully identified porous polypropylene hollow fibers. The preliminary results showed that the membrane contactor can bring the aqueous and the organic phase together without emulsion formation. After establishing the proof of concept, we plan to investigate the long-term performance process in a continuous mode of operation. Regarding solvent selection: Based on our preliminary investigation from molecular dynamic simulations and basic properties of organic solvents reported in the literature, we have identified two solvents; however, we plan to investigate other solvents with the support of molecular dynamic simulations. Regarding the hollow fiber selection, we have past experience in porous PP hollow fibers, as they have small pore size with high surface area, have hydrophobicity, and are relatively inexpensive. The PIs thank the reviewer for suggesting PVDF hollow fibers. We plan to identify and evaluate PVDF hollow fibers with comparable properties to PP as we progress with the project, especially processing real-life fermentation broth. After establishing the proof of concept in the first year of the project, we think it will be more appropriate to engage with industry partners.

- Comments: This project has made significant progress since the change in approach developed after the last Project Peer Review. The redirection and improved focus have resulted in what appears to be an initial demonstration of a practical, cost-effective means of separating 2,3-BDO from a dilute fermentation broth mixture, a technical problem that has resisted solution. Validation by an industry partner would improve the impact of the project and better demonstrate that the technical achievements illustrated to date have merit. The technology appears to have a valid pathway to scale-up and makes good use of computational methods to mitigate risk and speed up the development cycle in the solvent selection. More work needs to be done on the solvent recovery portion of the project, but the technical risks associated with that element of the project are low.

- Response: The PIs thank the reviewer for the positive comments. We will work on the solvent recovery process with the support of the computational team. The TEA/LCA work is in progress to evaluate the trade-offs for using hexanol versus oleyl alcohol. The computational team uses an ML approach and molecular dynamics simulation to identify organic solvent that has high affinity toward BDO. Previously, the computational team investigated the effectiveness of hexanol. Currently, the team is running a molecular dynamics simulation on oleyl alcohol as the organic solvent based on the thermodynamic properties, including BDO solubility and free energy. Lawrence Berkeley National Laboratory also performed a wiped film evaporation with hexanol and BDO and successfully recovered the hexanol. They plan to perform a wiped film evaporation for the separation of BDO from oleyl alcohol.

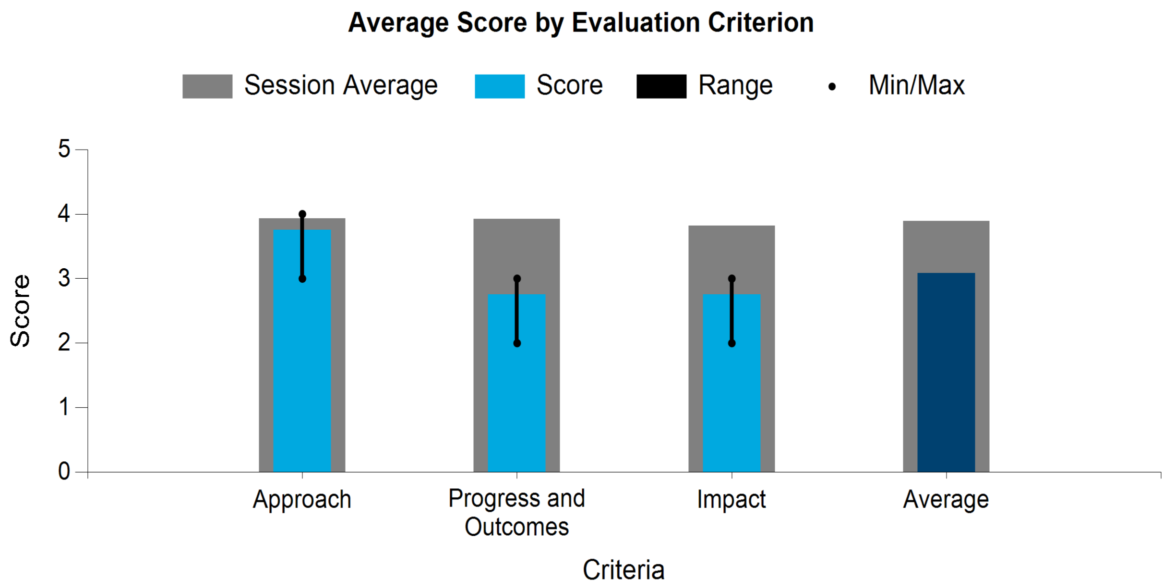
- Comments: I appreciate that the team is realizing the suggestions from the computational team to use hexane for the separations. It is always great to see computational models making suggestions that can have a real-world impact. The team should work closely with feedstock partners and offtake partners to ensure that their approach is relevant to industry, and they should check their assumptions in the TEA/LCA.

- Response: The PIs thank the reviewer for the positive comments. We plan to work with feedstock partners and offtake partners. Our team members have experience working with feedstock producers. We intend to work with more closely with these partners as the project progresses.

ELECTROCHEMICAL SEPARATION TECHNOLOGIES TO EXTRACT INTERMEDIATE ORGANIC COMPOUNDS

Separations Consortium

WBS:	SEP2.5
Presenter(s):	Yupo Lin
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$400,000



COMMENTS

- The project is on track. The team is trying to separate and recover medium-chain carboxylic acids from bioconversion streams for SAF and/or biochemical production using electrochemical separations. The previous and planned DEI activities look good. The team should address the main challenges (cost, process efficiency and selectivity, and the complexity of short- and medium-chain carboxyclic acids (SCCA and MCCA, respectively)) with electrochemical separation technologies. Is the process powered by renewable energy?

- It is very early in the project—the kickoff was in October 2022. The project has one of the strongest DEI plans, with four undergraduate interns, a separation activity for grade seven, participation in "Introduce a Girl to Engineering Day," and participation in Science Careers in Search of Women. Kudos for this! The project aims to design, fabricate, and operate a scalable shock wave electrolysis stack and scale a capacitive deionization system (by 10 times) to recover medium-chain carboxyclic acids from bioconversion streams. There are advantages to the electrochemical separation technique, including reduced fouling and resistance and lower GHG and use of water. Progress to date includes a shock wave electrolysis stack that has been successfully operated. Reversible electrosorption using capacitive deionization has also been demonstrated. The technology could be important in eliminating the fouling and transport resistance that is experienced with other membranes, with lower environmental impact.

There are good partnerships set up with the Agile BioFoundry and the industrial company Visolis to ensure the success of the project.

- This project would greatly benefit from some conceptual engineering to better illustrate a vision for how this technology could be deployed at scale. The pathway for commercialization is very unclear, and without some techno-economic guidance, the benefits of the approach are not clear. If we assume that the vision has been developed and the preliminary costs are defined, the approach appears to be valid and well thought out. The project is organized and well managed and shows good collaborative efforts across the labs. The project milestone states that the intent is to develop a “game-changing” technology for separations that, if successful, would have a tremendous impact on the bioproducts industry. The articulated risks are incomplete given the nascent state of development for this process and should be expanded, along with a more complete description of the mitigation strategy.

- The team is planning to do its TEA in the third year of the project. I would suggest that the team test the economic and environmental viability of the technology as soon as possible. This is a very early project, and the team is currently running their experiments with a potassium chloride salt solution. I would love to see this system use a more application-relevant feed stream to reach the goal of using real bioprocessing streams in the timeline of this project. To this end, the team should work with industry partners to source feed streams and enter into conversations with industry partners on the offtaker side. I believe that the self-assessment of TRL 3 at the project start is too high when the team is still using a model stream (potassium chloride salt solution) at bench scale.

PI RESPONSE TO REVIEWER COMMENTS

- We sincerely thank the reviewers for their thoughtful reviews and positive feedback. We appreciate the recognition of our efforts related to DEI. This positive feedback validates our ongoing commitment to promoting an inclusive environment, driving innovation, and achieving long-term success. We recognize the importance of addressing cost considerations to ensure the feasibility and adoption of these technologies. Previous internal consortium analyses indicated that the economic feasibility of another electrochemical technology (resin wafer electrodeionization) is comparable with that of other consortium technologies. As experimental performance results are generated in this task, we will feed these data into both techno-economic and sustainability analyses. We will explore potential scenarios in which electrochemical separations are powered by renewable energy to evaluate the cost and sustainability implications. Regarding process efficiency and selectivity, continuous R&D efforts are dedicated to refining these technologies to achieve higher efficiency and selectivity in the electrochemical separation processes. The progressive separation efficiency targets are listed in each milestone as measurement metrics. We fully understand the significance of conceptual engineering in providing a vision for the deployment of electrochemical separation technologies at scale. Although these are early-stage technologies, as mentioned during the presentation, slide 3 illustrates the biorefinery block flow diagram. We will work to develop a more detailed process flow diagram illustrating the key steps, equipment, and material flows involved in the electrochemical separation processes. The process flow diagram will serve as the basis for TEA to provide insights into the commercial viability of these technologies. Engaging with our industry partner, a potential end user, will help validate the technology’s value proposition and guide a potential commercialization strategy. Regarding the risks, shock wave electrolysis has been technically demonstrated by Martin Bazan’s group at the Massachusetts Institute of Technology, resulting in more than a dozen published articles for water desalination applications. Similarly, capacitive deionization is used at the industrial scale for water treatment but has not been demonstrated for biorefinery applications outside of the consortium. As noted in the Consortium Overview and Analysis task presentation, TEA and LCA are integrated throughout the R&D cycle to identify potential challenges and uncertainties. We agree with the reviewers that it is important to work with process-relevant streams; however, as these technologies are at an early stage, we are using synthetic mock solutions to provide initial insights into separation mechanisms, helping us understand the underlying science and optimize the technologies. As the work progresses, we will use mock solutions of increasing complexity and real-world process streams in our separation experiments.

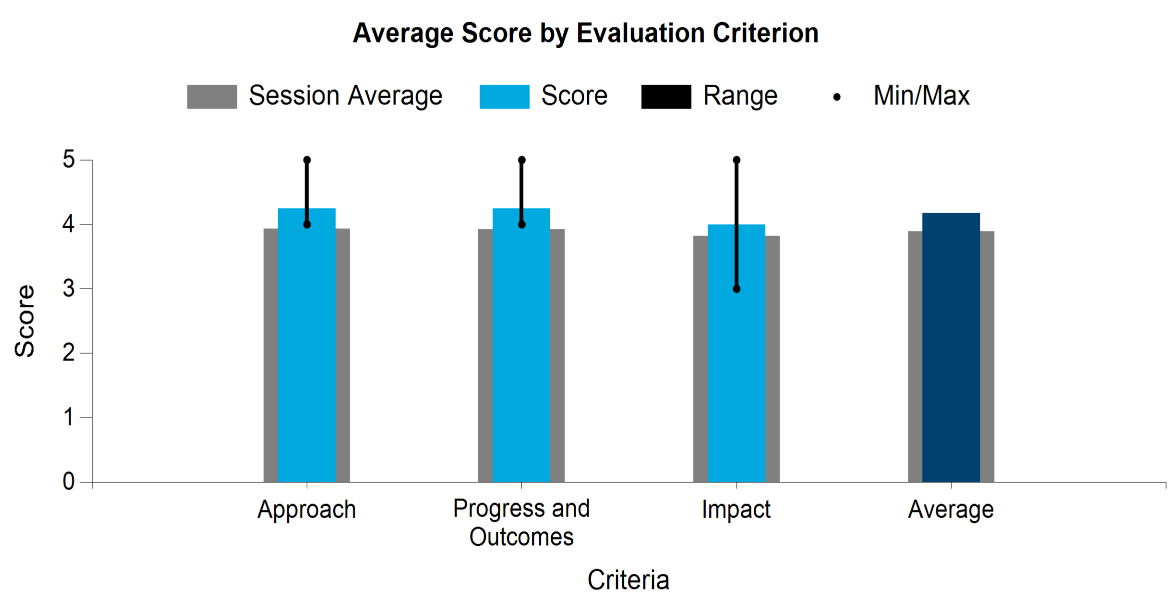
ENABLING SAF PRODUCTION BY ADSORPTIVE DENITROGENATION

Separations Consortium

WBS:	SEP2.6
Presenter(s):	Daniel Santosa
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$400,000

PROJECT DESCRIPTION

Hydrothermal liquefaction (HTL) of biocrude from wet waste biomass such as algae, manure, food, and sewage sludge inherently contains high amounts of nitrogen due to the starting protein content. Thus, nitrogen in hydrotreated biocrude includes a large variety of nitrogenated compounds, such as amides and amines, but also non-basic and more refractory indoles that require removal to achieve a <2-parts-per-million nitrogen level. This is a critical step to obtain ASTM approval of the wet waste HTL pathway for producing SAF. The HTL pathway can produce 3.9 billion gallons/year of SAF (>20% of the U.S. aviation demand in 2019) from wet wastes while reducing GHG emissions by >70% at a projected selling price of $3.15/gallon gasoline equivalent (2022); however, the current nitrogen removal method requires a severe hydrotreating step and consequently harsher operating conditions (increased temperature and pressure and/or lower space velocity) with increased H_2 requirements. This results in yield losses from undesired hydrocarbon cracking, and not many refiners have this capability. Alternatively, adsorbent development can be tailored for high selectivity toward small and refractory nitrogen molecules in complex biomass-derived liquids, coupled with regenerability and minimal yield loss. This technology is projected to be cost-competitive with the current SOA hydrotreating. In addition, this process requires no H_2 input and can improve the sustainability of refinery processes that adopt an HTL pathway. In this work, we will demonstrate an engineered sorbent system with tailored pore size, specific surface area, and selectivity targeted for high affinity and capacity for the sorption of target nitrogen molecules in a surrogate jet fuel, resulting in <2-parts-per-million nitrogen fuel. Future work will also demonstrate the selective adsorption of nitrogen-containing species from hydrotreated biocrude as well as minimal yield loss by continuous regeneration and lower carbon intensity due to lower hydrogen consumption.



COMMENTS

- The project is on track. There is huge potential to utilize 76 million tons/year of wet waste in the United States for conversion to ~400 thousand barrels per day SAF (~25% U.S. jet fuel demand). Are there any requirement(s) or limitation(s) for the incoming materials (wet waste) to optimize value from other HTL streams? TEA/LCA of an additional purification step using this method is critical. The PI needs to develop a DEI strategy and show the progress in the next review period or at the end of the project.

- The project started in October 2022, so it is in the very early stages. The DEI plan is multifaceted and includes three outreach activities, one student intern, and participation in Bioenergy to Bridge Program. The team has consulted with refineries to understand their concerns with adsorptive denitrogenation and gain their support, increasing the chances of project success. A good amount of data generated shows that Amberlyst resins have potential. The team is on track to down-select the most promising adsorbent materials. In summary, this is a solid project to remove nitrogen in HTL to produce lower-impact SAF.

- This is an impactful project that has shown significant potential to improve the manufacturability of SAFs in an industrially practical manner, with low energy inputs and a readily available adsorbent system that is scalable. A potential future technical challenge relates to the variability of wet waste and the impact of that variability on the separation technology employed here. Additionally, the successful use of a model biocrude, while valuable, could lead to underestimating the technical risk associated with a real-world stream that is variable. The state of the interaction with industry partners was also hard to ascertain. Some are listed on the collaboration slide, but their contributions and how they may be involved in the projects was not transparent from the presentation. Overall, the project is organized and well managed with a well-described technical approach.

- I would suggest that the team start using real-world wet waste and increase the capacity of the hydrotreated biocrude so that they can run this on more realistic samples. I would like the team to work with an offtake partner to confirm that its final fuels meet SAF requirements.

PI RESPONSE TO REVIEWER COMMENTS

- First, we thank the reviewers for taking their time and providing their thoughtful and insightful comments. Regarding the requirement for HTL, the current work on wet waste pretreatment for HTL includes dewatering to 25% or 20% and grounding/different feedstock mixing to make the stream homogeneous for pumping. Experimental tests are being conducted to de-ash the feedstock to avoid the potential engineering challenges of dealing with solids in the continuous process, such as plugging, fouling, vibration, and mechanical stress on the equipment. We believe that no additional pretreatment steps are needed to control the nitrogen content or make the adsorption technology suitable for denitrogenation, provided that the adsorbent can work for high nitrogen content as handled by hydrotreating. Our initial screening shows that candidate adsorbents have been proven to be able to work with high nitrogen content (up to 2,000 parts per million) in our simulated feed. The TEA and LCA effort will focus on identifying the adsorbent system with both the lowest environmental impact and the lowest capital and operational expenses. As for the key efforts to address DEI, we thank the reviewers for emphasizing its importance. Our team is actively engaging in three different outreach activities, including participating in the Bioenergy Bridge to Career Program, onboarding one summer student intern from an underserved community, and hosting a full-day virtual workshop this summer with seminars, panel discussions with our team of scientists, and hands-on learning sessions in computer programming for bioenergy science. This is part of the consortium-wide plan for this program, which was presented in the overview presentation. We are also in full agreement with the reviewer on using real-world wet waste. Our initial aim is to continue using model biocrude solutions to isolate specific variables, control experimental conditions, and gain a deeper understanding of underlying adsorption mechanisms. Subsequently, in the near future, we will apply the understanding gained above to test adsorbents and developed regeneration methods with real SAF fractions from upgraded biocrude derived from food waste. We would also like to thank the reviewer for their emphasis of the importance of collaboration and the transparency of our partnerships. Our partnership with Oak Ridge National Laboratory is critical in developing a scalable process. Using their continuous flow system will enable us to generate real-world adsorbent performance data for commercial process scale-up. We would also like to clarify that our partnership with industry is through gathering their critical feedback. They are concerned with recalcitrant nitrogen species that will require a severe hydrotreating step, which requires high-pressure hydrogen and special unit operations that are limited to larger refineries. Thus, the research is aimed at addressing an alternative that will enable smaller refiners to meet fuel quality requirements. We thank the reviewers for their encouragement of working with an offtake partner to confirm that the final fuels from biocrude meet the SAF requirements. We will continue to explore strategic collaborations to maximize the real-world impact of our work; however, we would also like to emphasize that the consortium’s core strength is in technology development. This project, in addition to several other BETO-funded projects, has been collaborating with SAF analysis experts such as Joshua Heyne from Washington State University to conduct a two-tiered prescreening process to demonstrate the suitability of the upgraded biocrude for SAF requirements, providing solid groundwork for future approvals and larger-scale demonstrations.

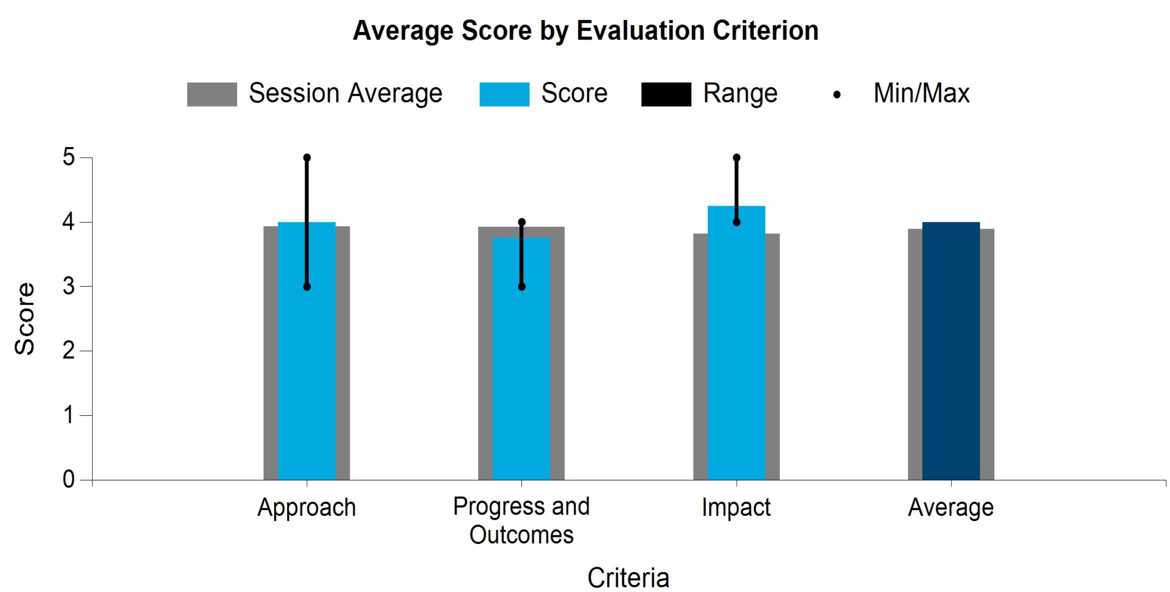
VOLATILE PRODUCTS RECOVERY

Separations Consortium

PROJECT DESCRIPTION

WBS:	SEP2.7
Presenter(s):	Phil Laible
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$650,000

Advances in strain engineering have enabled the biochemical production of a wide array of products. During aerobic fermentation, many of these molecules partition readily to the fermenter off-gas. Many of these are known to volatize fully during fermentation, while others volatilize less—but significantly—under typical conditions. This project utilizes advanced, high-surface-area materials for the recovery of volatile SAFs (and their precursors) by adsorption, with specificity achieved through tunable surface chemistries. This strategy thereby eliminates the energy-intensive steps (condensation/distillation) traditionally required to separate volatile organic products. Scaled adsorbent syntheses incorporating (1) macroporous structures capable of handling a high flow of fermentation off-gases while (2) retaining selective product recovery from bioreactors (= 10 liters) have been achieved. Performance with select volatile products has shown reproducible recoveries of ~85% of product from the vapor phase. Product is desorbed through compression with low energy forces (~20 psi, with materials reusable for >50 cycles). TEA and LCA demonstrate significant cost and environmental gains. Multiscale modeling enables mechanistic insights to optimize the recovery process for current and future products. Simple, inexpensive cartridge designs have facilitated successful, scaled validations—key metrics for industry stakeholders.



COMMENTS

- The project is on track. The team successfully demonstrated the use of xerogels (nanostructured adsorbents) with tunable surfaces in scalable, inexpensive capture cartridges to recover specific volatile products with little to no water. There was little or no info about xerogel chemistry. Scalability is a common challenge in structuring xerogels with specific structural profiles, such as mesoscale pores, high porosity, and high specific surface area. The team should integrate TEA for the scalability at the current stage. The previous and planned DEI activities look good.

- The team itself is diverse and has a very strong DEI plan in place to provide internships and learning experiences for DEI students. The development of vapor phase recovery will broaden the available products recovered from biorefining, so the project is important. The use of 3D printing to prototype cartridge geometry accelerates progress. There is good integration with the computational team and with other BETO projects so that specific volatile products can be retrieved, improving the overall success of the consortium. The industry collaboration looks really strong—there must be a lot of interest in recovering volatiles. The risks and mitigation strategies are clearly outlined. Milestones are on track. Are you thinking about ways to recycle or reuse the xerogel cartridges at EOL?
- This project has the potential to reduce the operating costs related to difficult bioproduct separations and has shown promise that good recoveries and purity can be obtained at a small scale. The project is well managed and appears to have good engagement with industry partners to meet the department's goals toward SAFs. The added complexity introduced by 3D printing does not seem to be adding significant value to the effort, and the scalability of that approach to meet the production volume goals for SAF does not seem to be well connected to the targets of the project. The overall research approach is rational, but a path toward scale-up is not clear. The project could benefit from a focus on the manufacturing of xerogel substrates, including surface modification, as well as the engineering requirements of the desorption step. The risk mitigation strategies for these scale-up issues could be strengthened.
- I appreciate that the team is actively collaborating with industry partners to use their capture technology within their systems to directly separate the volatile products of real reactions. I would like to see the team test their separations using real-world feedstocks and conditions, ideally in collaboration with their industry partners.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the review team for their interest in our technology, and we appreciate both their recognition of the success of our approach and their suggestions for future improvement. We agree that this project should be kept as industry-forward as possible, and we note that (1) it was originally born from discussions with industry across many levels, and (2) these discussions continue to inform our technical strategy. With regard to the concerns raised by the review team, we share an interest in demonstrating, via both modeling and experimental validation, that xerogel synthesis and use can be scaled beyond the bench scale. We have tested synthetic strategies for production and adsorbent gels with the capacity to recover several liters of product, and we have deliberately utilized approaches in these experiments that can easily be expanded to pilot scale and beyond. This data was used in scaled cost evaluations indicating that the xerogel off-gas strategy would be cost-competitive for the capture of commodity products, especially with the cycle resilience of the materials and their ability to be reused hundreds of times. We will focus more on these demonstrations in the future, including a goal of achieving pilot-scale adsorption at the Advanced Biofuels and Bioproducts Process Development Unit (ABPDU) by Quarter 4 of FY 2025. In addition, we have an FY 2023 Quarter 3 milestone that revolves around the engineering requirements of the desorption step. We concur with the review team that this unit operation is central to the long-term viability of the xerogel strategy and will become one of the most critical demonstrative requirements as the approach scales further in the future. Last, we have engaged with a variety of industry partners and are planning validation of this off-gas capture approach with a range of products and processes over the next 18 months. These industrial products will be screened utilizing bench-scale workflows within the Separations Consortium, with the most promising products spun out as independent demonstration projects.

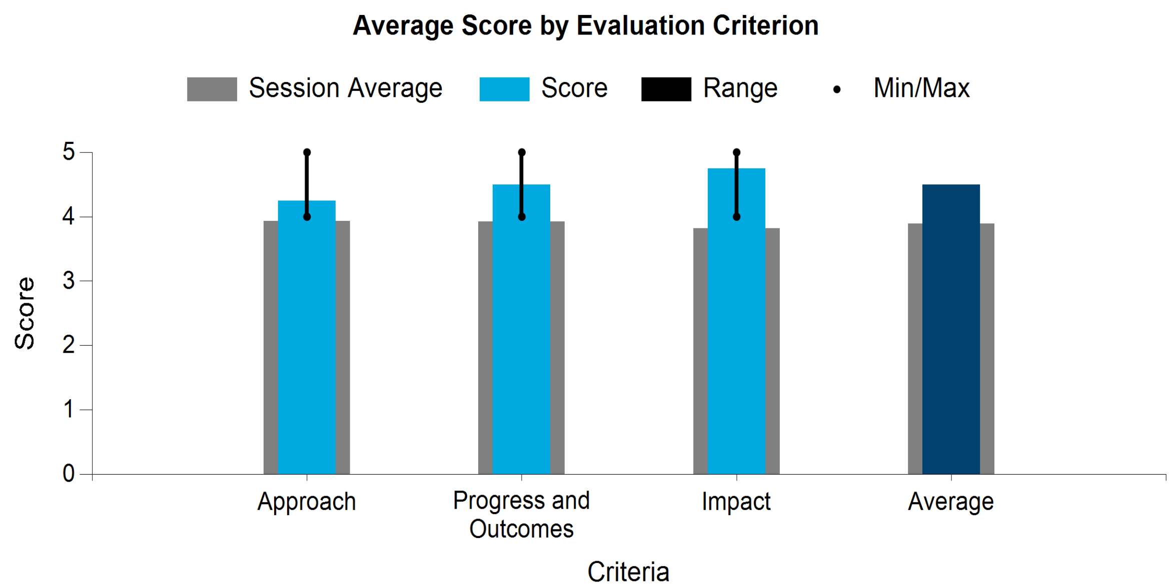
R&D-GUIDING TEA AND LCA

Separations Consortium

PROJECT DESCRIPTION

WBS:	SEP3.1
Presenter(s):	Jian Liu; Thathiana Benavides
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$825,000

TEA and LCA are used to guide and quantify the impacts of the Separations Consortium's R&D. The analysis team interfaces with experimental teams to illuminate the separation challenges that most influence the cost and environmental impacts of producing biofuels and bioproducts. This task quantifies the contributions to the cost and environmental footprint per fuel gallon equivalent or kilogram of product that these challenges are posing and compares them to defined baselines to assess the merits and drawbacks of the proposed technology. TEA is built on performance models developed in Aspen Plus and cost models in Excel using a discounted cash flow methodology. LCA uses biorefinery-level life cycle inventory data from the Aspen Plus models to determine sustainability impacts via calculations in the GREET model. During FY 2021 and FY 2022, the analysis team worked with the experimentalists addressing different challenges within the consortium and modeled the impacts of the various research efforts. Relative costs and sustainability outcomes were reviewed with the experimentalists. In this presentation, we describe the methodology around TEA/LCA for the Separations Consortium activities and present results for three different solutions of 2,3-BDO separations in support of the go/no-go milestone. A high-level challenge stream analysis was also conducted to identify separation challenges with high priority in the bioenergy processes and to reveal the maximum potential impact of using "ideal" separators.



COMMENTS

- The project is on track. The team collaborated with other BETO projects and industry partners. Understanding the trade-off between economic and environmental performance is crucial for sustainable practices, and integrating TEA and LCA is really important for evaluating emerging technologies at early TRLs. The team should be careful about any lack of consistent methodological guidelines, inconsistent system boundaries, limited data availability, and uncertainty for the integration of LCA and TEA. The team needs a clear plan on DEI initiatives.

- TEA and LCA were employed to assess and guide (recast) the BDO separations project and to optimize the research plan for the Separations Challenge project. Several significant project contributions resulted from the TEA/LCA, which highlighted cost and performance drivers for the processes. This is valuable feedback for the projects. Although this project functions as support to R&D, it provides critical guidance as projects progress to increase the likelihood of commercialization. Good and frequent communication between the LCA/TEA and experimental teams looks to be happening, which improves the progress and outcomes of all the projects. Milestones for BDO separation efficiency and the revised separation challenge streams were met. The DEI plan includes student internships, participation in the Bridge Program, and outreach activities.

- These analyses are essential to quantifying the technical merit of each project as well as ensuring that the outcomes satisfy the BETO strategy for technology development. It is apparent that these analyses are a key part of the other projects being reviewed and that the approach is widely adopted and considered a key element of the criteria for success for each project. The risks associated with performing these analyses at early stages of technology development are captured, and there appears to be a well-thought-out mitigation plan to address some risks. Additional risks to consider for these analyses are the fact that geography will often be a key driver for, e.g., energy costs or generation type, both of which will have a profound impact on the calculated cost and life cycle impact. The analyses were applied to great effect on the analysis of the 2,3-BDO separation process, which showed how the correct definition of the boundary conditions for the analysis drove the results. The impact greatly modified the approach applied to refining the development of the separation technology for that potentially valuable bioproduct.

- I appreciate how integrated the TEA/LCA work is in the go/no-go decisions for the rest of the projects. The example of how the TEA and LCA guided the development of the diol separations is a wonderful example of how to tie analysis into technology development. I think it would be helpful for the review to share the analysis team's milestones and timelines to better judge whether this team is on track as well. If the milestones are publication-based, for example, it would be great to share those numbers (goal versus actual) at the review.

PI RESPONSE TO REVIEWER COMMENTS

- "The team needs a clear plan for DEI initiatives": We thank the reviewer for this comment. Regarding the DEI initiative, we mentioned at the Project Peer Review that "we plan to participate in the Bioenergy Bridge to Career Program in FY 2023." We started working with the education programs at the different consortia labs to participate in the workforce development activities that will be conducted during summer 2023. This virtual workshop will occur every Friday starting July 14 and ending August 4. Among the activities we plan to participate in are selected topic webinars, panel discussions, and speed networking sessions, where we will interact with students from different backgrounds. Topics of discussion will include an introduction to the Bioprocessing Separations Consortium, bioenergy, LCA, and maximizing your digital and presence impact in social media, among others. Our team is also proud to have a strong representation of women, who have been traditionally underrepresented in STEM fields. This task has one female co-PI and supports a female postdoctoral researcher in her knowledge and skill development within bioenergy technologies.

- "I suggest the team include the impact of geography on the results of TEA and LCA": We agree with the reviewer regarding the point that regionalization will drive the results. Our current models are based on U.S. average costs, electricity grids, energy supplies, etc., and through our results, we can identify the key drivers of the cost and environmental metrics. We can vary parameters determined by the region, and this could be done by performing sensitivity analysis. In addition to sensitivity analysis, if necessary, TEA and LCA studies can also consider uncertainty characterization.

- "I suggest the team include milestones and a timeline for evaluation": We understand the reviewer's suggestion. Although economics and sustainability are strong considerations in the consortium's R&D, the consortium's deliverables to the project sponsor are primarily set based on the technical progress. As described in the overview presentation for the consortium, the analysis team worked closely with experimental researchers to develop internal analysis plans that align with the experiment timelines for all the tasks in the Separations Consortium at the beginning of the projects. We also track the TEA/LCA progress during biweekly meetings to ensure that the work is progressing toward our goals.

COMPUTATIONAL STUDIES SUPPORTING EXPERIMENTAL DESIGNS

Separations Consortium

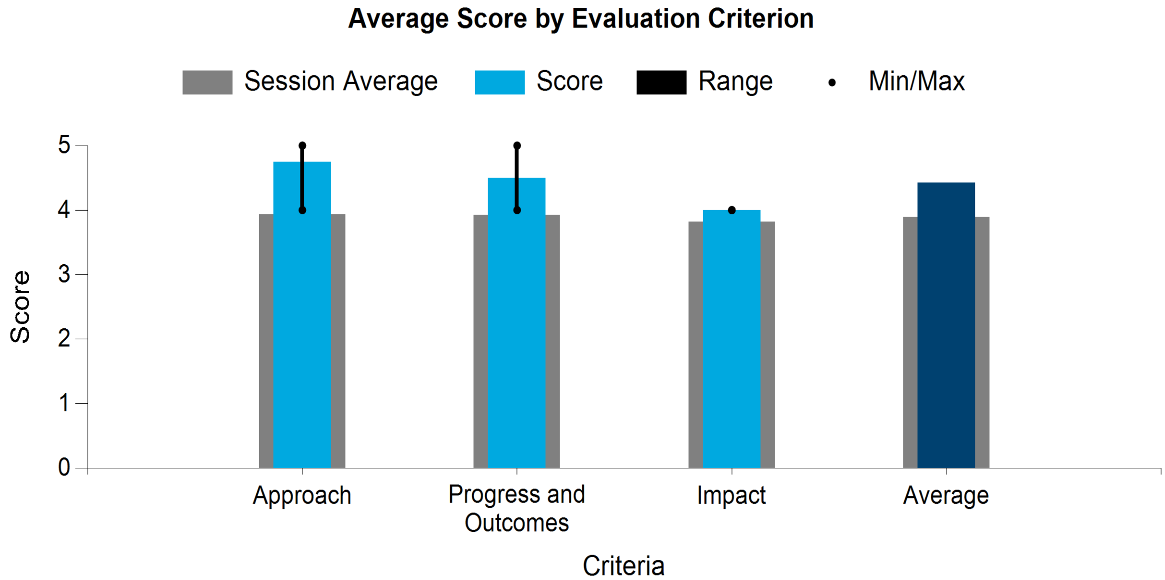
WBS:	SEP3.2
Presenter(s):	Difan Zhang
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$400,000

PROJECT DESCRIPTION

The separation of valuable compounds from complex biomass is hampered by high energy demands. Theoretical modeling and simulations can effectively accelerate the development of new materials and processes for efficient separation applications. Building on our collaborative work with the experimental consortium activities in FY 2020–FY 2022, we will combine atomistic-level modeling with data science tools to guide material selection and process optimization toward the design of novel separation technologies in collaboration with experimental teams.

The crosscutting computational task will interface with three experimental tasks to provide predictive guidance for down-selecting sorbent candidates and optimizing sorption processes. To achieve our goal, we will take input from our experimental partners on the specific separation task, including the target species; the desired properties of the sorbent materials; and other relevant information to establish the technology gaps that can be investigated by atomistic modeling. Atomistic-level modeling will be employed to characterize the sorbent/sorbate interactions and the key properties of sorbent materials corresponding to experimental conditions. Using these key properties as material features, we will apply high-throughput calculations to computationally screen candidate materials. Global optimization algorithms and ML technology will help accelerate our screening modeling. This screening will generate a list of potential material candidates tailored to target molecules and will inform fundamental insights into the governing factors in promising candidates. This knowledge will help the experimental teams narrow material candidates without needing to explore a wide experimental space, which is time-consuming and costly. In addition, TEA/LCA domain knowledge can be considered to further enhance our screening results by introducing more constraints in materials selection. On the other hand, our modeling results can refine the chemistry-guided parameters needed for TEA/LCA modeling.

The following specific tasks will be performed in collaboration with experiments: (1) computational screening of sorbent materials to understand the controlling factors of sorbents for deep nitrogen removal in experiments and to expedite the development of adsorption-based denitrogenation processes; (2) identification of new target volatile compounds and suitable functional groups in xerogels via computational modeling for the efficient capture of volatile compounds from off-gas streams; and (3) development of suitable solvent and membrane systems by computational modeling for large-scale 2,3-BDO separation from fermentation broth. We have identified three major challenges across these three tasks: the lack of high-quality data for complex sorbent systems, the trade-off between time cost and fidelity in the computational modeling of the bio-separation process, and the deficiency of fundamental knowledge for new technologies being developed in experimental teams. To address these challenges, we will carry out key molecular calculations and simulations as needed to fill the gap in data availability. To balance the trade-off between high accuracy and low cost, we will apply AI as the "last mile" tool to bridge the molecular modeling and experimental measurements. We will also pursue extensive collaborations with other BETO projects as well as industry partners to develop more fundamental knowledge about novel bio-separation technologies. By the end of the project, we will develop predictive modeling that expedites the search of solvent candidates for the solvent extraction of 2,3-BDO. Such methodology will be transferable to solvent solubility prediction in a wide range of industrial/BETO interests. We will also develop a molecular database to identify promising surface functional groups in resins for the efficient removal of both basic and non-basic nitrogen-containing compounds. Further, we will explore new research opportunities for functionalized xerogels to capture volatile compounds and guide the experimental synthesis of new xerogel materials. We expect that our computational modeling will offer guidance to expedite the advance of novel materials and processes in bio-separation. Theoretical tools will be made publicly available to interrogate bio-separation-relevant questions (e.g., solubility prediction for bio-separation process) and will pioneer new techniques for materials/processes in the decarbonization of transportation or industry. We will also disseminate our accomplishments in high-impact journals.



COMMENTS

- The project is on track. The team used the computational task to strategize and accelerate material/process discovery and design in bio-separation processes for three experimental tasks. A practical application of the computational screening/ML approach requires real-world case studies with sufficient data, which may be challenging for researchers; however, it could be a useful tool for the Performance-Advantaged Bioproducts and Bioprocessing Separations-related applications. Other than finding proper solvents, sorbents, and advanced materials with tailored surface groups, can we use ML to fill the data gaps of LCA? The PI did not present their DEI strategy and progress.

- This project is very new, kicking off in October 2022. The project will use computational modeling and AI to guide three projects and expedite the advances of materials and processes in bio-separations. The DEI plan includes topic development and the Bioenergy Bridge to Career internship. The team has already made progress in isolating promising solvent candidates for BDO extraction. In addition, the team has found that the Amberlyst resin could be a promising sorbate for denitrogenation and that long-chain alkyls on xerogels could provide better separation for limonene and isoprenol. These findings should help guide the experimental teams to accelerate their success.

- The project is a good example of how applied computational methods can reduce risk and increase the speed of the development cycle by providing better targeting and better fundamental understanding to improve the overall technical quality of multiple projects. In this case, applying these methods to solve problems in diol separation and adsorptive denitrogenation is particularly well thought out and impactful. The project efforts appear to have substantially advanced the SOA in both of those projects. The collaborative nature of this work is evident in the results. This work cannot proceed without excellent collaboration and work across diverse project teams. Excellent progress has been made, and a means of translating the successes of this effort to other projects should be developed and implemented to further advance both this project and the collaborative projects.

- I appreciate that the team is collaborating with the teams of Task 2.4 (Diol Separations), Task 2.6 (Enabling SAF Production by Adsorptive Denitrogenation), and Task 2.7 (Volatile Products Recovery). I would suggest that the team make their tool publicly available, if possible, to increase the impact of the fantastic work done here. Has the team explored industry collaborations for this model to work on industry-relevant problems? For the graphs of the computational screens, could you please mention what the desired feature is? On slides 6–8 in the presentation, please mark the desired quadrant, how close to the diagonal, etc.

PI RESPONSE TO REVIEWER COMMENTS

- The computational team thanks the reviewers for their thoughtful comments, valuable feedback, and encouragement. We appreciate that the reviewers value computational modeling, empowered by AI technology, in providing valuable insights to help guide experimental work and accelerate the technology goals set within the consortium. We have demonstrated good examples of how our computational modeling improves fundamental understanding in various bio-separation projects and how these new insights mitigate the risks of accelerating R&D in these projects. We are delighted that the reviewers found our computational work impactful and beneficial to advance the SOA in different projects. We strongly agree with the reviewers that our work cannot be achieved without excellent collaboration across diverse teams, and we remain determined to continue that in the future. We appreciate the constructive feedback on our presentation slides, and we will incorporate the suggested modifications in our future presentations to improve clarity. Several other specific comments are addressed below.

- The first reviewer asked if we could use ML to fill the data gaps of LCA. This is an excellent question! This is something we already considered several months ago, and we have initiated conversations with the TEA/LCA teams in the consortium. The idea would be to link the output from molecular modeling to AI tools to bridge the data gap and introduce more molecular-level insights in the TEA/LCA frameworks. With the reviewer's encouragement, we will continue developing this approach in the consortium.

- The first reviewer also commented that our DEI strategy and progress were not presented; however, the second reviewer noted our DEI approach. To clarify this, in slide 3 in our presentation, we indicated that we are deeply involved in the Bioenergy Bridge to Career Program by contributing to topic development and supporting student internships, as pointed out by a reviewer. The computational team members at PNNL and Oak Ridge National Laboratory will host a full-day virtual workshop with seminars, panel discussions, and hands-on learning sessions for programming in bioenergy science, and we will encourage the participation of underrepresented groups and students/postdocs. We have also reached out to local schools to host a Bioenergy Sciences for Students event. In addition, Vanda Glezakou is cochairing the next Gordon Research Conference in Chemical Separations on Jan. 21–26, 2024 (Galveston, Texas). The Gordon Research Conference is a premier conference with a very strong focus on DEI as well as mentoring of postdocs and early career scientists. We have requested a small contribution from the consortium (from FY 2024 funding) to support travel and registration for students/postdocs/early career scientists and underrepresented minority participants.

- The second reviewer's comment that the project is very new is only partially correct. The computational task was established in the previous cycle of the consortium (FY 2019–FY 2022) under the leadership of Vanda Glezakou, who also serves as the liaison between this consortium and the Consortium for Computational Physics and Chemistry. After Glezakou's move to Oak Ridge National Laboratory, Difan Zhang became the task lead, to provide the opportunity for leadership to an early career scientist.

- The third reviewer commented on the translation of our current success in the project to the other collaborative projects. We have strengthened the communication between different projects to ensure that the computational team's focus is on the core questions of our collaborators. We have also invited industry partners to join our advisory board to hear feedback from external voices and improve our connection to the other collaborative projects.

- The fourth reviewer suggested making our computational tool publicly available. In fact, we have been planning to make these tools available to the public once our paper is published. These tools will be shared via open-access platforms such as GitHub under the GNU license. This will also help us transfer our success in the current projects to the other projects, as the third reviewer commented.
- Further, a question was asked about whether we have explored industry collaborations for more industry-relevant problems. This activity is under development with the help of our experimental collaborators. For example, in our cooperation with the Volatile Product Recovery project, we have reached out to industry partners to identify new volatile compounds of interest, and the proper modeling for these compounds is currently under development.

ORGANIC WASTE CONVERSION

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Organic Waste Conversion Technology Area is one of 11 technology areas that were reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 18 presentations were reviewed in the Organic Waste Conversion session by five external experts from industry, academia, and other government agencies. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks (https://www.energy.gov/eere/bioenergy/organic-waste-conversion).

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $32,420,875, which represents approximately 6% of the BETO portfolio reviewed during the 2023 Project Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Beau Hoffman as the Organic Waste Conversion Technology Area review lead, with contractor support from Katie Davis (Lindahl Reed) and Brianna Farber (Boston Government Services). In this capacity, Beau Hoffman was responsible for all aspects of review planning and implementation.

ORGANIC WASTE CONVERSION REVIEW PANEL

Name	Affiliation
Samantha MacBride*	Baruch College
Aaron Fisher	Ernst Maier
Tim LaPara	University of Minnesota, Twin Cities
Musa Manga	University of North Carolina, Chapel Hill
Vanessa McKinney	U.S. Environmental Protection Agency

* Lead Reviewer

ORGANIC WASTE CONVERSION REVIEW PANEL SUMMARY REPORT

Prepared by the Organic Waste Conversion Review Panel

INTRODUCTION

Between April 3 and 7, 2023, BETO conducted a peer review conference to monitor, evaluate, and guide its portfolio of funded research and development projects. Projects were classified by area, with Organic Waste Conversion covering 18 projects. Five peer reviewers representing fields of microbiology, civil/environmental engineering, resource economics, and public policy convened over a 2-day period for presentations by representatives of each project team.

Organic Waste Conversion projects addressed novel methods to convert municipal and industrial organic wastes into bioproducts and biofuels. Targeted organic waste feedstocks included food waste; fats, oils, and grease; manure; treated wastewater solids; and paper mill sludge. Material throughputs addressed included lignocellulose, volatile fatty acids (VFAs), carbohydrates, and nutrients. A range of conversion processes were presented, including hydrothermal liquefaction (HTL), enzymatic hydrolysis, microbial electrosynthesis (MES), biomethanization, dark fermentation, cathodic electro-fermentation, and a range of pre- and post-treatments in conjunction with conventional and alternative approaches to anaerobic digestion (AD). Envisioned products included sustainable aviation fuel (SAF), a priority for DOE BETO, as well as a range of high-value products such as hexanoic acid, alcohol, and other precursors for chemical manufacturing/fuels or blendstocks of fuel products. Some projects also envisioned nutrient recovery of nitrogen and phosphorous for fertilizer applications.

Projects aimed to optimize carbon conversion efficiency (CCE) and to express market outcomes of conversion in terms of a minimum fuel selling price (MFSP) per gasoline gallon equivalent (GGE). Several projects considered the geographic context of project development, addressing the proximity of feedstocks to conversion facilities and to end markets, as well as local jurisdictional issues around facility hosting.

What follows is a compilation of general comments from the five peer reviewers on BETO program strategy and implementation, followed by recommendations for the future development of this program. Although there is broad overlap among the reviewer comments, some differences do exist within the Project Peer Review group. Bullets before paragraphs indicate different reviewer perspectives.

STRATEGY

- The review panel agrees that BETO's organic waste-to-energy (WTE) program is strong. There are numerous projects in diverse areas, increasing the likelihood of success. This program leverages academic researchers and researchers working at national laboratories well.

- The projects are nicely tackling the full array of wet organic wastes: food, treated municipal wastewater solids, and manure. In terms of conversion strategies and methodologies, the team seems to have a fairly comprehensive strategy. There do not seem to be any obvious missing pathways. All the products presented as part of the Project Peer Review begin with wet organic wastes. All of them are looking at deriving value from these streams. This includes deriving saleable products as well as minimizing waste. As a clearer strategy has come into play, the office has narrowed its focus on jet fuel and heavy vehicles as products that are difficult to decarbonize. The projects have responded well to these challenges and continue to demonstrate nimbleness and versatility. Each project is addressing key challenges around wet waste.

- BETO's programmatic goals are clear. BETO has set technical targets in their overall Multi-Year Program Plan process that make sense, including a focus on SAF as opposed to motor vehicle fuels, and an emphasis on small, "community-scale" AD. With regard to renewable natural gas (RNG) production from conversion operations, BETO has identified near-term supply bottlenecks that argue for growth in

RNG as a bioproduct. In focusing on SAF as a major targeted output, BETO has appropriately identified conversion technologies that stand to optimize the transformation of feedstocks into bioproducts that are less likely to compete with carbon-free renewable alternatives while minimizing unwanted byproducts.

- The projects that are being funded by the BETO program employ avant-garde techniques aimed at generating liquid fuel, products/chemicals, hydrogen gas, and RNG, which can be said to be the fuels of the future. Overall, BETO is pursing well-defined and highly impactful goals largely aimed at increasing environmental sustainability through the cultivation of energy sources such as RNG, liquid fuel, and hydrocarbons. In addition, these efforts mitigate decomposition in landfills, a leading source of greenhouse gas (GHG) emissions, as well as nutrient pollution from manure and wastewater management.

STRATEGY IMPLEMENTATION AND PROGRESS

Engaging Industry Stakeholders

- All projects require an industry (or similar) partner, which has merits. There may also be value in limiting industry partnerships for projects in their infancy and which display a low level of technology readiness. Such creative and/or risky projects would benefit from allowing the researchers simply to develop their ideas without partnering with an industry.

- Another positive is that teams are working with a range of industry professionals. The challenge is that the organic waste conversion industry is still nascent, particularly with regard to doing more with what most folks view as waste.

Extending Engagement to Other Stakeholders

- It is evident that BETO has considered industry input extensively. It has also acknowledged input from other stakeholders, including local utilities/management jurisdictions, businesses generating feedstocks and/or potentially consuming end products for particular projects, academia, and national laboratories. BETO should continue to guide researchers to seek greater degrees of input from local/regional utilities and service agencies, landowners, and community organizations, including those opposed to conversion technologies. Overall, there was good engagement with typical partners in project development, but more work is needed to provide stakeholders not directly engaged in R&D and finance to contribute to the selection and evaluation of projects as well as for researchers on selected projects to more proactively engage with local and regional stakeholders in these categories.

- One of the best features of BETO's strategy implementation is the launch of a technical assistance (TA) program geared to local/regional stakeholders in governments. BETO is to be commended for its emphasis on letting "communities define the problem statement" (as stated in slide 17 of BETO's Organic Wastes Session Overview presentation). BETO's partnerships with the Great Lakes Water Authority; Yarmouth, Massachusetts; and the city of Gainesville are excellent starts.

- BETO should also focus on promoting stronger stakeholder partnership to move these projects from the lab scale.

- The forced socialization of these projects to the broader community will be critical to overcoming the myriad challenges.

Using Techno-Economic Analysis (TEA) and Life Cycle Analysis (LCA) to Quantify Progress

- Reporting requirements for TEA and LCA were very helpful in a number of projects. In fact, the best projects took the LCA and TEA aspects of this work seriously and appropriately pivoted the direction of the project when the LCA and/or TEA indicated that they should.

- BETO positions ongoing work under organic waste conversion projects as having the potential for significant reductions in GHGs, including methane, carbon dioxide, and nitrous oxide. Overall, the structure of the individual project presentations did not allow for an apples-to-apples comparison of GHG profiles or projected impacts. Further, it would be helpful for reviewers and the public to have access to information on modeling assumptions used in the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) LCA tool or other tools used by researchers to estimate net GHG reductions. In particular, the goal of carbon neutrality through organic waste conversion heavily depends on assumptions of substitution between bioproducts and fossil-sourced products, especially in the case of fuels, to achieve a net system stabilization and overall GHG reduction. BETO must pay attention to the empirical verification of assumed substitutions once its funded technologies reach scale because of the possibility for net system growth due to bioproduct supply availability—regardless of the system stabilization envisioned in models.

- In generating energy from waste, the BETO program set economically and environmentally suitable targets that include reducing the levelized cost of energy (LCOE) by 25%, increasing the energy return of investment by 25%, improving CCE by at least 50%, and reducing the cost of disposal by >25%. To ensure that these set targets are well met, projects that are funded under the BETO program involve collaboration among industry experts, stakeholders, and researchers, which leads to the cross-fertilization of ideas and strategies. Also, the program includes projects that involve modeling, TEA, and LCA all aimed at finding optimized pathways (in terms of reducing cost and environmental contamination and increasing energy yield) for generating energy from waste. Further, the BETO program includes a WTE TA project where experts advise communities on the best avenues/methods for deploying WTE technologies.

Promoting Diversity, Equity, Inclusion, and Accessibility (DEIA)

- Overall, the requirements for DEIA were good, although some projects were better at appearing to have a DEIA component than demonstrating the implementation of DEIA initiatives. Many projects mentioned that key personnel came from underrepresented groups yet provided little additional information on these staff and/or their specific project contributions. Other projects required diversity, equity, and inclusion (DEI) training for project personnel. This approach is preferable because it is achievable and tangible.

- The current era (2020 to present) has been marked by three massive social upheavals that have affected nearly every aspect of political, social, and individual life. These include the COVID-19 epidemic; a new reckoning with justice that alternately recognizes, or denies, legacies and ongoing practices of harm to Black, Indigenous, and other people of color, LGBTQIA2S+, disabled, and migrant communities; and the now near-irreversible scale of the climate crisis, along with mass species extinction, the proliferation of new forms of toxicity, soil depletion and erosion, and air pollution. The combined impacts of these three upheavals have made clear, to varying degrees within some government agencies, that a more serious, complete, and inclusive approach to hearing and responding to local and regional concerns across a wide array of stakeholders is needed in public policy and planning. The establishment of DOE's Office of Energy Justice, and the recent incorporation of DEI and community engagement activities as criteria for funded project award and Project Peer Review criteria, reflect this trend but only in a nascent, unstructured manner with regard to organic waste conversion.

- With regard to the social impacts of organic waste processing, BETO is focused on siting inequities and disproportionate impacts falling on disadvantaged communities and recognizes the need for a "social license to operate" (slide 8 of BETO's Organic Wastes Session Overview presentation); however, it was not clear from the projects presented (1) that such inequities and impacts had been considered or (2) whether the project scopes even allowed for such consideration—because inequities and impacts typically appear upon reaching the commercialization scale, and not before. Moreover, there is more to gaining a social license to operate than siting considerations.

Project Management and Funding Mechanisms

- Project management and controls seem sufficient, although there were some delays due to COVID-19. All the projects are hitting their goals. The challenge is going to be integrating unit operations and finding sufficient human capital to make these projects go. Overall, funding mechanisms are sufficient. There is a good mix of funding opportunity announcement (FOA) and annual operating plan funding. There is a good mix of folks familiar with BETO and folks less familiar providing fresh perspectives.

- Another aspect of project management has to do with scaling up successful research. The challenge has been getting sufficient money to pilot/scale up these ideas and begin the long road to commercialization. The other challenge is addressing the potential downsides/risks with scale-up. For example, if a unit operation were to break at a wastewater treatment facility (WWTF), large quantities of treated solids would either need to be stored or disposed of. These kinds of contingencies are very difficult to handle within a research program's budget.

- One weakness in project management are the go/no-go interim goals. As a strong proponent of fundamental research, one reviewer felt that go/no-go metrics discouraged researchers from gaining a fundamental understanding of the issues and perhaps encouraged them to present their results in a way that was not entirely honest. Several projects seem to have been initially funded because they showed considerable promise; however, research often leads down dead ends, and negative results still have considerable importance. For these projects, a "completion" of the research to fully understand why these otherwise logical topics failed would be more beneficial than ending the project prematurely. Some researchers simply obviated the go/no-go requirements by setting an easily achievable go/no-go metric. Along these lines, a few of the projects were more focused on achieving a performance goal rather than learning how to optimize their process. In this sense, it would be beneficial to encourage more hypothesis-driven research rather than simply judging projects by cost/waste conversion/GHG emissions.

- So far, all the funded projects are showing tremendously good progress, indicating that the BETO program will meet its goals and targets. The level of progress of these projects was verified by the BETO program officials (Budget Phase I, Phase II, etc.). This gives credence to the fact that the BETO program is actively involved in managing the projects to obtain better outcomes. It is recommended that BETO finds a way of sustaining these projects beyond the assigned project periods. Also, it was observed that some of these projects are similar and apply the same techniques. These similar projects can be linked together because this will enable increased scale and wide applicability of the results from the projects.

Fostering Knowledge Transfer

- Many of these projects focus on the same technologies, such as HTL, AD, and biomethanization. Each process is basically being studied "empirically," meaning as part of a series of unit operations toward a specific goal. Each research has a slightly different research goal, so each process is investigated slightly differently. The problem with this approach is that there is relatively little transferrable knowledge from one project to another; alternatively, fundamental studies to understand how each process works over myriad conditions and feedstocks could lead to more transferrable knowledge and a better/more efficient pathway to producing commercially viable fuels from organic wastes.

Promoting Public Health

- Funded projects are mainly aimed at the protection of the environment. BETO can incorporate the protection of public health by including treated municipal wastewater solids as one of the wastes from which energy can be generated. Funds obtained from generating energy from human waste can serve as an incentive for properly treated municipal wastewater solids management and can, in turn, reduce the transmission of diseases. The projects should also consider monitoring the fate of pathogens and emerging contaminants in the biosolids and digestate.

- It can be noted that apart from producing fuels from the waste, the projects that generate energy from treated municipal wastewater solids have also started to consider the fate and removal of emerging contaminants in the waste (i.e., per- and polyfluoroalkyl substances [PFAS]) as well the generation of eco-friendly fertilizers. The funded projects make use of highly advanced and novel techniques. Some of the projects involve the incorporation of two or more innovative techniques in order to meet the program's strategic goals.

- The work that BETO has done since 2021 to advance HTL is of particular interest and value in light of the anticipated regulation of PFAS and other micropollutants in water resource recovery facilities (WRRFs), landfills, and potentially other generator outputs. The dimension of destruction of some or all PFAS species in these feedstocks will be a significant value add if landfilling, land application, and/or composting become unviable due to contaminants of concern and resulting costs and liabilities. BETO is encouraged to look closer at this dimension as it continues to advance HTL and potentially other high-heat technologies capable of PFAS destruction.

Integration with Solid Waste Management

- BETO recognizes the role of current solid waste management in the United States, especially for municipally sourced feedstocks such as food waste and treated municipal wastewater solids, and it has appropriately noted economic factors relating to hauling and landfill tip fee costs. This is evident in their solicitation and funding approaches.

- By virtue, waste is underutilized and undervalued. Converting this product to fuel and products is really critical to addressing sustainability challenges. Waste, though, has been a tantalizing target because of the tipping fees. The challenge has always been that waste is a bit of a catchall with a high degree of variability. This has always challenged processes. BETO has done an admirable job of forcing researchers to use real waste streams. Hopefully the efforts of the office continue to spur the development of an organic WTE industry.

RECOMMENDATIONS

Meeting Format

- These meetings are indeed expensive and take lots of planning, but they are worth it! I witnessed and hopefully contributed a few connections to resources and needs outside of the awareness of funded researchers. Contributions from reviewers will lead to furthered beneficial outcomes beyond those of what funded projects were doing on their own. (Examples: recommended deployment of technologies to remote areas with renewable energy abilities; ash from paper products potentially becoming a valuable input into energy-intensive concrete processes rather than a waste product.) All of this is to say that perhaps a similar, virtual review session could happen every other year, in between in-person meeting years.

- In the future, I recommend that all the presenters provide Gantt charts in their PowerPoint presentations tracking the progress of their work against the planned milestones.

Strengthen Approach to DEIA

- DEIA initiatives are clearly evolving as new funding opportunities become available. Training and substantive opportunities for those from underrepresented groups is a good baseline for all projects. Yet research, where reasonable, should also be deployed in communities where they can make the most difference. I struggle with assigning metrics to such a concept because applying DEIA to the rollout of new technologies in the field is complex. Deploying new technologies requires a baseline of infrastructure, personnel, and capacity on the ground that such communities typically do not have. But I do grow frustrated with training and hiring as a fallback. There are communities that have suffered from decades of disinvestment and disempowerment that need to see their government make a difference in their lives. These individuals cannot access benefits from training and hiring alone. We can only truly move forward in answering the challenges of climate change when everyone sees a benefit for their community.

- One of BETO's strategic goals is to "build diversity, equity, and inclusion into hiring and funding decisions, project plans, and community engagement" (BETO 2023 Multi-Year Program Plan). This is an area that needs to be better thought through and fleshed out with regard to providing guidance to research teams for selected projects. At a minimum, there is reviewer consensus that all funded project personnel be required to take DEIA trainings. BETO should also put together a robust guidance document for personnel on awarded projects that covers why DEIA is important in historical, political, and ethical contexts; covers how DEIA is achieved through formal and substantive (i.e. non-token) practices; and emphasizes the goal of DEIA to redress past exclusion of many groups in and outside U.S. society from senior-level roles in projects as opposed to primarily focusing on students and interns.

- In the area of organic solid wastes, there are specific concerns among disadvantaged communities, and others, regarding the diversion of potential feedstocks from composting and land application to bioproduct or biofuel uses. The value of soil-focused approaches, if compared on an LCA basis to alternatives such as AD and other conversion methods, may reveal inefficiencies, including higher rates of net GHG emissions; however, reliance on GHG-focused LCA comparison stands to exclude significant community benefits that are realized in terms of erosion remediation, soil improvement, and integration with locally reliant and resilient waste management and agricultural practices (which are, in turn, of increasing importance during periods of supply chain uncertainty, more frequent major weather events, and widespread hunger in the United States). Such community benefits are operationalized in community composting/urban agriculture projects and resiliency plans that are currently proliferating in the United States, in part as a response to health, justice, and environmental precarities that the three upheavals discussed above have made impossible to ignore. Such soil priorities may overlap with work that DOE and/or BETO is doing with the U.S. Department of Agriculture and U.S. Environmental Protection Agency. There is great room for improvement in BETO's overall approach to environmental justice and its relationship to community engagement and DEIA practice.

More Attention to Non-Market Project Benefits

- BETO's work to build a bioeconomy sourced with organic waste feedstocks has great potential but also needs to more fully consider the context of its mission. Researchers on BETO projects, including scientists and engineers, occupy an important role as pragmatic problem solvers focused on the development and optimization of carbon-neutral, environmentally safe energy technologies. To the extent that they are called upon to consider marketization potential through TEA, including metrics such as return on investment, equivalency pricing, or other cost metrics, this work may entail a focus on industrial profitability to the exclusion of more systemic consideration of appropriateness. Appropriateness here refers to a broader social and ecological context that represents interests and concerns outside the marketplace as well as within it. Among the most salient of these are questions of utilization and pollution of Indigenous lands; the siting of facilities in communities historically targeted for racial segregation and exclusion; and the transparency of industrial data reporting on material and energy flows, solid waste generation rates and fates, air and water emissions, and synergistic risks associated with old and new technological approaches.

ORGANIC WASTE CONVERSION PROGRAMMATIC RESPONSE

INTRODUCTION

The Organic Waste Conversion Program is grateful for the reviewers for their contributions, recommendations, questions, and feedback during the 2023 Organic Waste Conversion Project Peer Review session. The program recognizes that this is a significant investment of time to review the projects, travel, and prepare the reviews following the in-person meeting. The program appreciates that each reviewer was willing to contribute their time and expertise to this meeting. In particular, the program is grateful for the diverse perspectives that the individual reviewers brought to the meeting on matters of urban design, public health, sanitation, and national policy.

The program would first note that the work presented in these 18 presentations is comprehensive of all projects that contain organic wastes. For example, the Renewable Carbon Resources Program conducts work on preprocessing of fractions of municipal solid waste (MSW) bound for landfills. The Data Modeling and Analysis Program conducts various forms of air quality analysis and LCA. The intention of this session was to present groups of work funded by the Organic Waste Conversion R&D program focused on the conversion aspects of these waste streams.

The program is pleased to hear that the reviewers feel the overall strategy and grouping of projects is sound and strong. Over the years, the program has shifted its focus into several areas:

- Improvements to AD (including RNG)
- Production of liquid fuels from waste
- Production of products from waste
- Community-led project implementation.

With regard to fostering knowledge transfer, the program appreciates suggestions from the 2021 peer reviewers on how to do this. This served as some of the inspiration for the community-led projects and funding opportunities, and the program intends to continue those opportunities. In recent years, several technologies have since "graduated" from the program and are being scaled up using other DOE/federal funds and/or private equity funds. It is gratifying to see these successes make their way into the marketplace; however, reviewers might not have insight to that based on the information provided from these project presentations. In future Project Peer Review sessions, the program will include updates on past work that has concluded and its current status. The program would also note that several technologies developed from this portfolio are only just beginning with industry or community partners, and it was premature to invite them to present given that they have yet to begin.

In the response, the program did note some comments with regard to early-stage research and concerns about the expectations for these types of projects. While the program appreciates the sentiment of this comment and recognizes that overly prescriptive requirements or project management oversight can impact the overall technical progress, too much freedom goes against the program's ethos. In the past, the Organic Waste Conversion Program has received comments that the quantitative metrics were prescriptive to the point that it took away from the main mission of technology development. For this reason, the program has moved away from esoteric FOA requirements to the extent possible; however, other requirements, such as industry or end user engagement, really are critical to ensure that the technologies being developed (1) have engineering feasibility and (2) solve problems identified by the end users (see response to Recommendation 3 below).

Recommendation 1: Meeting Format

The program is pleased to hear that the meeting was indeed valuable and fostered collaborations and networking. The in-person element of this meeting, unlike what was possible in 2021, was highly beneficial and is another reason for this; however, the program has no intention to increase the frequency of the Project Peer Review because it is quite burdensome on the project teams and requires extensive logistical planning.

Recommendation 2: Strengthen Approach to DEIA

The program recognizes and concurs that work remains to be done with regard to DEIA efforts in the funded research. BETO has distributed a new set of guidance to national laboratory projects for the fiscal year (FY) 2024 cycle to provide examples of ways that research teams can integrate these values into their research. The program has recognized the unique environmental justice issues associated with organic wastes and has sought to incorporate these efforts into recent community-focused solicitations. The program also appreciates that there are sustainability indicators beyond just GHGs that are germane to this field, and projects going forward are now required to incorporate their tracking in their work, including PFAS, air quality, truck traffic, and others. Generally speaking, there is a dearth of publicly available research on these indicators at a local level, and the program recognizes the need and opportunity to support this area. The program intends to continue the TA program and other efforts that bridge the gap between applied research and the communities that will/could adopt these technologies.

Recommendation 3: More Attention to Non-Market Project Benefits

The program strongly concurs that the value proposition of organic waste conversion technologies extends far beyond those of economics. Organic wastes represent environmental and social liabilities, and it is critical to recognize that there is a need to ameliorate some of these impacts in the course of technology development. BETO would note that the metrics and desired outcomes from recent solicitations reflect metrics other than purely economic outcomes. Moreover, recent solicitations have had eligibility restrictions to increase the likelihood that projects are being led by the communities themselves as opposed to being based purely on profitability for entities that are looking to deploy technologies.

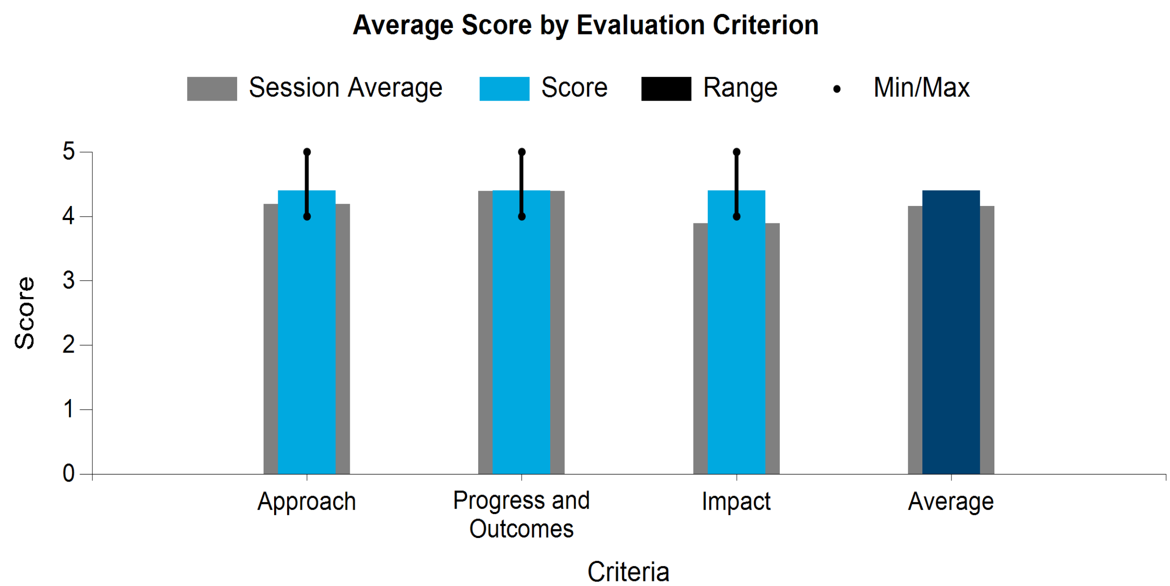
WASTE-TO-ENERGY TECHNICAL ASSISTANCE

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.1.0.112
Presenter(s):	Anelia Milbrandt
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$1,200,000

The goal of this project is to mobilize data, information, and knowledge generated about organic waste streams to local governments and support their decision making. It builds on previous work related to wet organic waste resources (food waste, sludge, manure, waste fats, and oils). The project provides an improved understanding of local waste challenges and priorities to inform BETO's R&D strategies and decision making. It also supports local governments' goals and plans related to sustainable waste management, enables energy and/or resource recovery project development at the municipal level, and facilitates public-private partnerships. A key challenge is associated with more activities requested by entities than the program allows, which is mitigated by prioritization by the requesting agency. All FY 2021 and FY 2022 TA requests have been completed. Major accomplishments include (1) 34 requests managed in the past 2 years and (2) distilled key challenges faced by communities. Key outcomes include strong community participation since the inception of the program, a dedicated program website, deliverables tailored to communities' needs, and distribution materials (e.g., fact sheets, brochures) for a broader audience.



COMMENTS

- I want to better understand the impacts of the TA. I'm trying to judge if the advice was heard and taken. In this vein, advice heeded to not do something could be just as valuable as advice to do something. This presentation should be structured more like a bunch of case studies instead of speaking in general dimensions.
- The approach is sound. Overwhelming interest from communities. There were more meritorious applicants than money/time to address these issues. Project is oversubscribed going into the 2023 cohort.

- Good that there is a selection process. Engagement and communication strategies seem reasonable. Would desire a clearer presentation of expectations.
- DEI issues are well woven into this project. Looking at both staff assisting and the communities being assisted. Good geographic and socioeconomic factors.
- Engagements seem to lead to wider circles of involvement from the communities. It is great that it reached so many communities with diversity of location, size, etc.
- These slides read more like strategy/approach and less like progress/outcomes. Would expect more progress/outcomes for a project this far into its life cycle.
- Certainly believe this work is valuable and important.
- Overview/impact:
    - This project is the first WTE TA for local governments on the most appropriate WTE technologies and practices to adopt. The project provides assistance on a wide range of issues spanning land constraints, environmental justice issues, and organic waste management. This project provides a nuanced but relevant aspect of organic waste management. It involves garnering relevant information about different organic waste streams to provide the information needed for decision making by local governments. The project also gathers information about organic waste management challenges faced by different communities that will help inform the prioritization of projects by DOE.
    - Considerable progress has been made so far in this project, and the researchers have addressed a wide range of topics since the project began in 2021. They have completed all the milestones that they had set out at the beginning of the project; however, looking at all the approaches employed in the project, I do not see any novel or unique approach, as everything put forth by the research team is well known. Also, the researchers keep on mentioning what they did but did not clearly explain how they undertook the work.
- Strengths: It can be said to be the first study that provides WTE TA for local governments. The project team has a clear communication and management plan. Also, the fact that the selection process for applications in the project takes into consideration geographic and demographic diversity is commendable, as it ensures diversity and inclusivity, which is a core goal of BETO.
- Weaknesses: I feel the risks and the risk management strategies outlined in this study are weak, as the researchers only outlined factors that are related to the staff. Expected risks in this kind of project should include inaccessibility to relevant information and community pushbacks. Second, in the PowerPoint presentation, the researchers indicated that they had stakeholder outreach and engagement, and I am wondering if they could provide more information about the stakeholders who were involved in the community engagement activities and how they were selected.
- Questions: While presenting the progress and outcomes of the project on slide 7, the researchers indicated that they carried out a cost-benefit analysis on food waste comparing landfilling, AD, and composting. It will be great if the researchers can give more elaboration on how they carried out the cost-benefit analysis. In the same vein, I am wondering if the researchers have clear guidelines for communities to follow as they prepare these cost-benefit analyses to avoid missing or ignoring some key items or cost elements.
- This project consists of a TA program geared to local governments, which will support systemic analysis, planning, and tech evaluation around various WTE technologies. This is a very useful and needed project that will greatly aid localities, large and small, in critically evaluating new technology pitched to them by

private sector actors. This program will support localities in seeking funding and making community-informed decisions.

- In the last funding cycle, there were 17 community recipients with good geographic diversity. This program badly needs increased funding and staffing so that more municipalities can be reached. Over and above the resources offered, developing and providing technical expertise in the areas of cross-agency collaborations, agency siloing mitigation, novel and accelerated forms of municipal procurement, and data management/sharing will further assist localities grapple with the gap between federal funding availability, workforce shortages, infrastructural aging, and local institutional capacity.
- This project is a TA plan for public entities trying to increase their WTE output for various reasons.
- This appears to be a highly qualified team with a good risk management plan. The DEI approach is very good, covering multiple definitions of "diversity and inclusion," such as rural to urban, early to late career, gender, and race. This is definitely a strength of this project.
- The team provides 40 hours of TA per project. There seems to be far more interest by municipalities in receiving TA than there is opportunity to provide it.
- Perhaps most importantly, a lot of knowledge is gained by performing these projects; project personnel help disseminate this knowledge by producing fact sheets that are made available on their website, and these can be downloaded by other interested individuals.
- The project has clear targets, goals, and mission. As the project enters this next phase, it would be good to know how the project can convert their on-the-ground experience with municipalities into an actionable framework for future outreach. Are we starting to gain insight into which factors best help to categorize or standardize municipal bioenergy possibilities across the United States? For example, does a community's size, region, climate, or other factors (if any) best determine which actions it can take to move local wastes to energy? Can a tool be built to streamline the technical outreach that is offered to municipalities and leverage work from the Pacific Northwest National Laboratory's (PNNL's) project WBS 2.1.0.113: Waste-to-Energy: Optimized Feedstock Aggregation and Blending at Scale?
- The project is being managed well to ensure beneficial outcomes for the performer and the government. Outreach and education at this scale, with technical experts, to learn U.S.-wide lessons would be difficult to do without BETO funding, as well as the project's initial investigation into bioenergy technology workable solutions or offerings.
- This project is ambitious and has done a great deal to consider multiple technologies and their unique applications to various scenarios. The aggregation of data at this scale could help develop and coalescence a suite of organic waste technology offerings on the ground, an important strategic outcome. The project also sought to bring new technologies into offering as it considered the uniqueness of the requested topic in its applicants.
- This project offers the possibility of an important strategic outcome in how WTE options can be evaluated by analyzing outcomes of direct TA. This project's results could inform future outreach and education and potentially provide a suite of tools to streamline organic waste project development at the community level.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their time and valuable feedback. It is gratifying that the review recognized the value and importance of the WTE TA program and approved of the approach and progress/outcomes. One reviewer noted that we should have provided more information on progress/outcomes and structured the presentation in the form of case studies. We recognize and apologize for leaving some detail out of the presentation. This was done to protect confidential information, as many communities are not willing to share the specifics of their TA request. We are unclear about the comment about providing clear expectations. Would that be from BETO or the communities? In any case, we would like to think that expectations have been met on both ends, and testaments of that are both positive feedback from BETO and results from participating community surveys. With regard to the comment, “I don’t see any novel or unique approach, as everything put forth by the research team is well known,” we politely disagree. This is the first (and to the best of our knowledge the only) WTE TA program, which makes it unique. We agree that everything put forth by the research team is well known, which is the purpose of a TA program—to disseminate knowledge and provide technical transfer based on previous experiences. We apologize for not providing enough clarity on how we undertook the work and more specifically how we carried out the cost-benefit analysis. There was simply not enough time to do this given the prescriptive presentation formatting and mandatory content requirements for the BETO Project Peer Review. Each request was different, and it would take a long time to describe, even briefly, how we undertook 34 tasks within the given time frame. As noted in the presentation, the program builds on existing work, and in the case of the cost-benefit analysis, we ran a model we previously developed for communities that requested it with input data and scenarios provided by those communities. While most reviewers approved of our risk management plan, one comment was that we “only outlined factors that are related to the staff. Expected risks in this kind of project should include inaccessibility to relevant information and community pushbacks.” While we agree that there may be expected risks with this kind of project, we did not encounter them. Our only challenges were related to staffing on both sides, the participating community and NREL. We have not had any issues related to data availability or pushback from communities. One of the reviewers asks us to “provide more information about the stakeholders who were involved in the community engagement activities and how they were selected.” Many entities that participated in the program had a team that includes various stakeholders, such as external advisors, boards, and private citizens, connected to the local community. This is an excellent question: “How can the project convert their on-the-ground experience with municipalities into an actionable framework for future outreach? Are we starting to gain insight into which factors help to best categorize or standardize municipal bioenergy possibilities across the United States?” The insights gained through the program will inform not only future outreach but also future R&D activities. At the end of this 3-year cycle, we will analyze exactly that and present BETO with a written report summarizing our findings. We agree with the statement that “this project’s results could inform future outreach and education and potentially provide a suite of tools to streamline organic waste project development at the community level.”

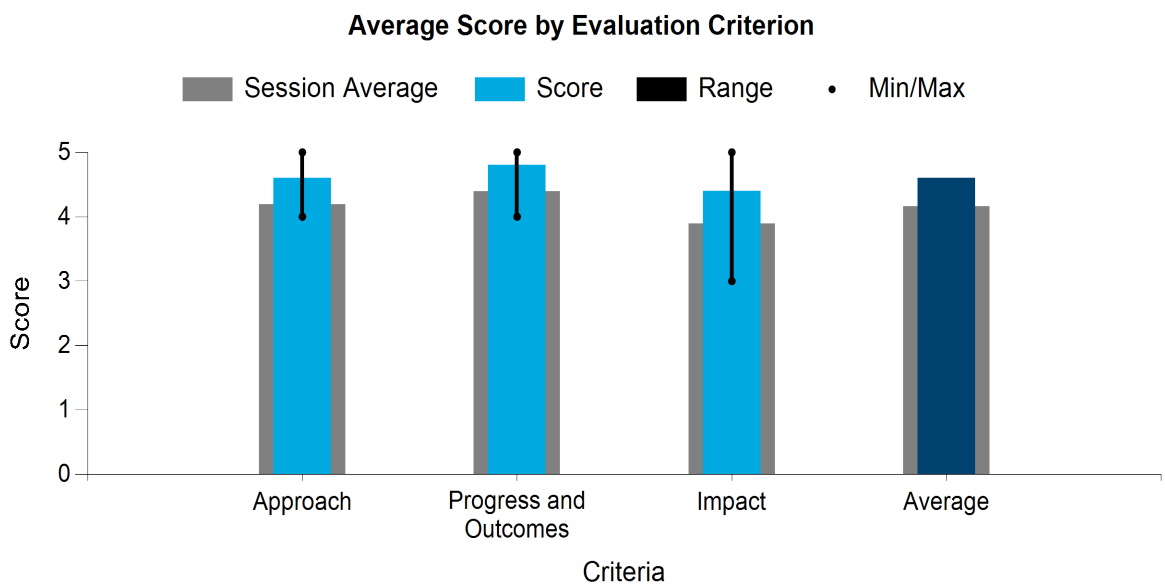
WASTE-TO-ENERGY: OPTIMIZED FEEDSTOCK AGGREGATION AND BLENDING AT SCALE

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.1.0.113
Presenter(s):	Karthikeyan Ramasamy; Katarina Younkin; Michele R Jensen; Tim Seiple
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$900,000

Wet organic wastes such as municipal sludges, manures, food waste, and fats, oils, and greases are considered priority feedstocks for conversion to biofuels. Feedstock costs have a major impact on the feasible scale of the proposed conversion and biorefining facilities and the final fuel price. BETO's 2019 draft Multi-Year Program Plan establishes an MFSP target of $2.50/GGE or less for biofuels by 2030. To validate whether proposed conversion pathways can meet this target, our project will deliver and apply a reusable, data-driven, geo-economic framework to identify practical and cost-effective opportunities for pilot- to commercial-scale deployments. Despite risks from imperfect engineering, spatial, and market data, our work improves understanding of the real-world possibilities to increase plant scale by combining waste feedstocks, thereby reducing the cost of biofuels.



COMMENTS

- Really great to see transportation handled on a micro/local level. The impact of this element of logistics is very local.
- With regard to the very large site data, does the model take into account truck turnaround times? It is a very big deal to be able to make 2–3 runs in a day from a personnel perspective. Also, is average traffic factored into this?
- Very impressed with the improvements since 2021. Think this model has great value.

- Great that the team is now looking at helping communities to develop their own plans. Would like to see targeted engagement as part of the DEI.
- Interesting to be including the national Freight Analysis Framework to minimize the impact of communities by trucking.
- Maps and graphics are great for conveying information. Great visuals.
- Want to ensure the tools are easy to use to maximize impact.
- The project is an analysis task and is not necessarily meant to be commercialized but rather to assist folks.
- Really great capabilities of this model around transportation costs, multimodal. Certainly would be interested in optimizing those issues, but acknowledge the cost and trade-offs. Understand that it would probably be best to incorporate this with community engagement because of rail challenges.
- Tim, you do not need to read the slides to us. Wanted you to cover more of the project's accomplishments
- Would be interested to see how the rest of the organic waste projects confirm these values/models with their independent activities—that is, to see how well the insights align. I do not think it is worthwhile to have a perfect model, but this should be enough to give confidence to folks commercializing WTE technologies.
- Need better engagement with communities and interaction with the TA program. Think this project is ready to engage with stakeholders.
- Overview/impact:
    - The researchers investigated how empirical data from novel WTE techniques obtained from laboratory experiments can be fused with real-world resource data to find viable WTE deployment opportunities and locations for siting energy generation plants. They achieved this using geospatial techniques to identify hot spots for cost-effective biofuel substrates, which they integrated with empirical technology and data costs, travel costs, and real-world resource data. The approach used by the researchers is inventive, as the model developed in the project has very insightful outputs, such as the net profit, total waste disposal savings, total fuel production, and total travel costs, which can be used to inform decision making when siting WTE generation plants. This project has a relevant impact on the waste management sector, as many WTE experiments usually end at the laboratory or pilot scale and are never scaled up; thus, having a project like this will serve as a basis for checking the feasibility of scaling up projects.
    - So far, the project has shown considerable progress and improvement since its inception—as the developed model has been adjusted to include dynamic feedstock pricing, realistic supply logistics, and fungible energy, price, and technology variables.
- Strengths: The project makes use of data-driven and scenario-based models, which means that the developed model is not rigid and can be applied/transferred to different scenarios. Also, an adept communication plan is applied in this project, as there is stakeholder communication with waste regulators and researchers as well as city leaders.
- Weaknesses: In discussing the model they are using in the project, the researchers provided the different variables and factors that were used in developing the model as well as the outputs expected from the project; however, they did not clearly describe the nitty-gritty of the model, such as how the different

factors (inputs) were applied/used in the model. Further, the researchers should also consider incorporating data trends in their model so that the changes in the supply of feedstocks and/or their characteristics could be captured, as in the past we have seen huge treatment plants constructed in locations with low feedstock supplies, and these plants failed as they never operated at the optimum loading rate.

- Questions: In slide 8 of the presentation, one of the milestones marked as 100% complete is model verification; however, there is nothing in the presentation showing how the verification was carried out. It will be highly appreciated if the researchers could shed more light on this.
- This project focuses on understanding wasteshed geography for multiple wet waste streams that can be converted to biofuels and products. This type of generation and flow analysis is crucially needed in all aspects of waste management to understand which flows or feedstocks make sense to consolidate, where, and at what scale. Regardless of the processing technology ultimately used (WTE variations or other treatments), a geographic model of this kind will be extremely useful for regional, state, and, in some cases, municipal waste management planning.
- The team is to be commended for consulting with stakeholders in a range of waste-related industries (refuse hauling, biosolids trade associations, plant operators, etc.). Seeking this input should be continued and expanded to the widest range possible of stakeholders, including municipal, state, and regional planners, as well as constituents engaged in regenerative and non-regenerative agriculture and livestock raising, community composting and food sovereignty groups and activists, and university cooperative extensions.
- The researchers note imperfect resource (presumably waste flow) data, which is typical of the distributed, heterogeneous, and localized nature of waste management in the United States. Another value add to government planners and other stakeholders would be to improve and publicize datasets publicly.
- The fact that the deliverable from this project is a dynamic model that can accept varying inputs and does not provide a single “right” answer is a plus, reflecting the realism of the approach. It opens the door to the productive consideration of various scenarios by stakeholders of all types who might in the future be able to use this tool, or a version of it, to engage in community-informed planning.
- This is a fantastic project with a lot of potential for cross-fertilization and future applicability to real-world cases all over the United States.
- This appears to be a very important project. In addition to developing the technologies for converting WTE, it is also critically important to identify various locations where the organic wastes are produced versus the locations of the facilities that can convert these wastes. Essentially, the researchers developed a very complex model that incorporated data regarding the locations and quantities of various organic wastes, transportation costs, conversion factors, etc. The results of this work essentially identify potential locations where WTE facilities could be located and profitable. Alternatively, this work could be used to exclude locations for WTE conversion because they are unlikely to be successful/profitable.
- These researchers appear to be highly responsive to previous review comments by the BETO panel and by others. Similarly, the researchers seem to understand that they have uncovered some very important and practical knowledge, and they are now focused on identifying entities/people who can take advantage of this knowledge.
- The project has clear targets, goals, and a mission. There is the potential for this project to have large impacts on the management of wet waste nationwide.

- The team's recommendation to move forward with designing a standard reporting package for city leaders, and potentially build dashboards, if budget permits, has a clear overlap with work from WBS 2.1.0.112: Waste-to-Energy Technical Assistance for Local Governments. Incorporating lessons learned from direct TA into a standard reporting package for cities would help address common upfront hurdles and considerations to assist municipalities in moving forward with organic waste reduction technologies that best fit their needs.
- This project is ambitious, and the aggregation of data at this scale could help develop and coalescence a suite of organic waste technology offerings on the ground, an important strategic outcome. The model that has been built is robust on many decision-making factors in policy, incentives, transportation, and geospatial optimization.
- The project is being managed well to ensure beneficial outcomes for the performer and the government. This is the leading edge of the comprehensive modeling of available wastes and technologies at this scale, and it would be difficult to do without BETO funding for this effort.
- The beneficial outcomes of this project have far-reaching positive outcomes for the reduction of waste landfilled, the intervention of methane emissions from wet organic waste degradation, and the potential of supporting large-scale bioenergy creation to further decrease the prices and availability of these fuels nationwide. This project offers the possibility of an important strategic outcome in how WTE options can be built out nationwide to achieve large-scale bioenergy nationwide. This project's results could inform future outreach and education, especially through the creation of a standard reporting package, that will streamline organic waste project development at the community level.

PI RESPONSE TO REVIEWER COMMENTS

- We greatly appreciate the personal investment made by each reviewer to improve the quality of our research. We are also thankful for your recognition that our work is impactful and relevant, and we look forward to continuing to serve the public.
- DEI focus and stakeholder engagement: We agree on the need to focus more on DEI and stakeholder engagement. The BETO DEI requirements were developed after our previous project cycle began (FY 2021–FY 2023); however, our FY 2024 project renewal proposal focuses entirely on partnering with and providing analysis support for waste-impacted underserved communities. If funded, this work will include a strong stakeholder focus when developing standard communication products and assessing the impacts of various waste management strategies. We are also committed to hiring staff from groups underrepresented in STEM to participate in model design and implementation to broaden the perspectives of our approach and improve our impact.
- Modeling traffic conditions: We account for average traffic conditions in our model, but we do not model traffic explicitly, which is resource- and cost-intensive. Instead, we represent average traffic conditions implicitly in the transportation network model in the form of variable truck speed limits assigned by road segment type, which are based on literature values. Speed limits also encourage trucks to find suitable highway routes as fast as possible and avoid neighborhood-level streets. Changing speed limit factors is easy but does require solving the network model again. We are exploring various traffic impact assessment methods on a related clean energy project, which could inform our model to improve travel time estimation and eventually estimate the impacts of potential neighborhood-level increases or decreases in truck travel associated with diverting wastes to energy recovery facilities. In the real world, waste transport is carefully scheduled to maximize truck and driver utility and reduce cost. This includes aggregating waste into larger vehicles at waste transfer stations. Due to limitations in our scope and budget, we cannot model optimized fleet and collection route management; however, we can carefully configure the input data to divert waste from intermediate diversion points—such as transfer stations, landfills, or similar collection/transfer/disposal locations—to represent likely waste diversion scenarios.

It is important to acknowledge that most wastes in the United States are handled through trucking with costs borne by ratepayers. This may also be the case in the future. Therefore, we are most interested in the difference between business-as-usual and projected traffic and cost impacts.

- Truck turnaround times: The transport model does account for truck turnaround times. Our current research focus is on modeling typical daily trucking requirements to estimate total annual delivery costs for wet organic wastes. We make the simplifying assumption that the number of trucks and drivers required will always be available. Waste pickups occur at prearranged places and times and are typically much faster than terminal or drayage turnaround services. Our specific method for estimating turnaround and total travel times is as follows. For each feedstock source, we know the location, type, and dry mass, and we can specify the "as-delivered" moisture content and density, truck type, truck capacity, truck charge-out rate, total fixed wait time (load + unload), and loading rate (e.g., gal/min). Dry waste mass is converted to a wet volume using moisture and density factors. Depending on the waste type and format (liquid, slurry, semisolid, solid), we may either assume a fixed wait time or estimate it dynamically based on a waste pump/loading rate. Load and unload times are assumed to be equivalent. The total wait time is then multiplied by the truck charge-out rate to determine the total turnaround cost. The turnaround cost is then added to the total two-way truck travel cost, represented by the modeled routing distance (i.e., least-cost network path plus on-/off-network connection costs). Finally, the total annual transport costs for each waste source are estimated by multiplying the per-trip costs by the total number of required trips per year as a function of truck capacity and waste volume. The model also supports the use of a default total wait time (e.g., 30 minutes) for all waste sources regardless of type. If the waste source and energy facility are collocated, the total travel cost is zero. We do not explicitly include factors for anomalous conditions such as site access issues, traffic congestion, and accidents; however, all model transportation factors can be easily modified to represent alternative truck turnaround assumptions. Further, we can represent turnarounds for other modes of travel (i.e., barge and rail), but implementing these modes of travel requires specific local knowledge regarding likely operating conditions and cost, which is why we do not yet use these modes in our national assessment scenarios, but we do plan to use them in planned local scenarios in FY 2024, if funded.

- Methodology details: We apologize for not sharing more details regarding the network and geospatially optimized siting models. We are in the process of preparing peer-reviewed manuscripts that will fully document and share our methodology, detailed model formulation, and underlying data. In the meantime, a more thorough description is offered here. Siting analysis is a two-step process, including (1) calculating realistic travel routes and costs and (2) using those data as the basis for a geospatial optimization to determine possible optimal facility and waste utilization solutions. The network modeling ("routing") was performed using parallelized automation routines we developed to iteratively execute the "pgr_dijkstraCost" function within the "pgRouting" extension of PostgreSQL 14 to calculate the least-cost path (travel time in hours) between each biorefinery siting candidate and its potential waste producers (i.e., neighboring waste generators) by traversing a roads network developed based on the U.S. Census Bureau's 2021 MAF/TIGER state-level edges datasets. For regional to local scales, we can use the routing data directly in the optimization model. But for national-scale assessment, we perform a regression on the travel costs by geographic region to enable the computational feasibility of the geospatial optimization (make it efficient) and to make the problem differentiable (continuous). The regression equations are then used as the primary input, along with the waste resource data, to the geospatially optimized siting model. The siting model is formulated as a (large) nonlinear optimization problem, which we solve using a standard open-source interior point algorithm (Ipopt: https://coin-or.github.io/Ipopt). Currently, the optimization is set up to maximize systemwide profitability, thereby determining the best use of each unit of feedstock when in proximity to multiple candidate facilities. But the objective function can be changed quite easily in the model.

- Model verification and alignment of results: We apologize for not sharing more details regarding the model verification. The following tests and quantitative metrics were designed and applied to evaluate the accuracy and consistency of the routing and siting models. We will describe the model verification in our planned peer-reviewed publications.

- Routing model accuracy and consistency: We performed a suite of manual, automated, and statistical tests to validate the routing model:
  - Run the "pgr_analyzeGraph" function to test the network topology.
  - A random sample of automated routing solutions was visually compared to manually queried route segments using the QGIS desktop to ensure 100% reproducibility.
  - Stress testing was performed to solve for all possible routes to identify potential network topology, software errors, or memory issues.
  - Auto-testing was performed to evaluate cumulative route error by ensuring that estimated travel times between all U.S. state capitals were within 2% of results from the Google Routes API.
  - Summary statistics were computed to (1) ensure 100% of routes had a solution and (2) assess average on- and off-network connection costs and total travel costs across all routing solutions to identify potential outliers, which may indicate network topology issues.
  - When used, the travel cost regression ends up being a linear regression, so its solution and associated error are well defined. Further, once we solve for an optimal siting solution, we can put the sited facility back through the more precise routing model to get a better estimate of true travel costs, if necessary.
- Geospatial facility siting model accuracy and consistency: The geospatial optimization relies on previously documented cost curves, calibrated parameters ("factors"), and constraints. The quality of the optimization solutions will be as good as the input data. Although not a perfect model, this approach enables us to quickly generate reasonable upper- and lower-cost and performance boundaries on emerging technologies to help reduce uncertainty and provide industry with confidence to take on transformative clean energy projects. Due to the unique combination of literature-based technology cost and performance data with actual waste mass and logistics data, a baseline for the direct comparison of our national siting projections does not exist. Although we cannot make 1:1 comparisons of our modeled feedstock gate price, energy productivity, or profitability estimates to previous experimental or empirical results, we can design special scenarios that allow us to approximate published cost and performance data for a particular technology at a specific engineering scale. For example, we can limit waste producers in our model to represent 100 dry metric tons of available sludge at a single site (or a few proximal sites), which should result in a sited HTL plant with similar total capital investment costs and net present value as the same sized HTL plant evaluated in the BETO HTL design study (https://www.pnnl.gov/main/publications/external/technical_reports/PNNL-27186.pdf), which was prepared using a detailed discounted cash flow analysis. It is not a perfect match because our feedstock prices are dynamic compared to the fixed feedstock prices used in the earlier studies. Measuring siting model consistency is a little more straightforward. Because this is a nonlinear optimization, a gradient-based algorithm like Ipopt will converge to the nearest local optima, which could be one of many, and is not guaranteed to be the global optimum. Finding the global optimum of a nonlinear, nonconvex problem (like this one) is NP-hard and infeasible for the size of problem we are considering. Instead, to improve our chances of finding the global optimum, we may solve the same scenario many times and statistically compare the results. Randomness in how the model generates candidate facility siting locations ensures that each model solution is different, which is desirable because it helps us better explore the solution space. In practice, if we observe

(1) objective function values for all solutions within 3% and (2) Rand index = 0.9, it indicates robust results (similar siting solutions across model runs) and gives us some confidence that even if we missed the global optimum, it would not be much better than the solutions we are finding.

- Support for data trends: We agree, adding support for temporal variability would be useful. Modulating waste flows, costs, and performance inputs improves our ability to investigate impacts from population growth, waste policies, market dynamics, etc. Currently, we are working with average annual values to maximize profit for an average year. This approach meets our current need for rapid sensitivity analysis; however, if our project is renewed in 2024, we could easily incorporate input variability in several ways, each with their own advantages and disadvantages and with some computational cost:
    - Adding an explicit temporal component to the model by accepting input data arrays and evaluating each timestep of the time horizon
    - Treating waste sources as random variables with known distributions that account for variability (or uncertainty) without an explicit representation of time (i.e., value changes each iteration)
    - Use either method to modulate facility capacity factors, which provides an integrated control on productivity, not just from changes in feedstock supply.
- Data and findings dissemination and improvement: We agree that disseminating results is critical. We do our best to ensure that published findings and data are easy to retrieve and cite by publishing the data in multiple common spatial and nonspatial formats. Our current baseline for feedstock data is the National Wet Waste Inventory, which we published as a peer-reviewed open-source dataset jointly with NREL in 2020 (https://doi.org/10.17632/f4dxm3mb94.1). The sludge estimates were subsequently updated based on more detailed wastewater treatment modeling and published online, including mass and energy flow estimates by waste phase (https://doi.org/10.1016/j.jenvman.2020.110852). At the end of our current project (FY 2023), we plan to publish our findings in a peer-reviewed article with a link to data on Mendeley. If funded, our FY 2024 project renewal plan includes scope to build some prototype (web) tools to help end users explore WTE data and results more easily. Successfully developing, deploying, and maintaining software requires careful life cycle planning to ensure that tools can be available after the end of a particular project. Regarding improving our source data, we can improve some data but not others. The National Wet Waste Inventory dataset was the result of a multi-lab, multiyear national resource assessment. It remains the best publicly available national inventory of wet organic wastes. The waste flow data for sludges and manures are high-precision point-based data. Food waste and waste fats, oils, and grease were prepared at a mix of spatial scales from point to county level and were downscaled to representative point locations. Updating the national inventory would require a level of effort equivalent to the original assessment and is not something we can tackle on an analysis project; however, on another project, we are working on a methodology for modeling food waste in a new way that could substantially reduce spatial uncertainty for nonresidential food waste. If successful, we could request funding to apply the methodology to update the National Wet Waste Inventory. The remainder of our input data come from the literature or publicly available data published by federal and state agencies. We inherit the data quality from these sources.
- TA program coordination: It is not our goal to compete with or start a new TA program. Rather, we hope to leverage the synergy between our project and the TA program to maximize impact for the public. We deliberately scope our analysis and model-building activities to facilitate the development of results and tools that can eventually be deployed to serve the public through the TA program. In fact, our FY 2024 project renewal proposal is specifically designed to integrate all our data, models, and lessons learned to deploy a demonstration workflow through the TA program that helps underserved communities perform and explore the results from siting, impacts, and trade-off analyses using easy-to-access tools and a standardized reporting package. In return, we can leverage the learning done through the TA program to guide our communication deliverables and tool development.

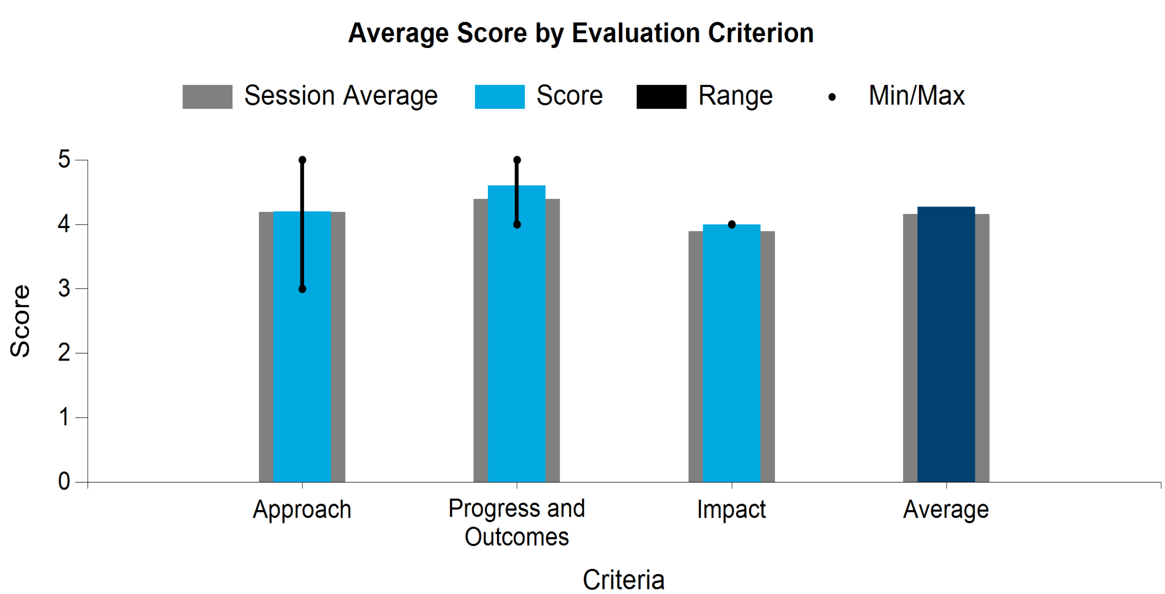
ANALYSIS AND SUSTAINABILITY INTERFACE

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.1.0.301
Presenter(s):	Karthikeyan Ramasamy; Katarina Younkin; Lesley Snowden-Swan; Michele R Jensen
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,800,000

This project provides technical, economic, and sustainability analysis support for several biomass conversion routes to hydrocarbon fuels and chemicals. In the context of the Organic Waste Conversion area, this presentation focuses on the project's wet waste HTL task. Building on previous wood and algae work, PNNL began testing, modeling, and TEA of the wet waste HTL and biocrude upgrading process in FY 2016. The design case projecting the 2022 cost target for the pathway was published in 2017, and annual state of technology (SOT) assessments were conducted since then to guide the research and track the modeled performance, GHG emissions, and MFSP toward BETO's targets. Data availability is a risk mitigated by frequent interaction with the team to continually review sustainable cost reduction strategies. The combined experimental/analysis efforts reduced the modeled SOT MFSP by $0.67/GGE and developed an initial assessment of jet blendstock production from HTL. Modeled SOT GHG emissions for the pathway are 77% lower than petroleum. Several options for the treatment of the aqueous phase were assessed, and our HTL reduced-order model was bolstered to include 29 continuous run datasets. Work in FY 2023 and beyond is focused on the development of business cases that will serve to bridge the gap between traditional SOT assessments and the needs of key external stakeholders to help accelerate technology adoption.



COMMENTS

- There is a clear management plan, communication strategy, and DEI goals to approach this work. The work has clearly incorporated a lot of learnings from HTL projects that BETO and others have funded. They seem to be incorporating them within a reasonable time frame.

- The team regularly incorporates the learning from the experimental members to update the SOT. This engagement and connection is valuable for the success of this project and also helping to unintentionally pass learnings between other projects. The project has achieved progress toward its goals and outcomes.
- While the dollars are fixed to a year, I'm curious about the impact of inflation around equipment, items, and labor versus general inflation.
- As an analysis task, this project is not intended to be commercialized by itself. The other challenge is that the commercial WTE space is still nascent, which would provide real-world feedback. The next phase of this project will address much of this, which should lead to an increased score in impact. Just the way the project is phased results in more of a wait-and-see score for impact.
- The team has reduced the Aspen model about HTL production to a publicly available Excel sheet. This simplified form makes the insights and analysis more accessible.
- The amount of 110 dry tons/day is a fairly large scale. The sensitivity of MFSP to this value will be critical. Not advocating for much smaller, but maybe one-third the size.
- Overview/impact:
    - This project generally aimed at optimizing the pathways through which bioenergy is obtained from wet waste with regard to cost reduction, increasing bioenergy yields, and reducing environmental contamination. To achieve this, the researchers used experimental values to develop HTL models and carried out TEA and LCA to obtain critical data, key cost drivers, and key techniques required for scaling up WTE techniques applied in the laboratory. They also used the aforesaid techniques to determine the most sustainable and environmentally friendly techniques for waste valorization to energy. GHG emissions that can emanate from HTL systems were also assessed. The approach applied in this project is very pragmatic, as HTL model parameters are based on real data and not on assumptions.
    - So far, within the short period of time the project has been operational, it has progressed well. For the first phase of the project, the researchers have been able to model a pathway that reduces MFSP by \$0.67/GGE and GHG emissions to 21 g CO_2e/MJ, which is 77% lower than the petroleum baseline value.
- Strengths: The project has very good management and communication plans. Also, the project has a good DEI plan that ensures that underrepresented and marginalized people/groups are well represented through their inclusion.
- Questions: One aim of the project was to assess the quantity/volume of GHGs that emanate from HTL—the researchers presented GHG reduction values predicted using their model; however, the researchers did not show the key elements of GHGs that were included in the model. Also, in slide 7, where the process flow of the model is presented, it can be noted that the solids from the HTL unit and those from treating the aqueous-phase units are sent to the landfill. Is there no other way the solids can be better managed? Further, the scenarios considered in the study make a lot of sense; however, some of the assumptions used are superficial (e.g., the assumed scale of the HTL unit is too big). The researchers should consider conducting a sensitivity analysis to assess the impact of different HTL unit scales on the economic viability of the system. In slide 13, the researchers present the sensitivity analysis results; however, it would be great if the researchers could also use other methods for assessing the economic viability of HTL units, such as breakeven point and net present value.
- This project provides useful contextual research for HTL and biocrude upgrading projects, taking an iterative approach to identifying and sharing insights on cost drivers and real-world operations as

research in these areas progresses. They are to be commended for including waste generators as stakeholders to inform this research direction. Among positives of this important work are leveraging the modeling/analysis work across other BETO projects and industry/university collaborations. The project's FY 2023 plans to engage a broader audience of stakeholders are good.

- The DEI aspect of the project plan could be strengthened. The stated goal of hiring only one student intern from an underrepresented group and/or disadvantaged community is a start of what should be a more comprehensive effort to pursue representation among project staff at multiple levels as well as to proactively consider community impacts of projects that will involve infrastructure, wastes, and emissions
- This project (as I understand it) is primarily a TEA for the application of HTL to convert organic wastes into SAF. This project basically seems to be a more practical envisioning of how organic wastes to SAF (via HTL) could occur. For example, an initial assumption might be that the WWTFs would house the HTL facility, but this is not likely feasible given that wastewater treatment personnel are poorly suited/trained (and they are already busy) to produce SAF. The outcome of this work is more reasonable/achievable visions for how organic wastes to SAF can be achieved.
- The project has an excellent team with a very good project management plan. The project has an appropriate focus on DEI with numerous internships going to women and to various underrepresented groups. I expect very high impacts from this work, although this has yet to be achieved because the project is still relatively new (i.e., about halfway through the project period).
- Similar ambitious goals to WBS 2.1.0.112 and WBS 2.1.0.113; together, these analyses can inform the information modeled and shared with local governments and industry to further reduce organic wastes to produce bioenergy.
- The project has clear goals and targets to convert dry wastes through HTL to SAF. The project has provided a survey to industry to ask what information they need to analyze the project's viability, demonstrating collaboration with industry to guide project deliverables.
- How have initial assumptions of HTL owned by the municipality set back TEA/MFSP? WRRFs could continue to pay tipping fees for sludge removal, but would the demonstration of the profitable conversion of wastes presumably lower tipping fee expenses for WRRFs?
- Looking forward to developments as this new project continues. The characterization of wastes at this scale will enable large shifts in production and GHG reductions and lead to decreasing costs of bioenergy-derived fuels.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the time spent by the reviewers and for all their insightful feedback.
- Response to Reviewer 1: Thank you for your acknowledgement of our contribution to multiple BETO projects, efforts in management, communications, and the value of the open-access HTL process model from the reviewer. We regret that under the time constraints we did not emphasize the efforts of evaluating our technology at multiple pricing years. The impacts of inflation around equipment, items, and labor on the sludge HTL process can be found by comparing the results shown in slide 10 (2016 pricing basis) and slide 13 (2020 pricing basis). The modeled MFSP increased from \$2.85/GGE to \$3.15/GGE (10.5%) when moving from a 2016 to 2020 pricing basis. The general inflation from 2016 to 2020 is 7.8% according to the U.S. Bureau of Labor Statistics. The increase in MFSP is slightly higher than the general inflation rate (10.5% vs. 7.8%) because different indexes were used for chemical, labor, and equipment in the TEA model. We appreciate the reviewer's acknowledgement in our ongoing business case study and its potential to address feedback from the commercial WTE space. Industry

partners are actively participating in the project to establish specific sites of interest, key metrics, and priority outputs for deployment. We agree that the sensitivity of MFSP on the plant scale is critical. Due to the time limitation, we did not present related sensitivity studies in our previous works and other projects. The 2021 SOT study (https://doi.org/10.2172/1863608) presented a sensitivity study on a 2016 pricing basis regarding the plant scale. The modeled minimum biocrude selling prices are $1.7/GGE at a scale of 110 dry tons/day, $2.8/GGE at 50 dry tons/day, and $5.0/GGE at 20 dry tons/day. We would like to emphasize that the sensitivity of MFSP on the plant scale will change as the HTL technology keeps advancing. It is valuable to understand the impact with the most recent SOT. We are working closely with our industry partners and the Waste-to-Energy: Optimized Feedstock Blending at Scale project to understand the real-world supply and infrastructure of organic wastes and determine the plant scale for the baseline and sensitivity study.

- Response to Reviewer 2: Thank you for highlighting our effort in using real data instead of assumptions for modeling and our management, communication, and DEI plans. We would like to acknowledge that the GHG reduction evaluation of the sludge HTL process was conducted by our collaborators at Argonne National Laboratory. Details were presented by Argonne in another talk under the Data, Modeling, and Analysis session during the Project Peer Review ("Life Cycle Analysis of Biofuels and Bioproducts and GREET Development"). The key GHG emissions contributors can be found in slide 17, including natural gas, quicklime, and electricity. The modeled process improvements in the SOT over the past 2 years significantly reduced the chemical and utility demand, resulting in GHG reductions increasing from 53% for the 2020 SOT to 77% for the 2022 SOT. Thank you for pointing out the gaps in solids treatment. PNNL's HTL experimental team is actively investigating valorization options for the solid product (i.e., fertilizer production). We would like to emphasize that in this project, process modeling and TEA were performed based on actual data. We will follow our communication plan and include alternative options for the solid products once we receive quantitative results from the experimental team. Regarding the plant scale, a survey of existing wastewater treatment plant scales was conducted in our 2017 design case study (https://doi.org/10.2172/1415710), where a scale of 110 tons/day was selected in the base case due to the concern of economic feasibility. A number of U.S. wastewater treatment plants have scales greater than or equal to 110 tons/day, including the Great Lakes Water Authority, the specific site selected for this year's business case study. In addition, a sensitivity study varying plant scale from 20 to 500 dry tons/day is presented in our 2021 SOT report (https://doi.org/10.2172/1863608, Figure 13). As the HTL technology keeps advancing, it is important to revisit the sensitivity study regarding the plant scale. Moving forward, we will work closely with our industry partners and the resource analysis projects to determine the most relevant base case scale and range of scales for sensitivity studies. Thank you for suggesting other economic methods. Actually, this is included in the scope of our FY 2023 work as a critical component. Particularly, the team will study the economics of a first-of-a-kind plant for the specific site application, including the metrics of most value to partners, such as MFSP, net present value, payback period, and/or breakeven fuel price.

- Response to Reviewer 3: Thank you for highlighting the value of this project and our collaborations with other BETO projects, industries, and universities. We regret that due to the time limitation, we did not get a chance to present the organization-level plan of DEI. PNNL's strategic philosophy entails more than just looking at the demographic numbers related to diversity but also focusing on developing leadership competencies that create and maintain an inclusive culture. The bioenergy research area at PNNL is woman-led by Sector Manager Corinne Drennan. We are using the FY 2022 BETO Lab Call to increase the involvement of members from underrepresented STEM groups as project leads. In the current portfolio, 28% of co-PIs are women. In the response to the current lab call, 33% of responses are women-led, and 43% of co-PIs are women. For pursuing representation among staff at multiple levels, we will require contributions from multiple projects instead of one single project, and an organization-level plan. Environmental justice is not within the scope of this project; however, a team of experts at PNNL has developed the environmental justice LCA capability that complements conventional LCA by considering geospatial and community-level impacts. We are actively collaborating with the environmental justice LCA team at PNNL to evaluate the community impacts of sludge HTL regarding infrastructure, wastes, and emissions under different projects.

- Response to Reviewer 4: Thank you for highlighting our achievement in the past 2 years. In the remaining project period, we will increase the impacts from this work by including more collaborations with industry stakeholders, first-of-a-kind plant costing for a specific site, carbon credits, sensitivity study, and uncertainty quantification into the FY 2023 design/business case study.
- Response to Reviewer 5: Thank you for highlighting our collaboration with the waste resource analysis projects and potential impacts at scale. Regarding your question, the change in system boundary assumption with the inclusion of a $40/wet-ton tipping fee and waste disposal fees resulted in a $0.76/GGE reduction in modeled MFSP ($3.61/GGE for old system boundary vs. $2.85/GGE for the new system boundary). We regret that we did not emphasize our investigation on the tipping fee assumption and sensitivity study. In the base case, the tipping fee was set based on a survey of the present market status, of which the value is also within the typical range of organic waste landfill cost. We agree that the demonstration of the profitable conversion of wastes presumably may lower tipping fee expenses for WRRFs. At the same time, regulations for waste disposal are becoming stricter and may potentially result in higher landfill costs and therefore higher tipping fees. Due to the uncertainties in market scenarios, a sensitivity study was conducted in the 2021 SOT study (https://doi.org/10.2172/1863608, please refer to Figure 13), where sludge credit varied from $0 to $350/dry ton. The modeled minimum biocrude selling price would decrease by $1/GGE with a $100/dry-ton increase in the sludge credit.

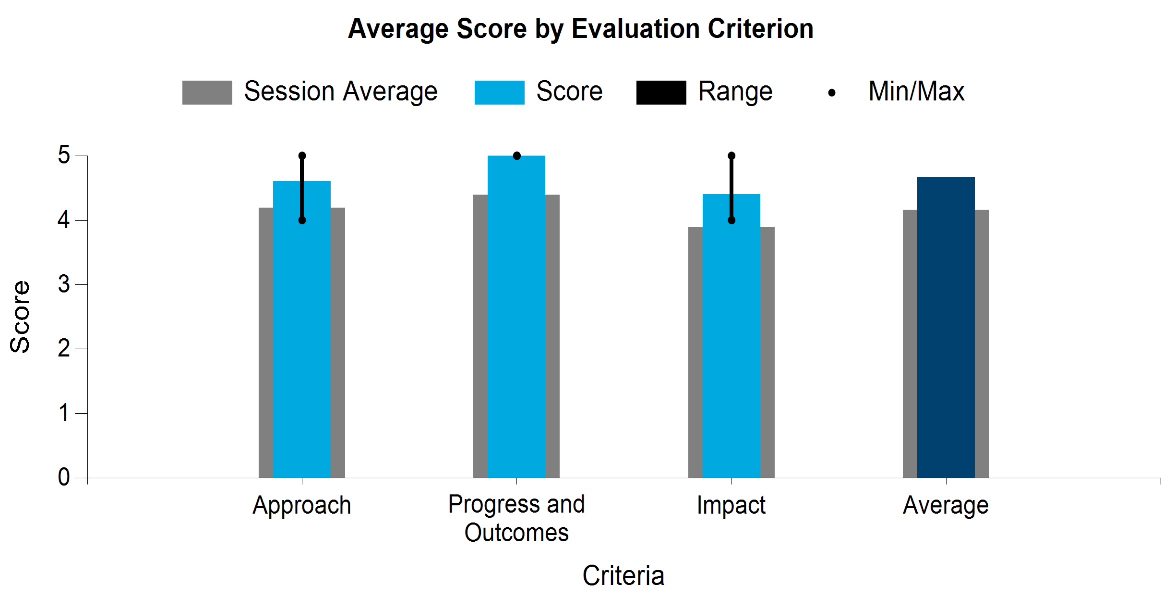
BENCH-SCALE HTL OF WET WASTES

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	2.2.2.302
Presenter(s):	Karthikeyan Ramasamy; Katarina Younkin; Michael Thorson; Michele R Jensen
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,200,000

HTL can solve the wet waste disposal problem by converting wet wastes to fuel with the potential for 5.5 billion gallons/year of transportation fuel in the United States. The focus of this project is to advance HTL to enable the conversion of waste feedstocks to biofuel intermediates that can meet industry-relevant cost and performance requirements with a focus on SAF capable of >70% reduction in GHG emissions. This project has made key advances by (1) demonstrating the industrially relevant and stable hydrotreating of the HTL biocrude to fuels (2,000 hours of hydrotreating) and (2) demonstrating the potential for regional blending of wet wastes to improve process yield and performance. Current research efforts are focused on (1) side stream disposal, including aqueous and solid streams, which are crucial barriers for commercial deployment; (2) forever chemical destruction, including PFAS and perfluorooctane sulfonic acid (PFOS); and (3) nutrient recovery of P/N for fertilizer applications. Thus far, this project has demonstrated the applicability of a mild wet air oxidation process to increase the bioavailability of the HTL aqueous stream by converting organic content to carboxylic acids with a high yield (>60%), improving ammonia capture, and reducing the volume of residual solids. This project tracks forever chemicals through all HTL process steps to quantify the destruction and partitioning of residual PFAS through hydrotreating, wet air oxidation, and struvite recovery.



COMMENTS

- Addressing some of the significant remaining barriers to commercialization: aqueous waste stream, nutrient recovery, catalyst life, and scale.
- Also tackling a big use case in addressing PFAS chemicals, as this is going to substantially increase treatment costs and/or land disposal/tipping fees.

- Progress has been clearly made on these items, as witnessed by the data and the substantial decreases in the SOT values.
- Tackling SAF clearly has value with the coming electrification of most vehicle fleets. The pivot and proof around the quality of the fuel shows high promise for this technology.
- Appreciated the layout of the goals and the show of progress. Clean and easy to follow.
- Incorporation and execution of DEI goals.
- HTL is coming up against the limits of commercialization that can be done by a national laboratory. Private projects have developed slowly for myriad reasons, which is less than ideal.
- Curious to understand more about the fate of the F atoms from the PFAS.
- Overview/impact/progress:
    - The project examined the feasibility of using HTL as a means of treating and managing wet waste while simultaneously generating biofuel SAF. Using HTL to convert wet waste to fuel eliminates the need for drying, which is one of the most expensive steps in the process of converting WTE.
    - What makes this project particularly interesting and impactful is that the researchers are addressing key issues, such as the fate and removal of emerging contaminants (i.e., PFAS) from wet waste (i.e., sewage sludge) during HTL as well as the extraction of nutrients (phosphorus and nitrogen) from the resulting HTL side stream. They also apply mild oxidation for treating the aqueous-phase liquid resulting from the HTL process, which removes recalcitrant contaminants, thereby making it recyclable. In sum, the researchers are also looking at how to make the use of HTL more sustainable. The project is highly relevant to the aviation and energy sector, as it is aimed at increasing the proportion of jet fuel that is made from renewable energy, leading to the gradual decarbonization of the aviation transport sector.
    - So far, the researchers have made considerable progress in this project. The researchers were able to achieve stable continuous hydrotreating of biocrudes from mixed fuels (>1,500 h) and >75% extraction of phosphorus from HTL solids.
- Strengths: The researchers are employing a multi-integrated framework, as they are collaborating with industry partners, and they use the results of their research to inform the commercial design of hydrothermal liquefiers.
- Weaknesses: In the presentation, the researchers indicated what they want to do and how much progress they have made so far; however, they did not clearly present the steps/process they used in achieving the set objectives. For instance, one objective of the study was to develop a process to extract valuable fertilizer coproduct from HTL side stream, and they were able to extract >75% phosphorus, but they did not provide the methods they used in doing this. The researchers also need to consider the feasibility of scaling up the proposed technique. Further, the researchers indicated that they made use of catalysts in the conversion process and that they achieved industrially relevant catalyst lifetimes; however, they did not mention the type of catalyst they used in the process and why.
- This project tackles a timely and important topic, which is the conversion of treated wastewater sludge and other dirty wet waste feedstocks into usable fuels, with the essential added-value aspect of PFAS destruction and N and P recovery. This suite of approaches, if scaled and economically viable, and proven in a transparent, public fashion, stands to be a game changer in wastewater treatment as the understanding of PFAS risks throughout the food web increases. It also poises WRRFs for a new role as

net withdrawers of PFAS and other forever chemicals from ecosystemic circulation, which is also a massive system improvement at this time in the history of human-induced ecological collapse.

- The researchers are encouraged to document the destruction rates of as many PFAS/PFOS compounds as possible, not only those that are currently identified by the U.S. Environmental Protection Agency for designation as hazardous, and to include steps to verify that the resulting biocrude is indeed hydrotreated, commenting on the presence of HF in the resulting product, which was mentioned. The worst thing that resulting work from this project could do is to provide WRRFs with the assurance of PFAS destruction without complete and transparent end-to-end verification.
- With respect to the DEI aspects of the project, the team should go well beyond hiring one student from an underrepresented group to engage students from schools, colleges, and universities that serve Black, Indigenous, and other people of color communities, including historically Black colleges and universities (HBCUs) and tribal colleges, with attention to outreach, recruitment, retention, and promotion, as well as building an understanding of the context of industrial operations such as are studied in the project for diverse communities and stakeholders. While staff have taken required trainings, they are encouraged to consult DEI practice literature around the history of racism, sexism, and other forms of systemic exclusion in the field of environmental engineering R&D to refine their approach.
- To the extent they have not yet done so, the researchers are encouraged to make contacts with water/wastewater trade associations, such as the Water Environment Federation and Water Research Foundation, as part of future community engagement, as well as with trade associations seeking to continue land application of biosolids, such as Northwest Biosolids, whose business model stands to be destabilized by near future PFAS regulation, as well as the emergence of HTL as a treatment alternative at scale.
- This project focuses on the HTL of sewage sludge and/or food waste to produce SAF. One major outcome of the work was to demonstrate the stable, long-term processing of waste to fuel (1,500 hours). Another aspect of the product focused on the nitrogen and phosphorus content of the waste stream/feedstock. One solution was to precipitate this material as struvite, which is a mineral sometimes intentionally produced at municipal WWTFs (and it is attractive as a fertilizer). Much of this work is driven by TEA and LCA, with the goal of producing cost-competitive SAF via HTL. After watching this presentation, I am optimistic that this goal is achievable.
- The project is well managed, organized, and highly productive. The DEI goals appear to have been met; I am particularly pleased that DEI training is part of the requirements for participating in the proposed project. I like this because other metrics of DEI “success” appear to be easily manipulated, whereas the completion of a DEI training program is tangible.
- The project demonstrates HTL treatment processes that create fuel, usable solids, the destruction of PFAS-group chemicals, and the recovery of fertilizers (P and N) to further reduce the need for expensive, fossil-fuel-derived fertilizers that are prone to supply shocks.
- The research has utilized many partners for deployment and feedstock analysis to ensure full consideration of real-world fuel types. Results are showing clear benefit for the performer and government while providing valuable SAF. PFAS will be an emerging expense for municipalities in treating organic waste streams. This process offers the ability to finance facility upgrades by creating several revenue streams and offers a solution to reduce the flow of PFAS-containing water and biosolids into other areas of our natural environment.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful feedback on our project. We are grateful for the recognition of the progress we have made (“Progress has been clearly made on these items, as witnessed by the data and the substantial decreases in the SOT values"), that we "are addressing key issues such as the fate and removal of emerging contaminants (i.e., PFAS)," that this "project is highly relevant to the aviation and energy sector," and that "the researchers have made considerable progress in this project."

- Barriers to commercialization: We acknowledge the significant remaining barriers to commercialization, including the aqueous waste stream, nutrient recovery, catalyst life, and scale. We are actively addressing these challenges and making progress in overcoming them. The data presented in our work demonstrate substantial decreases in the model SOT costs, indicating clear advancements in these areas.
- PFAS chemicals: We recognize the importance of addressing PFAS chemicals in our project. We are aware that their presence can substantially increase treatment costs and land disposal fees. Our research aims to tackle this issue and find effective solutions to minimize PFAS contamination. We will continue to provide updates on the fate of F atoms from PFAS and include more information in our future reports to enhance understanding.
- DEI goals and community engagement: We value the importance of incorporating DEI goals into our project. We agree that our DEI impact needs to extend beyond hiring one student, and we are actively engaging with the broader community. We will leverage our contacts with water/wastewater trade associations and biosolids trade associations to foster community engagement and address the concerns of diverse communities and stakeholders.
- Complete PFAS destruction: We acknowledge the need for complete and transparent verification of our PFAS destruction results. As noted by Reviewer 3, "The worst thing that resulting work from this project could do is to provide WRRFs with the assurance of PFAS destruction without complete and transparent end-to-end verification." We will ensure that destruction rates of various PFAS compounds are documented, and we will include WRRFs in the workflow process to ensure that we provide complete and transparent verification of our PFAS destruction results. Again, we sincerely appreciate your positive feedback and insightful suggestions.

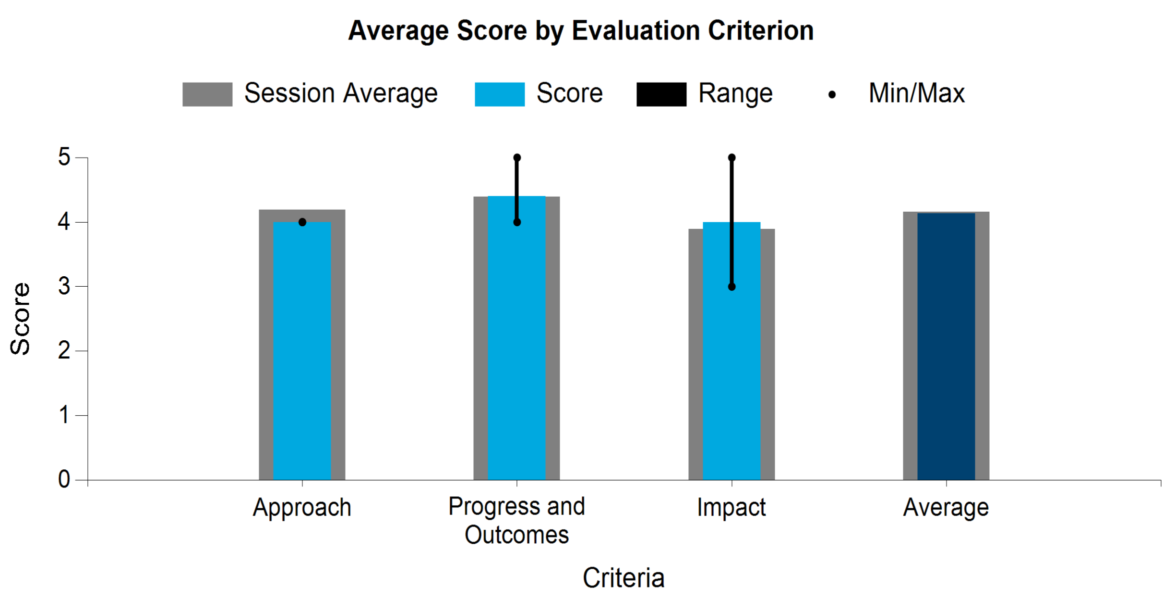
CATALYTIC UPGRADING OF CARBOHYDRATES IN WASTE STREAMS TO HYDROCARBONS

North Carolina State University

PROJECT DESCRIPTION

WBS:	2.3.1.209
Presenter(s):	Rosemary Loycano; Sunkyu Park
Project Start Date:	10/01/2018
Planned Project End Date:	09/30/2023
Total Funding:	$3,094,759

The primary objective is to develop a technology for converting the carbohydrates in paper sludge, a wet organic industrial waste stream, into a hydrocarbon biofuel, both economically and sustainably. BETO has identified wet organic waste streams as valuable potential feedstocks for the bioeconomy. This project will develop an integrated process using wet paper sludge where no drying of the feedstock is needed. The process includes (1) ash removal from paper sludge, (2) enzymatic hydrolysis of carbohydrates to monosaccharides, (3) dehydration of pentoses and hexoses to furfural and hydroxymethylfurfural, (4) aldol condensation of furans with ketones to intermediates having molecules with 10–14 carbons, (5) hydrodeoxygenation of the intermediates to paraffins with excellent properties for blending in jet or diesel fuel, and (6) robust TEA and LCA to focus research on developing cost-effective routes to address key cost barriers and ensure the sustainability of the process. The developed process will be validated at a relevant scale to produce sufficient hydrocarbon biofuel for fuel property testing.



COMMENTS

- It is really quite refreshing to see all the contact that was done to paper mills. The team took the time to visit plants and speak with staff. These kinds of conversations are the most invaluable kinds of customer discoveries.

- The team then took the time to solicit real feedstocks and do the characterization. Subsequent tests were done with one of the actual feedstocks, which is ideal. Truly appreciate the effort around this issue.

- Pulp and paper waste is certainly a big challenge to turn into SAF relative to a lot of other feedstocks. The team is tackling quite an important issue, alongside the other feedstocks being tackled by BETO projects.
- The team has a good management, communication, and risk plan. There did not seem to be any DEI elements as part of the project plan.
- The team did a lot to pivot from diesel to SAF part of the way through the project, and they navigated those changes fairly well.
- Relative to many other WTE feedstocks/conversion processes, this material seems to have a much higher MFSP.
- The technology seems to be at an earlier stage; it will require a lot of valorization of other streams. Certainly see a lot of promise in being a supplementary cementitious material if it as rich in Ca as it is.
- Does not necessarily seem like it is ready to be commercialized/deployed immediately following this program. Also does not seem to have an involved commercialization partner.
- The project has met all the goals as they have been set out, and it appears on target to meet its final objectives/deliverables.
- Overview/impact:
    - The researchers in this project developed a sustainable and economic technique for transforming the carbohydrates in paper sludge into hydrocarbon using a combination of enzymatic hydrolysis, aldol condensation, and hydrodeoxygenation. The production of fuel from paper sludge serves as a means of incentivizing and sustaining the proper management of paper sludge. The approach used in this study is futuristic and will help with the effective management of paper sludge produced by mushrooming paper industries.
    - Considerable progress has been made in this work, and most set targets have been met. In the pretreatment of the paper sludge, the researchers were able to obtain about >90% ash removal and >65% carbohydrate retention. The project findings suggest that carbohydrates in the sludge could be converted to 150 million gallons of diesel fuel, showing that this project aligns with DOE's strategy for the production of high-performance biofuels from waste feedstocks.
- Strengths: The project involves the collaboration of several academic and industry partners. Also, the channels of communication used in this project are highly commendable.
- Weaknesses: The researchers did not indicate anything about the originality and novelty of their work. In the presentation, it is indicated that a lot of progress has been made with respect to the set objectives; however, the PowerPoint presentation does not provide a clear overview of how each of the objectives was achieved. Further, the catalytic upgrading of carbohydrates in waste streams to hydrocarbons using enzymatic hydrolysis is a novel approach; however, I am wondering if the researchers have considered its applicability to the existing paper production facilities for sludge management. In slide 23, the TEA provides an MFSP of about $5.67/GGE, and this seems high. I am wondering if researchers could consider other economic benefits associated with their proposed technique that would help reduce the fuel selling price. For example, costs associated with the disposal of paper sludge should be considered. Last, in slide 10, the researchers present the ash percentage in the paper sludge; however, these values significantly varied. Therefore, characteristics of the paper sludge should be given a high priority in the scaling up of the technique, as this will have a significant effect on the ash content and viability of the proposed technique.

- Recommendations: The authors made mention of examining three different paper sludge types and developing solutions that fit each sludge type; however, it would have been good if the authors consider using the chemical composition of these sludge types and the way they react to the catalytic upgrading to develop models that can fit different sludge types and not just the three sludge types they plan to examine. This is done as a way of tackling sludge variation between mills.
- The project seeks to develop an economic and sustainable process for the conversion of carbohydrates in paper sludge into a biocrude output that can be refined into SAF considering this feedstock's high ash content. Researchers showed good engagement with industry participants and regular communication among project partners.
- As the project proceeds, researchers should take note of major differences in pulp composition from virgin versus recycled feedstocks. Recycled papers contain, among other things, varying levels of added PFAS and microplastics used in coatings and finishings. Researchers should also contrast project cases with alternative pathways for carbohydrate conversion, including fermentation. Finally, the researchers should draft a DEI engagement plan for project staffing and outreach that includes students from underrepresented groups at levels between the high school and doctoral levels.
- The goal of this project was to convert organic wastes from the pulp/paper industry to hydrocarbons. Paper sludge is about 10% of the raw product used, but the disposal of the remainder costs about $30 per wet ton, which translated to about $250,000,000 per year for waste disposal for the industry. The project is a collaboration among researchers at North Carolina State, Yale, and NREL. There were regular (monthly) online meetings among the project participants as well as less frequent in-person meetings with all collaborators.
- NREL does conversion of paper to hydrocarbons. Trying to make biofuel from paper. In Year 3 of the project (about 6 months left). Monthly meetings. In-person meetings with all collaborators.
- The project approach was very linear and logical. The investigators have done a nice job meeting all their various milestones. I was particularly pleased that the TEA (and LCA) process identified a financial bottleneck, which the researchers identified and then pivoted to reduce the cost of the process (i.e., shift from using dioxane to acetone).
- Really nice application of the TEA driving a modification of the plan to get a more reasonable price to produce the jet fuel.
- In many ways, this seemed like a nice example of how BETO's various requirements (i.e., required partnerships, LCA, and TEA) can work very well.
- The team is actively managing the project and includes clear roles and interactions among researchers and the inclusion of industry partners. The project includes waste from 11 facilities that produce paper sludge to analyze input factors and design a treatment solution. Risk in ash management and alternative methods to manage high-ash waste has been an issue, but the project has found a simple, low-cost, low-input way to separate ash.
- This project has the potential to create high-value SAF bioenergy from typically low-potential, high-moisture waste, moving 8 million metric tons of waste from current disposal practices (land application, lagoons, and incineration) while separating ash product that may further reduce energy inputs in the concrete industry.
- The project in its remaining months will need to consider the incentives available for the creation of renewable SAF and valorize ash resources in order to move this technology further toward deployment and increase its impact.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the review panel for their supportive and constructive comments regarding this project.
- The reason that DEI elements are not currently included in this project's plan is that DEI objectives were not required when the request for project proposals was made in 2018. All the organizations currently taking part in this project are aware that the importance of DEI has become recognized since then and are looking to involve underrepresented groups in the research being conducted in projects such as ours.
- As the reviewers noted, there are some scenarios where the MFSP is relatively high ($5.67/GGE) for the base case; however, we have changed our solvent system to acetone after the intermediate verification, which considerably reduces the calculated MFSP to $3.49/GGE.
- A recommendation was made for us to consider how the chemical composition of different sludge types might affect the catalytic upgrading of the carbohydrates to hydrocarbons. In our work to date, we have determined the carbohydrate, lignin, and ash contents of the paper sludge samples we have obtained, plus the elements present in the inorganic component of the sludges, which is mostly Ca from the $CaCO_3$ filler used in making paper. A large fraction of this inorganic component is removed during deashing. Residual $CaCO_3$/ash does affect how much HCl must be added to get the proper pH for efficient enzymatic hydrolysis of the carbohydrate; however, it has not so far appeared to affect downstream catalytic processes. Elemental analyses of used hydrodeoxygenation catalysts have not found levels of elements (such as Ca, K, Mg, Na, P, S, Sr, Cu, and Cr) significantly higher than those found in unused catalysts.
- So far, we have not identified the presence of PFAS or microplastics in the paper sludges we have obtained, nor any effect they might have on our catalytic processes. One sample of low-ash-content sludge we received from a mill making paper tissue was resistant to enzymatic hydrolysis. We think this was due to the addition of a polymer (wet strength agent) that coated the paper fibers, restricting access of enzymes to the fibers.
- The main variable we have encountered between different paper sludge samples is their ash contents, and we believe that the side hill screen provides an efficient means of removing the ash from most paper sludges, allowing subsequent downstream operations to convert the carbohydrate component into hydrocarbons without a problem.

NOVEL AND VIABLE TECHNOLOGIES FOR CONVERTING WET ORGANIC WASTE STREAMS TO HIGHER-VALUE PRODUCTS

The Research Foundation of SUNY, University of Albany

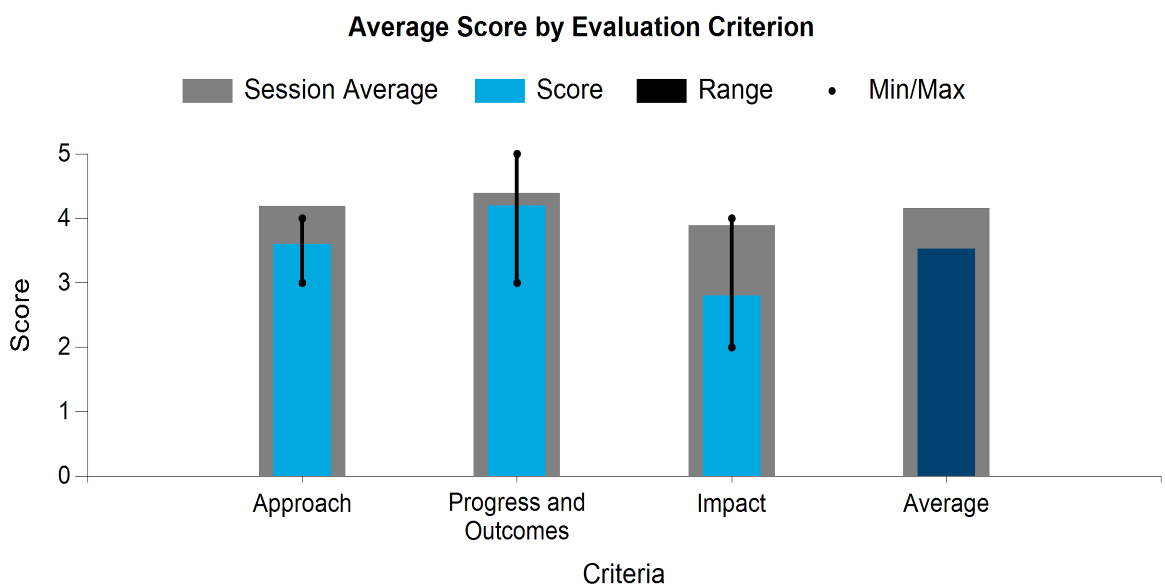
PROJECT DESCRIPTION

WBS:	2.3.2.226
Presenter(s):	Yanna Liang
Project Start Date:	10/01/2019
Planned Project End Date:	05/31/2023
Total Funding:	$3,408,092

The overarching goal of this project is to develop an integrated and efficient process for converting wet organic wastes to VFAs. To achieve this goal, we aim to accomplish seven different objectives:

1. Identify the optimal pretreatment method for each target waste stream.
2. Determine the best process parameters for arrested methanogenesis.
3. Evaluate the product yield and titer of VFAs from the waste streams separately through MES with CO_2 capture and conversion.
4. Develop an innovative membrane-based liquid-liquid extraction process for extracting VFAs and carboxylic acids out of the fermentation broth.
5. Perform preliminary LCA and TEA for each process block and the overall process.
6. Operate the integrated process continuously at a 5-liter scale for at least 3 months.
7. Operate the integrated process continuously at a 50-liter scale for at least 100 hours. TEA and LCA will be performed for this operation.

Upon finishing all the proposed objectives, we expect to have developed one of the first scalable, economically competitive, and environmentally sound processes for converting wet organic waste streams to high-value products.



COMMENTS

- The team did quite well at arresting methanogenesis in this project and driving production toward VFA production.
- The modeling analysis was quite strong, and it shows potential in describing what was seen experimentally.
- It would be curious to see, if a different wet organic waste stream were chosen, if the model would be robust enough to still function reasonably well.
- The project seemed to fastidiously proceed through the individual steps and is well positioned to complete their final goals around the 50-L reactor.
- Glad to see that someone explained that H_2 has demonstrated greater electron efficiency than direct contact.
- Given the early technology readiness level (TRL), I'm not sure about the commercial potential. Also, this team did not seem to engage with commercial entities.
- The research accomplished its goals and presents an opportunity for this team or others to continue.
- The GHG emissions savings for these products appear to be important, but does it also make financial sense?
- Not really sure about the integration of these unit operations at industrially relevant scales.
- The research is solid; the challenge is with programmatic offices at DOE, it needs to be applied.
- Did not seem to spend much time discussing project management, but given its performance to date, success is inferred.
- Did not see any comments on DEI or outreach.
- Engaging with local WRRF.
- Overview/impact/progress:
  - The researchers investigated the use of a novel technique: membrane-based liquid-liquid extraction for the continuous extraction of VFAs from wet organic waste streams. The novel technique was applied after improved VFA production from wet organic waste streams through MES and arrested methanogenesis. The project is highly impactful as it entails the conversion of food waste and sewage sludge to biofuel, thereby serving as a way to avoid the negative impacts associated with landfilling the waste.
  - The project is on track, as all the milestones that were set out at the beginning have been reached. Also, the plethora of presentations, awards, patents, and publications associated with this project shows that the project is of high importance to the scientific community.
- Strengths: It can be said that the researchers developed a vanguard technique for continuous VFA production from organic waste, which is very laudable.
- Questions/weaknesses: The researchers indicated that the overarching goal of the project is to systematically evaluate the whole process of converting organic wastes to high-value products, but from the presentation, the only high-value target product is VFA, as they did not make mention of any other

product. In the PowerPoint presentation, it can be noted that the researchers were dealing with the extraction and conversion of VFAs from food waste and sewage sludge; however, the methodology used is not clear—everything seems jumbled up, as there is no logical flow from one step to another. Also, the researchers state that they are converting the organic wastes to high-value products, and in this case, VFA using different methods. I expected the researchers to take the initiative of explaining/examining the composition of different VFAs they obtained from different methods to know which method gives the best results. Further, I am wondering if the researchers have considered the variability of the feedstock and its effect on the performance of the system. It would be great if they could assess the effect of feedstock type and characteristics on the performance of the system. Last, the researchers should consider assessing the feasibility of scaling up this technique or incorporating it into the existing system.

- This project is a systematic evaluation of wet waste conversion to high-value outputs such as biomethane and biocrude, with emphasis on the capture of VFAs. Among the project's strengths are that it addresses both food and wastewater residuals as feedstocks, and it proposes a continuous process to produce VFAs that can be valorized as bioproducts. The GHG profile of this process, compared to a fossil benchmark, heavily depends on pretreatment with arrested methanogenesis. Researchers should keep the viability of this treatment configuration (integrated system), in terms of commercialization and community acceptance, in mind as the progress progresses.

- The award was made prior to BETO's DEI requirements, but the researchers should start to develop a proactive DEI strategy that includes outreach and staffing, targeting students from the high school through doctoral levels, to ensure continuous participation of underrepresented groups on the project team.

- The idea is to operate an anaerobic digester fed with food waste at very short residence time to limit methanogenesis and then primarily produce VFAs. These VFAs could then be used to help make various value-added products. The researchers also tried to use MES on the residual waste (i.e., after partial treatment) to produce hydrogen gas to enable the growth of acetogenic microorganisms. The researchers then used LCA and TEA to help guide the optimization of these processes to reduce cost and GHG emissions.

- The project seems to be well managed and generally successful.

- Research seeks a strategic/novel goal to target VFAs for separation to provide revenue streams for organic waste processes. The interesting ultrasonication approach differs from other methods that require a high thermal load and additional reactor cost. The TEA indicates that capital and operating costs are on the same order as the other unit processes, with ultrasonication less energy-intensive than hydrothermal treatment, which could reduce energy inputs once proven at a larger scale, above 50 L over 4 days. With the project drawing to a close, it is unclear if there is potential for significant impact and outcomes of this technologies to commercial applications; however, there are lessons learned that can be applied to other technologies in organic waste processing and reuse.

PI RESPONSE TO REVIEWER COMMENTS

- We deeply appreciate the reviewers' time and effort in providing critical evaluation and valuable feedback for this project. In particular, we appreciate the strengths, uniqueness, and potential impact raised by the reviewers. All five reviewers gave no weaknesses regarding the technologies, approaches taken, and progress made so far. The impression is that the reviewers are satisfied with what has been accomplished so far. Four of the five reviewers commented on commercialization. The project team does desire to see the technologies commercialized in the near future. The process commercialization, however, is not the goal of this project. The final milestone of this project is to test the whole system at a 50-L scale. At present, we have been in communication with a local city to perform a test at 1,000 gallons. Whether we can get this done or not depends on the available budget and other logistics, such as collecting enough organic wastes and how to deal with the residual wastes. Two reviewers commented on DEI. As one reviewer pointed out, DEI is not a requirement of this project, starting from October 2019. Although as researchers, all team members have been engaging students from K–12 and especially those from disadvantaged communities, but implementing DEI for this project has been severely affected by the pandemic, as universities were shut down immediately after the initial verification in March 2020. As a result, most project tasks were accomplished during the pandemic, and recruiting high school students to work in the lab has been nearly impossible until recently. One reviewer commented on how different feedstocks may affect the composition of VFAs and which method can give the best results. These questions are specifically tied to the viability of food waste. Throughout the project, we have collected different types of food waste, such as wasted food from dining halls, grocery waste, and kitchen waste. Different food wastes have different compositions and lead to different VFA profiles after arrested methanogenesis. Typically, acetic acid and butyric acid are the dominant ones. The change of VFA compositions can be minimized or eliminated when the process is scaled up. On an industrial scale, as food waste from different sources are blended, mixed, and digested, the variability of the feedstocks will be minimal. At this scale, the VFA profile should be stable and predictable.

ADVANCED PRETREATMENT/ANAEROBIC DIGESTION

Washington State University

PROJECT DESCRIPTION

WBS:	2.3.2.228
Presenter(s):	Birgitte Ahring
Project Start Date:	10/01/2019
Planned Project End Date:	10/31/2023
Total Funding:	$3,035,351

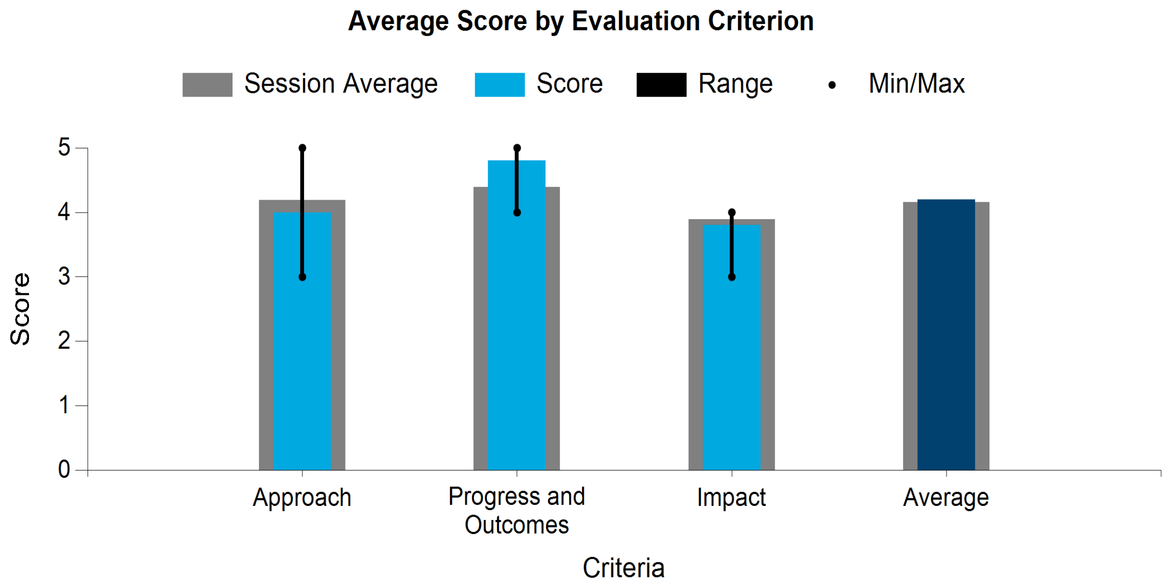
The goal of the Advanced Pretreatment and Anaerobic Digestion (APAD) project is to significantly improve the CCE of AD of sewage sludge by implementing pretreatment technology in the form of Advanced Wet Oxidation and Steam Explosion (AWOEx) pretreatment. This pretreatment has been shown to be superior for pretreating lignocellulosic materials, but it has not previously been tested on sewage sludge.

In addition, the project aims to convert CO_2 from the biogas (approximately 40% of the gas) to methane with the addition of hydrogen. This process will further increase the methane yield of the sewage sludge and produce RNG, which can be used as a transportation fuel.

The end goal of the project is to increase the CCE by 50% or more and to further produce a final biogas with maximum 5% residual CO_2. This will increase the amount of methane produced by the APAD process by an extra 134% compared to the methane produced by conventional AD.

The results from Budget Period 2 (BP2), which finished at the end of spring 2022, showed that the APAD process worked very well on sewage sludge and resulted in a CCE of 60.4%, far exceeding the end goal for the project. The CO_2 conversion further produced a biogas with 5% or less CO_2, which was the end goal for this task. Overall, the project showed 84% conversion of the organics in the sewage sludge by the APAD process, leading to more than 100% more methane, while the upgrading further increased the methane production with 115% extra, leading to a final extra production of methane of 215% compared to conventional AD.

The project is now in BP3, consisting of a small pilot testing. The pilot facility is expected to be in full operation later this spring. We expect to finish the work in the pilot mid-September 2023, after which the final mass and energy balance will be produced. The project is therefore on track for closing as planned at the end of October 2023.



COMMENTS

- Solid work.
- Demonstrated significant improvements on all measured metrics/baselines.
- Would be better to frame this research relative to the true state of the industry.
- Curious as to the baseline of some of the other AD-enhancing strategies being considered by WRRFs: thermal hydrolysis processing (THP) (Cambi), chemical pretreatment, etc. (slides 21 and 24).
- Overview/impact:
    - This project investigated approaches for improving the CCE of sewage sludge by at least 50% and upgrading biogas to RNG.
    - The investigators used a novel APAD technology that involves the use of AWOEx on the remaining biosolids after the first AD followed by a second AD.
    - The investigators have made significant progress against the project goals, especially in BP2 and BP3. The project results show that using the APAD technology helps to improve the methane production rate in the AD system for sewage sludge. Further, the investigated APAD technology for the increased conversion of sewage sludge to bio-natural gas in small-scale wastewater plants is an innovative technique that is relevant to the DOE program goals, and it can be easily integrated into the existing wastewater AD facilities for sewage sludge treatment.
- Strengths: The technique applied in the project is novel and improves the CCE of sewage sludge by AD to approximately 60% and the methane yield by about three times, thus reducing the costs of waste disposal. Further, the communication plan and the collaboration and diversity activities are highly commendable.
- Weaknesses:
    - In this study, the researchers did not report the characteristics of the digestate from the first AD process. The researchers need to note that the characteristics of digestate from the first AD may

vary depending on the feedstock, and I am wondering if we could see the same results when this type of pretreatment is used/applied to the digestate of different characteristics. Also, the researchers noted that to solve the challenge of concentrating the AD-digested sewage sludge, they used other flocculants and concentration methods; however, they need to be careful with the addition of chemicals in the process, as this has a significant effect on the quality of the end products and sometimes the AD process itself.

- Second, on slide 24, the researchers indicated that their APAD technique generates Class A biosolids; however, I am wondering if they considered the other emerging contaminants (e.g., PFAS) in the biosolids before claiming that their technique generates Class A biosolids.
- On slide 2, the researchers recommend the optimal pretreatment conditions of AWOEx; however, I am wondering if these conditions apply to all types of digestate from different sewage sludge ADs. Ideally, the characteristics of sludge significantly vary, and therefore I expect the effectiveness or optimal pretreatment conditions of AWOEx to vary too. Therefore, a series of more studies are needed to determine the optimal conditions with a 95% confidence interval.

- Questions: The advanced pretreatment stage only occurs before the second digester; what about the first digester? Is it really economic to run two digesters? Further, the aim of any project is to ensure that the results are transferable and applicable to other similar products; is this advanced pretreatment process applicable to other kinds of sludges or organic wastes? Looking at the flowchart provided for the APAD process on slide 3. Why is the liquid digestate from the second anaerobic digester sent to the biogas upgradation stage? And what happens to the liquid digestate after the biogas upgrade? Last, the authors made mention of operating the methanogenic fermentation process in two steps after each other to increase the overall efficiency of converting methane to carbon dioxide, but they do not categorically state how they did so. In addition, as part of the impact statements, the investigators stated that the major steps in the process were optimized separately, but the results of the optimization process are not provided anywhere in the slides.
- This project seeks to improve the CCE of AD of sewage sludge through pretreatment. This project was well managed and had a well-developed communication plan. Among its strengths was stakeholder involvement with the host municipality, the city of Walla Walla. The project showed good progress toward the goals of improved CCE and the biomethanization of CO_2. Among suggestions for future improvements, the researchers are encouraged to go beyond hiring students from unrepresented groups generally, to specifically reaching out to Black and Indigenous Americans, as well as provide guidance to existing students on a pipeline of study to professional employment. The acceptability of this approach to small-quantity WRRFs may be limited by the need for two AD reactors in terms of capital and footprint. This may not be avoidable in future iterations of the project, but it is something to keep in mind.
- The goal of this project was to improve the conversion efficiency of carbon to methane during the AD of sewage sludge and to increase the methane content of the biogas so that it is more amenable for commercial applications. The proposed solution was to treat sewage sludge via conventional AD, sending the biogas from this process to a “biogas upgradation” process and sending the treated material to a liquid/solids separator. The concentrated solids material was then treated via an AWOEx process, which had been previously used to make lignin more bioavailable. The AWOEx-treated solids were then remixed with some of the digestate (from the liquid-solid separation) and treated by a second (thermophilic) AD process. The biogas from this AD process was then also processed by a “biogas upgradation” process to increase the methane content. The research demonstrated that the process was able to achieve its goals as far as CCE and methane content of the biogas. There are plans to design and implement the process at full scale at the Walla Walla, Washington, WWTF.
- The project is a success in many ways because the investigators reached their metrics and they achieved their goals, particularly when this process is compared to conventional AD; however, it remains unclear

whether this type of design would be better (e.g., incorporating cost, reductions in GHG emissions) than other designs also intended to achieve greater CCE and high-methane-content biogas (RNG). The investigators provided excellent information on the optimization of the AWOEx process; however, it is not clear whether similar optimizations were considered for the first-stage anaerobic digester, the second-stage anaerobic digester, or the biogas upgradation process. It would be very interesting to learn the results of a TEA considering each of these unit operations to identify an optimal strategy. In contrast, the TEA that was performed seemed to consider the inclusion or exclusion of each unit operation.

- The project has clear targets, goals, and a mission. A biosolids reduction of 59% and a levelized cost of sludge treatment at $79 could greatly impact WRRF processes and budgets for the better. What is the landscape of applying this technology to operations smaller or larger than Walla Walla?

- Does this project have updated information on the destruction of PFAS-group chemicals? Although this is not the primary focus of this research project, concerns continue to grow about PFAS-group chemicals, and this technology could provide multiple bottom-line benefits. An integrated process that can be employed at WRRFs could greatly reduce the flow of PFAS-containing water and biosolids into other areas of our natural environment.

- The project is being managed well to ensure beneficial outcomes for the performer and the government. There are HTL opportunities employed at larger WWTFs. The economics can be difficult to pencil out at medium- and smaller-sized WRRFs, as RNG incentive values do currently and will continue to change in the future. It is important that lessons learned through this effort are incorporated over time into existing facilities, reducing cost and complexities for smaller-size operations with smaller-sized budgets.

- The overall goals of this project could solve a reoccurring issue at municipal WRRFs and forgo many tons of waste in already decreasing landfill space, all while providing RNG to support the needs of WRRFs and the greater community.

PI RESPONSE TO REVIEWER COMMENTS

- We are truly thankful for your many positive remarks from the reviewers as well as their constructive suggestions!

- Response to comments from Reviewer 1. Frame the research toward the true state of the industry: From slide 12, it is obvious that thermic hydrolysis followed by steam explosion of digested sewage sludge as performed by Cambi will not deliver the same positive impact as we have seen (we found less than 25% more methane with THP at 175°C and approximately 10% more at 165°C as normally used during THP compared to simple AD of the input digested sludge material). In contrast, the AWOEx process delivers an increase of approximately 130% more methane compared to the digestion of sewage sludge without any treatment and 85% higher methane production compared to THP at 175°C. It is important to understand that our APAD test setup is different than the process operated by THP in general. We do not pretreat the raw material, and we use higher process temperatures for shorter times. Unfortunately, due to the lack of public data, we do not currently know what the TEA and LCA are of the currently used THP processes; however, we know from our study that the effect of this pretreatment on the recalcitrant parts of sewage sludge is limited and that the effect on reducing the amount of biosolids out of the WWTF is further limited. Using AWOEx up front instead of after AD 1 would overall produce the same methane production, but the cost would be higher due to the higher throughput; however, as AWOEx is developed as a continuous process, this would have a lower impact compared to companies such as Cambi, which operates in batch mode with long retention times. The technology is approaching the commercialization phase, and new team members are needed; we fully agree with this statement, and our company partner Clean-Vantage is working on a commercialization plan for getting the technology to the market.

- Response to comments/questions from Reviewer 2. Thank you for seeing the novelty and value of the project. Weakness. Characteristics of the sludge used are not shown: The characteristics of the sludge and the composition analysis of the sludge before and after AWOEx and AD 2 were unfortunately part of the slides but eliminated due to the time constraints for the presentation (the data are, however, in the publications described on slide 26). We agree with the reviewer that these slides should have been kept at least in the appendix. As discussed at the meeting, we did further test sludge from another small WWTF (the one in Richland, Washington) and found similar results as found for Walla Walla. We are therefore convinced that our results will show the same trends for sludge from other WWTFs. Flocculant: Additional chemicals can have negative effects. We presented our test of the different flocculants/coagulants used at the last review meeting 2 years ago just after the startup of the project. We found no inhibitions on methane production for the concentrations used in our experiments. We do, however, agree with the reviewer that additives should be avoided as much as possible. Class A biosolids: Must know about of fate of PFAS in the sludge to claim Class A. Class A biosolids are defined by the concentrations of pathogens in the sludge, not the amount of chemicals. We do meet all the requirements for Class A biosolids after AWOEx pretreatment. The U.S. Environmental Protection Agency does, however, further regulate the amounts of heavy metals for use of the sludge for land application. Right now, there are no regulations or guidance for PFAS-contaminated biosolids; however, some counties are setting up their own rules for use. Questions: Is it economic to run two bioreactors? The setup is based on the fact that over 50% of all WWTFs already have AD installed. In these systems, the AD plants convert all the easily digestible parts of the biosolids and leave the recalcitrant part behind. After AWOEx, the rheology is changed, and the second AD can be operated with high solids loading using a far smaller AD 2 system compared to the AD 1 bioreactor. Modeling of the cost of upfront pretreatment before the AD bioreactor compared to our APAD setup clearly demonstrates that APAD gives a higher reduction in cost. Why is digestate sent to the biogas upgrading? Good question! We use parts of the upfront separated liquid from the concentration of the digested biosolids before AWOEx as the liquid stream for operating the trickling bed bioreactor for biogas upgrading. We have data demonstrating that our methanogen grows with similar doubling rates in this stream compared to laboratory media. This will further reduce the cost of operating the upgrading process, and no supplements need to be added for operating the process! As shown in slide 3, this liquid stream goes back to the wastewater treatment units after use. Operating the biogas upgrading in two steps? No—it is a one-step process. This was one of the solutions we suggested if our process was not efficient enough; however, our results were very promising, and we managed to operate the trickling bed reactor for several months with 98% CO_2 conversion efficiency with a 4:1 relationship of H_2:CO_2. This was higher than the 95%, which was the original end goal for the project. Some optimization steps are not presented in detail: We operate several processes in the APAD project, where the main aim was to show over 50% improvement of the CCE over conventional AD. The presentation therefore focused on demonstrating the effect of AWOEx on the CCE. The tasks related to the concentration of digested sludge and the upgrading of biogas are further presented with several slides. Seen in the light of the time constraints for the presentation, as well as the priority of the FOA we responded to, we find that our presentation is well balanced.

- Response to Reviewer 3. Potential problem with having two AD reactors: The cost of landfilling of sewage sludge is significant (see slide 25). The advantage of producing far less sewage sludge, which needs final disposal (15% compared to 50%), while at the same time producing far more biogas or RNG is significant! The data shown in this slide include all the capital and operational costs involved! The data clearly show that the APAD process with all its extra cost is far less costly for the community than sending the sludge for landfilling!

- Response to Reviewer 4: No optimization of AD 1: Sewage sludge contains some parts that are easily digestible and parts that are recalcitrant (the first part is mainly primary sludge, while the second part is waste-activated sludge). Most conventional biogas systems in WWTF are operated with low solids loading and long retention times, which might be optimized, for instance, by operating at thermophilic temperatures instead of mesophilic conditions or by concentrating the sludge upfront; however, overall, this would not significantly affect the CCE of this treatment. We can optimize AD 2 and operate with high solids loading as demonstrated because of the changed rheology. The results from our biogas upgrading test are right now better than what has been published in the literature. The TEA needs the full process for understanding the impact of the different parts. For instance, it does not really make sense to model biogas upgrading without understanding the nature of the needed hydrogen source.

- Response to Reviewer 5: Thank you for seeing the impact of the project. Any destruction of PFAS: The team has planned to do some measurements of potential PFA/PFOS degradation during the pilot testing, which is currently in progress.

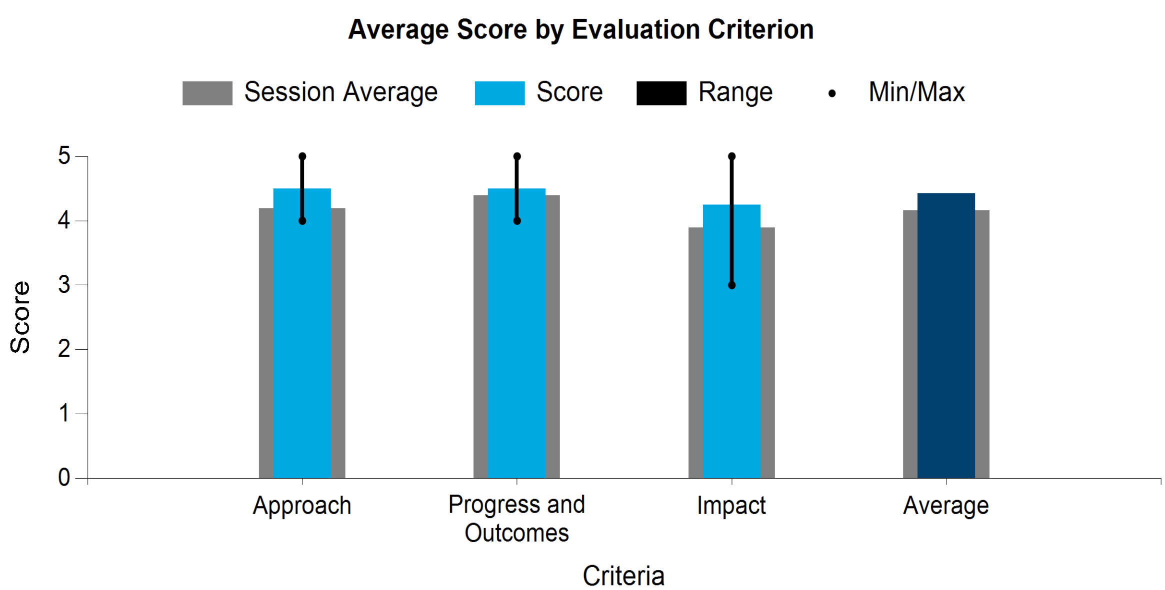
INNOVATIVE POLYHYDROXYALKANOATE (PHA) PRODUCTION WITH MICROBIAL-ELECTROCHEMICAL TECHNOLOGY

University of Maryland

PROJECT DESCRIPTION

WBS:	2.3.2.230
Presenter(s):	Stephanie Lansing
Project Start Date:	10/01/2020
Planned Project End Date:	03/31/2024
Total Funding:	$2,481,536

The project goal is to valorize food waste by shunting traditional AD toward value-added bioplastics (PHAs) to improve the economics of community-scale systems treating wet organic wastes. We are currently moving from intermediate verification to BP3 to meet our end goals of increasing value by 25% and carbon conversion by 50% (from 36% to 56%) through PHA formation from food waste compared to AD. This project valorizes wet organic waste streams for the bioeconomy and manages wastes locally, resulting in a profit from waste and increased sustainability. We have exceeded expectations for dark fermentation, with our robust bacterial consortium creating high VFA concentrations (>30 g/L) over long-term operation (>1 year), exceeding our 3-g/L target. The use of a novel *Haloferax mediterranei* bacteria effectively created extractible PHAs using a 78-day semicontinuous reactor, with a maximum polyhydroxybutyrate co-valerate (PHBV) content of 65% wt/wt and polyhydroxyvalerate (PHV) content of 10% wt/wt, exceeding our combined 30% target. The team of researchers from universities, national labs, and industry is overcoming challenges in blending high-salinity food waste for PHA production, which increases the profit margin and decreases the salt content needed for the halophilic *H. mediterranei* bacteria. The team will be the first to operate a continuous-flow reactor system (50 L) for PHA production from food waste for at least 100 hours, with TEA and LCA informing process effectiveness.



COMMENTS

- One would think there are numerous high-salinity water streams. Curious about the widespread availability of this feedstock, and if any are particularly better than others.

- PHA as a commodity good/product needs to be discussed. Does what is being produced meet industrial specs? Or is an organization willing to take off-spec?
- This project has commercial potential and will address BETO's goals of offsetting significant carbon intensity in plastics production. It also valorizes wet waste.
- Really promising piece on VFA concentration via dark fermentation.
- Have met all technical goals for BP2. The project team seems to coordinate well. Plans include DEI goals and staff investment in these outcomes. The project is advancing to BP3.
- Efforts around dark fermentation have been quite successful in advancing the state of knowledge.
- Commercialization efforts were not discussed, but should have been given the ending TRL.
- DEI goals have been well met. Engaged numerous underrepresented students of science backgrounds.
- Significant increase in VFA production—good job on the arrested methanogenesis piece.
- Seem to have made a lot of positive insights and adjustments as the project has progressed.
- The team has done good work socializing the research as part of the presentation. Will be good to get formal academic publications into the literature.
- Unit operations have significant time online, well beyond what is required for the project. Bodes well for commercialization.
- Would have liked to see more about the involvement/engagement of a partner in the commercialization. Curious about the timeline they see to get to market.
- Overview/impact/progress:
    - The researchers on this project apply a novel and innovative technique for the production of PHAs that are fungible with plastics from food waste. They combined microbial electrolytic technology and dark fermentation to optimize the continuous production of VFAs and PHAs. A lot of inventiveness is shown in the project, as the researchers made use of halophilic cultures (*Haloferax mediterranei*) to produce PHAs as opposed to conventionally used mixed cultures. The project is designed in such a way that the technique can be deployed beyond laboratory-, bench-, or pilot-scale experiments. Producing PHA from waste will help reduce the dependence on fossil fuel for plastic production, and since microbial-electrochemical technology produces a clean form of energy, it will also reduce the release of GHGs into the environment.
    - So far, within the past 3 years of its inception, the project has shown good progress and is on track. The intermediate verification of enhanced VFA and PHA production at the lab scale has occurred and was successful. Also, compared to baseline values, the applied technique in this project produces >100% increase in VFAs.
- Strengths: The steps outlined in this project have good flow and follow a logical pattern. The researchers showed the methods of the project in a detailed and concise manner. The project involves collaboration between researchers from different universities and industry experts, which results in cross-fertilization of ideas. In addition, the project incorporates the DEI plan of the BETO program as underrepresented groups comprise part of the staff.
- Weaknesses/question: Though the researchers have outlined different logical steps for the project, the characterization of organic wastes to be treated, which should be a major step before all other steps in the

project, is not included in the study. In the TEA model, the researchers made an assumption that the bioreactor will be a continuous stirred-tank reactor. Why? What advantages does it have over the types of reactors that it has to be used?

- The goal of this project is to produce PHA, a biodegradable, compostable polymer, from VFA derived from food waste. The project acknowledges BETO's goal of organic waste valorization at local scales of waste management. This is an important consideration for any tech dealing with food waste.
- The project team has integrated good DEI actions into their project staffing plan. Something to consider: When reporting DEI efforts, show denominators (e.g., of *X* students working on this project, *Y* are from underrepresented groups; of *XX* team members in professional roles on the project, *YY*% are from underrepresented groups), rather than listing staff by race and gender.
- Net revenue from PHA production was estimated at four times the cost of disposal. This is reasonable, as PHA markets are growing, especially in Europe, and increased demand is forecast. Should this project's approach be used with municipal food waste, ensuring community benefits from PHA production will be crucial.
- The goal of the project was to convert food waste into VFAs and PHAs (bioplastics). The work on the VFA production was performed at the University of Maryland, and then the conversion of VFAs to PHAs was performed at Virginia Tech. The TEA and LCA were performed at Idaho National Laboratory. The baseline comparison was traditional AD of the food waste.
- A portion of the project focused on high-salinity food wastes, which is something of a niche but also a nice opportunity. The research on the conversion VFAs to PHAs seemed to be rigorously tested under numerous conditions. This was excellent. The work was partially guided by the LCA and TEA results, which is a strength.
- Project management seemed to be good, and there were a number of DEI-related hires. The project partners (industry) appear to be well suited and strong participants.

PI RESPONSE TO REVIEWER COMMENTS

- We agree that this project is a novel and innovative method for PHA production, with the use of a halophilic bacterial strain at the pilot scale. As stated by the reviewers, this project has commercial potential and will address BETO's goals of offsetting significant carbon intensity in plastics production while valorizing wet waste. We also agree that the VFA concentrations achieved via dark fermentation are very promising and have advanced the state of knowledge, with positive insights as the project has progressed on track with operational capacity of more than 1 year (more than what was required). Additionally, as stated by a reviewer, the conversion of VFAs to PHAs was rigorously tested under numerous conditions. As stated, we have met all technical goals for BP2, with a logical project flow, solid project coordination, and real staff investment in meeting our DEI goals. In the future reporting of our DEI efforts, we will state that of the 18 team members in professional roles on the project, 22% are from underrepresented groups and 39% are female (rather than listing staff by race and gender). There are numerous high-salinity water streams available, which can be hard to properly dispose of or treat. As stated by one reviewer, having one portion of the project focusing on high-salinity food waste is a niche but also a nice opportunity. We assessed one high-salinity waste stream from one of Quasar Energy Group's current vendors. We are sourcing more high-salinity waste streams and comparing their performance on PHA production as part of BP3. High-salinity feedstocks can be fermented and produce VFAs to PHAs but are usually detrimental to anaerobic digesters due to the low salt tolerance of methanogens. Having an avenue to utilize this waste stream would be profitable. Properties of the real organic waste streams (both high-salinity and regular food waste substrates) have been properly characterized prior to feeding the fermenters, with the results included in the DOE quarterly reports.

Specifically, the regular food waste had the following composition (pH: 4.60; total solids: 24.6%; volatile solids: 23.5%; phosphorus: 1.95 g/L; total nitrogen: 7.15 g/L; ammonium: 0.03 g/L; sodium: 1.79 g/L). The high-salinity food waste had higher salt content, less volatile solids, lower nutrients, and a higher pH (pH: 10.04; total solids: 35.9%; volatile solids: 10.2%; phosphorus: 0.68 g/L; nitrogen: 0.25 g/L; ammonium: 0.0001 g/L; sodium: 113 g/L). For BP3, we will examine various blends of the two waste streams guided by the TEA, estimate the availability of the waste streams, and evaluate the value of processing more of the economically favorable high-salinity waste and reducing salt inputs for the PHA process against any reductions in overall PHA production with high salt inputs. Some companies, including our own partner Quasar Energy, have interest in our VFA-derived PHA polymers; however, they will need to have kilograms of products for testing and evaluation. We will invite industry partners to visit during our pilot-scale testing and evaluate the performance against their specifications during BP3. As PHA will be used as an ingredient for copolymer, the blending recipes can be tuned to meet the specification of the final product. As stated by one reviewer, the estimation of net revenue from PHA production at four times the cost of disposal was reasonable, as PHA markets are growing, especially in Europe, and increased demand is forecasted. As stated by the reviewer, when using municipal food waste, we need to be clear on elucidating the community benefits from PHA production. As stated by a reviewer, the work was guided by the LCA and TEA results, which was a strength. In the TEA model, the assumption that the bioreactor will be a continuous stirred-tank reactor was made because we designed based on experiments that used batch and sequencing batch reactors, and the closest continuous system to these systems is a continuous stirred-tank reactor. The specific advantage over other reactors is that it provides the residence time required for the reactor in a continuous mode of operation.

DENITROGENATION OF WET WASTE-DERIVED BIOCRUDE TO MEET SAF SPECIFICATIONS

Pacific Northwest National Laboratory

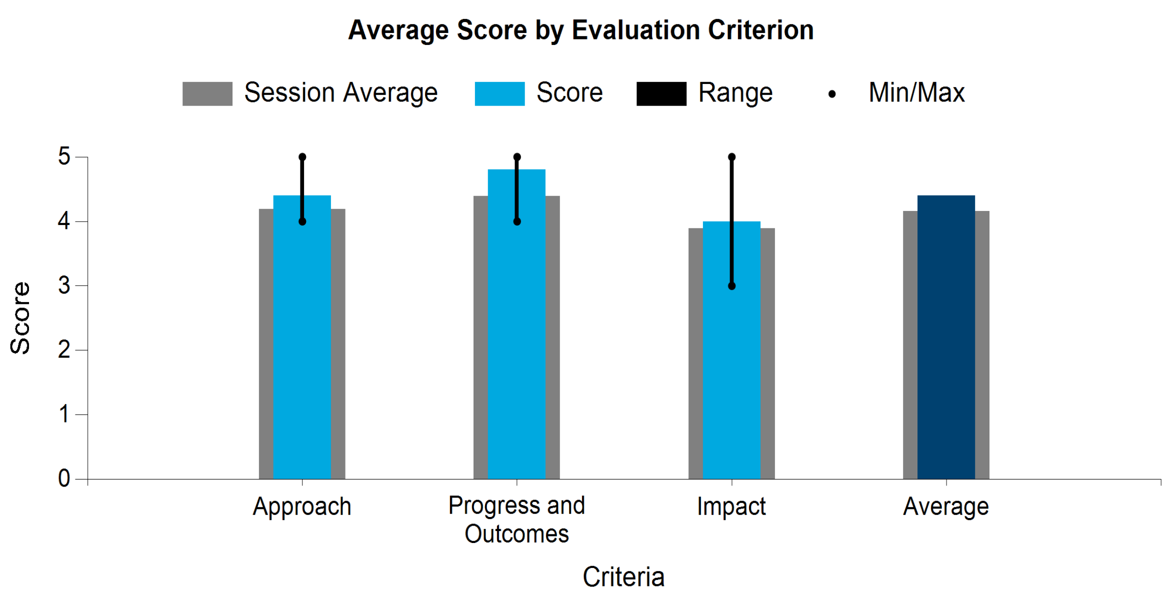
PROJECT DESCRIPTION

WBS:	2.3.3.301
Presenter(s):	Karthikeyan Ramasamy; Katarina Younkin; Michael Thorson; Michele R Jensen
Project Start Date:	10/01/2022
Planned Project End Date:	09/30/2025
Total Funding:	$1,155,000

Wet waste feedstocks have the potential to produce approximately 4 billion gal/yr of SAF (>20% of the total U.S. aviation demand in 2019) via HTL. We will enable the efficient conversion of wet wastes to SAF through HTL by addressing the key challenges associated with nitrogen removal and jet fuel yield in addition to studying the impact of nitrogen from HTL on SAF fuel stability. This project will address the following needs: (1) determine the impact of nitrogen (N) on fuel stability in SAF derived from HTL, and (2) develop a pathway to reduce the N content to <2 ppm.

Using the conventional approach, N-containing molecules are difficult to hydrotreat. This necessitates research to address the removal of these species or the addition of a polishing step to remove trace components to meet the ASTM requirement. In conjunction with Topsoe, we will demonstrate the ability to reduce the nitrogen content from 6 wt % to 2 ppm in a two-stage hydrotreater.

The N specification for all approved SAF pathways (synthetic paraffinic kerosene, synthetic isoparaffin, and alcohol-to-jet) is 2 ppm, likely because these pathways use feedstocks containing no N. Common guidance is that an HTL SAF specification should meet a 2-ppm N level based on precedent from other SAF pathways. No data on thermal stability for HTL SAF fuels currently exist, and this task will provide those data to help assess the importance of N reduction for fuel stability.



COMMENTS

- Early work on framing the topic is good. Clear what is being addressed. Did not spend any funds in FY 2022. Not clear why this project is being evaluated so early after starting.

- Plan looks solid with clear goals to get HTL SAF to something that is compatible with the existing market. Plan includes DEI goals.
- Important collaboration with an industrial catalyst company.
- Score reflects uncertainty on how to judge the impact of something so early in its life cycle.
- Preliminary progress was able to reduce N from 60,000 to 5,000 to 50 ppm. Confident they can meet the 2-ppm standard.
- Interesting conversation about N limit in jet fuel.
- Milestone should include preparation of the data for the ASTM standard for HTL-derived jet fuel. While PNNL cannot do it alone, this is too big of a barrier to commercialization to wholly ignore.
- Overview/impact:
    - The researchers assessed the use of HTL to convert wet waste to SAF to act as an eco-friendly substitute for jet fuel. They used hydrocracking to improve the yield and quality of the resulting fuel (reduced nitrogen content), thereby addressing a major limitation in nitrogen sulfur interactions in the use of biomass biofuel for jet fuel. Using biofuel as jet fuel will help reduce overreliance on fossil fuel and enhance the decarbonization of the aviation industry, thereby reducing the amount of GHG emitted by the industry.
    - Within a short period of time, the project has made appropriate progress toward addressing the project goals. The researchers were able to obtain about 25% of the upgraded fuel in the jet range and also reduced the nitrogen concentration from 60,000 ppm to 53 ppm in the produced SAF.
- Strengths: The researchers are collaborating with a plethora of industry partners who have different expertise and skills, which leads to cross-fertilization of ideas needed to improve the quality and suitability of the biofuel that will be produced. The researchers applied a DEI plan that involves hiring students from underrepresented communities and training PIs and task leads on diversity, inclusion, and belonging. Further, commercialization efforts are being made to increase the marketability of the biofuel that will be developed in the project. It is also commendable that the researchers were able to reduce nitrogen content in SAF by 97%, thereby increasing the stability of the SAF produced.
- Weaknesses: In presenting the tasks that have been carried out for the DEI aspect of the project, the researchers indicated that all the PIs and task leads completed courses on diversity, inclusion, and belonging with documentable action; however, it is not clear to me what documentable action was taken. Jet fuels have stringent fuel requirements, and the process of approving the fuel is very complicated. I am worried that this may limit the process of scaling up the proposed technique. Therefore, I am wondering if the researchers have carefully evaluated the approval process. And, if so, what steps have they taken in trying to overcome these approval process barriers? Further, the researchers proposed a novel approach for reducing nitrogen content in SAF so that all SAF pathways have a nitrogen spec of 2 ppm, which is a stringent jet fuel requirement. I am wondering if the researchers could try different feedstocks with low nitrogen content, as this may not complicate the process of reducing the N content in SAF. Second, the researchers should also consider assessing the economic viability of using different feedstocks with low nitrogen content. Last, I am wondering if the researchers have evaluated the feasibility of scaling up the process of reducing nitrogen content in the SAF to 2 ppm.
- This project tackles a timely and important topic of relevance to the conversion of treated wastewater sludge and other dirty wet waste feedstocks into usable fuels, specifically addressing the denitrification of fuels. The research team is making good progress on the project goals at this relatively early stage in

the project. DEI efforts and community engagement efforts can be strengthened beyond basic training and hiring one student, as noted in comments on the related WBS 2.2.2.302.

- This project focuses on the problem of nitrogen being in the waste during a WTE conversion via HTL. This problem is essentially unavoidable because virtually all organic wastes will have some nitrogen content (i.e., it is part of most cellular material). Simultaneously, the presence of this nitrogen is a major bottleneck for the production of SAF from organic wastes.

- The team does a really nice job of handling DEI. Like other projects, they try to hire a diverse group of people. Beyond that, though, they require DEI training for all project personnel, which I like because it is tangible.

- The initial progress of this research is fantastic. The investigators have been able to reduce the N levels to approximately 50 ppm at an estimated cost of $0.04/GGE. Similarly, the HTL of sewage sludge also appears to be insensitive to the presence of the PFOS, which should likely partition to the biofuel and then be combusted during flight. This latter issue is much more attractive than applying sewage sludge to land, where the PFOS could enter the food chain.

- The project seeks to understand additional barriers to nitrogen sulfur interactions on fuel thermal stability and to achieve stringent fuels standards. Compositional changes in Jet A/A-1 fuels would delay the introduction of sustainable/decarbonized fuel deployment. SAF needs to meet ASTM fuel specification D7566-18, but no nitrogen content (derived from organics) is typically present in fossil fuel Jet A.

- Samples indicate an average of 2 ppm in fossil Jet A, and many partners have provided input for the project in the initial 6-month stage to guide research needs, including N reduction testing, analysis, and the assessment of economic viability of the reduction to determine what is the acceptable N content in SAF. Minor quibble, but recommend researchers continue to investigate barriers in aviation alternative fuel deployment and policy barriers (e.g., unleaded general aviation fuel has recently been approved by the Federal Aviation Administration, yet challenges to its deployment nationwide remain).

- If SAF standards are achieved on par with existing Jet A/A-1 fuels, significant GHG reductions will be possible, quicker, through the use of existing infrastructure and approved equipment, providing beneficial outcomes for the performer and the government. Promising early results in N reduction indicate further N reductions are possible and to what extent those reductions are needed. Excited to continue to see research progress, given the work and accomplishments achieved in the first few months of the project.

- The project has demonstrated actionable DEI outcomes from training to improve hiring questions, and it strives for a more inclusive research environment.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their valuable feedback. We appreciate the positive comments and the recognition of our early progress in addressing the challenges associated with nitrogen content in HTL for SAF. We would like to address the comments based on the different topics raised.

- Framing and goals: “Early work on framing the topic is good. Clear what is being addressed. Did not spend any funds in FY 2022. Not clear why this project is being evaluated so early after starting.” We are glad to hear that the early work on framing the topic was well received and that our goals are clear. We acknowledge the concern about the evaluation timing, as the project kicked off in FY 2023. Hopefully, in the FY 2025 Project Peer Review, we will be at the end of the project cycle and will have a lot more to update the committee on.

- DEI efforts: "In presenting the tasks that have been carried out for the DEI aspect of the project, the researchers indicated that all the PIs and task leads completed course diversity, inclusion, and belonging with documentable action; however, it is not clear to me what documentable action was taken." We appreciate your recognition of our commitment to DEI. Two actions after completing DEI training included creating consistent interview questions for candidates to eliminate bias in the hiring process and participating in a seminar workshop series at Columbia Basin Community College, a minority-serving institution, to share examples of pathways into STEM.
- Nitrogen reduction and fuel standards: We appreciate the concerns raised by the reviewers regarding the complexity of the fuel approval process and the need to carefully evaluate and overcome the barriers associated with meeting stringent fuel standards. We are committed to meeting the stringent jet fuel requirements and ensuring that our SAF complies with the ASTM standard for HTL-derived jet fuel. Further, we are actively engaged with industry partners and fuel testing experts regarding the fuel approval process, which is why we are focusing on thermal stability testing of the produced SAF.
- Feedstock selection and economic viability: We have completed extensive HTL and upgrading of organic wet wastes and have found that all classes of organic wet wastes include nitrogen in the biocrude because all organic wet waste classes contain proteins. Wood or cellulosic feedstocks not containing nitrogen are a very different value proposition. While this is an exciting area of research, we believe that the waste disposal advantages of organic wet wastes make it a much more attractive feedstock for HTL.
- Scaling up and approval process: We acknowledge the concerns raised about the scalability of the process for reducing nitrogen content and the complexity of the approval process. As such, we are limiting our denitrogenation to using existing hydroprocessing unit operations, and hydrotreaters focused on hydrodenitrogenation, such that this process will be scalable at refineries.

ELECTRO-ENHANCED CONVERSION OF WET WASTE TO PRODUCTS BEYOND METHANE

Colorado State University

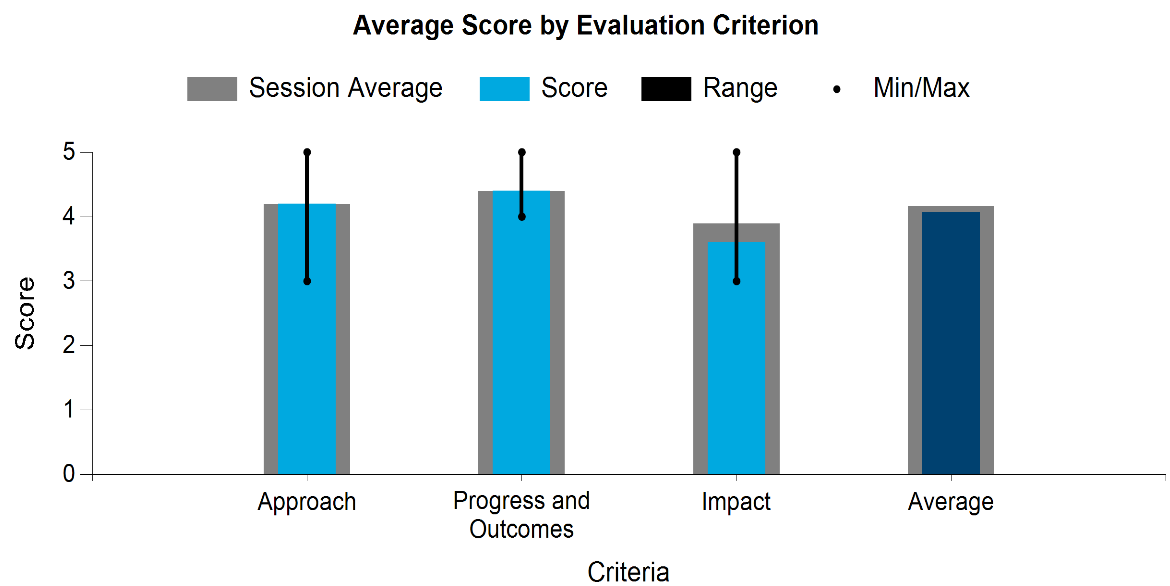
PROJECT DESCRIPTION

WBS:	2.3.4.605
Presenter(s):	Ken Reardon
Project Start Date:	10/01/2019
Planned Project End Date:	10/31/2025
Total Funding:	$6,335,445

Wet organic wastes present problems in disposal cost and environmental impact and represent lost opportunities as inexpensive feedstocks to displace fossil-based products. AD, composting, and incineration strategies are limited by their CO_2 production (wasted C) and low-value/uncaptured methane production. Surplus renewable electricity could provide inexpensive electrons to enhance wet waste processing and generate drop-in liquid transportation fuels.

The goal of this project is to improve wet waste conversion by inhibiting methanogenesis, increasing the production of VFAs, and elongating VFA chains to produce higher-value medium-chain fatty acids and iso-butanol. This interdisciplinary project is designed to achieve the project goal through four objectives: (1) enhance VFA production in AD, (2) upgrade AD gaseous and liquid product streams, (3) evaluate and optimize the system to assess economic viability, and (4) integrate education with research.

Technical accomplishments to date include the identification of conditions yielding high VFA levels, including high levels of C4 and higher acids; the conversion of acids to alcohols using synthetic biology; the development of software that relates microbiome composition to VFA production; the demonstration of scale-up from 2-L to 600-L bioreactors; and TEA and LCA based on a comprehensive process model.



COMMENTS

- Significant figures seem to change in the goals. Is that level of precision even necessary or real?
- Good use of TEA/LCA to identify inoculum that has an MFSP that meets the goals of this project.

- Significant improvement demonstrated in most metrics, particularly around C6–C8 production.
- Approach to improving upon AD seems to be fairly all-inclusive of ideas/techniques.
- The omics analysis in the backup slides looked quite interesting.
- There did not seem to be any conversation about the commercialization or other entity. Leprino Foods just seems to be an interested party, but not the commercialization party.
- There is a lot of outreach with undergraduates and students as well as strong communication activities.
- The team relies a lot on the basics of this project for impact—that is, it is a bit more detached from the real implementation and commercialization that would be needed to take something like this to market. A more nonacademic/non-research-focused partner would help provide the necessary advice.
- AD is a commercial technology; improvements should be easy to commercialize. The difficulty is that this changes the unit operations and products significantly enough.
- Looking at adding CO_2 to drive additional VFA production.
- Looking at process intensification, combining some of the unit operations, and potentially avoiding separations.
- Overview/impact/progress:
    - In this project, the researchers are using renewable electrons to facilitate targeted pathways in the AD of wet organic wastes (manure and food wastes) to produce energy and other high-value products, such as hexanoic acid and alcohol. This is a very insightful and innovative project. The project will help in reducing GHGs that emanate from the AD process. Apart from the environmental benefits of the project, it also has economic benefits as the LCOE can be enhanced with it. The researchers demonstrate a lot of technical expertise as they apply avant-garde techniques such as arrested methanogenesis, electro-enhanced AD, and electro-elongation of MES to increase the quantity of VFA that can be generated from the AD process. The researchers also employ advanced molecular biology techniques to improve the efficiency of the process.
    - The researchers have made a lot of progress in this project, and the results provided in the presentation show that the implemented technique is exceeding the set target values; greater than 50% increase in VFA production was achieved.
- Strengths: The researchers clearly outlined the steps that are being used in the project in a detailed and concise manner. They also provided means through which the results of the project can be verified and validated to ensure that it is economically feasible. In addition, the project provides hands-on practical training for undergraduate, graduate, and postdoctoral students who are participating in the project and helping to disseminate the results of the study to their colleagues.
- Questions: In reporting the progress of the work in slide 22, the researchers state that they constructed *E. coli* capable of converting C4–C6 acids to alcohols. I would like them to give more elaboration on what they mean by constructed *E. coli* and how this will be used in scaling up the technique. In addition, it will be great if the researchers can investigate further why the amount of VFA generated using only food waste as the substrate is higher than that generated when food waste and animal manure are co-digested; could it be that co-digestion is not suitable for the process? In the economic analysis, the researchers should try to compare the benefits of producing VFA from the AD process to those of producing methane.

- The goal of the project is to improve the efficiency of wet waste treatment through AD by maximizing VFA production and conversion to commodity fuel blends and chemicals. The researchers made good progress and met milestones toward project goals. A few suggestions. First, the project mentions “renewable electrons.” In future presentations, especially to nontechnical stakeholders, researchers should take care to fully contextualize and define this term to avoid confusion with renewable energy as commonly understood. Second, the research team is to be commended for inclusiveness and outreach among students. As the project progresses, they should build on this work to proactively seek to include students at the high school through Ph.D. levels, in particular students from underrepresented backgrounds, including outreach to HBCUs and universities serving tribal communities and students.

- This project is relatively early in its time frame. It involves personnel at Colorado State University, South Dakota School of Mines, University of California Irvine, and NREL. The project management seems to be good. There are numerous project partners, but there are strong ties because there is sharing of data, methods, and materials among partners. There are biweekly meetings (electronic).

- The goal of the project is to make medium-chain organic acids and alcohols from organic wastes (food waste and animal manure). Solid-liquid separation is achieved via centrifugation. The production of VFAs is achieved by optimizing pH and identifying the appropriate inoculum (termites!). Cathodic electro-fermentation is used to produce the medium-chain organic acids and alcohols. A lot of work has been performed in optimizing the inoculum. I am skeptical of this work, specifically because it essentially is trying to extrapolate 16S rRNA gene profiles (i.e., microbiome) to “metagenomic” information, although it is well understood that suggested metabolic potential via 16S rRNA gene sequences is likely spurious (with a few exceptions that do not apply to this situation).

- The work has met its pertinent milestones to date. The work is also guided by LCA and TEA, and there appears to be good adherence to DEI principles.

- Research targets arrested the AD process to develop more refined pathways for organic waste conversion to products other than methane. Products include needed precursors for chemical manufacturing/fuels or blendstocks of fuel products, which can diversify organic waste revenue streams in volatile energy markets with changing policy incentives.

- Researchers have investigated improved microbial biomes to increase VFA production, yielding higher productivity of VFAs. The microbiome scales well to larger reactors. Testing of microbiome community has found interesting susceptibility to shear in the population, but given that mixing adds complexity and cost to AD of organic waste, it would serve to only lower TEA and LCA of potential future deployment.

- Recommend partnership with other industry or municipality to investigate the technology’s applicability to other waste streams (e.g., use of microbiome with termite gut bacteria, although useful in high-lignin feedstock, may impact VFA results when processing other wastes).

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments, and we appreciate that they have recognized the innovation of our project and the progress we have made. In the following paragraphs, we provide responses to these reviewer comments.

- Commercialization partner: We are searching for an appropriate partner to commercialize our findings. As noted, the process we are developing would present changes to standard unit operations, and thus not all current AD technology providers will have an interest.

- DEI: We appreciate the suggestions for enhancing the diversity and inclusion aspects of our project. While the FOA under which our project was funded did not have a DEI requirement, our team is committed to the principles of DEI. We make efforts to recruit a diverse set of students, especially undergraduates, to participate in this project, and our outreach efforts at Colorado State University's Spur campus in Denver allow us to connect with K–12 students and their families from a wide range of backgrounds.

- Research scale: One reviewer commented that our work is at the level of basic research and is detached from real implementation; however, we have already conducted experiments at 700 L in a pilot-scale bioreactor with a capacity of 2,000 L, and more research at this scale is planned for BP3.
- Information on the strain developed for alcohol production: An *E. coli* strain has been metabolically engineered to convert organic acids to alcohols. Two pathways and a variety of sources for each enzyme in each pathway were evaluated. The best strain from this work has been shown to convert C2–C6 organic acids to the corresponding alcohols and to be tolerant to both electrodialysis-purified digestate and the digestate itself. Current research is directed toward developing a bioreactor configuration that would allow this strain to be used in a scaled-up bioprocess.
- Higher yields of VFAs from food waste than from co-digestion of food waste and manure: The reason the yields are lower in the co-digestion case is that yields from manure are lower. This is a common observation that stems from the lower content of readily digestible carbon in manure compared with food waste.
- Economic analysis: A reviewer suggests that we compare the benefits of producing VFAs (and alcohols) to standard biogas production via AD. We are doing that analysis because it is our baseline case for calculating the improvements that are among the project metrics. The TEA presented focused on the economic trade-offs of different pathways because that information helps steer our experimental work.
- Inoculum optimization: A reviewer commented that inoculum optimization from 16S data may have challenges because it assumes an accurate extrapolation from phylogenetics to metabolic potential. This is a reasonable concern, and we are aware of that potential limitation; however, our modeling incorporates our experimental data and some published metagenomic data, and the results to date are encouraging. All methods have limitations. For example, the best approach for inoculum modeling would be multi-omics analyses that include proteomics—but this would be very expensive and time-consuming. We seek to extract information from methods that are simpler and less expensive, but we are also incorporating some data from methods that provide more detail and accuracy.

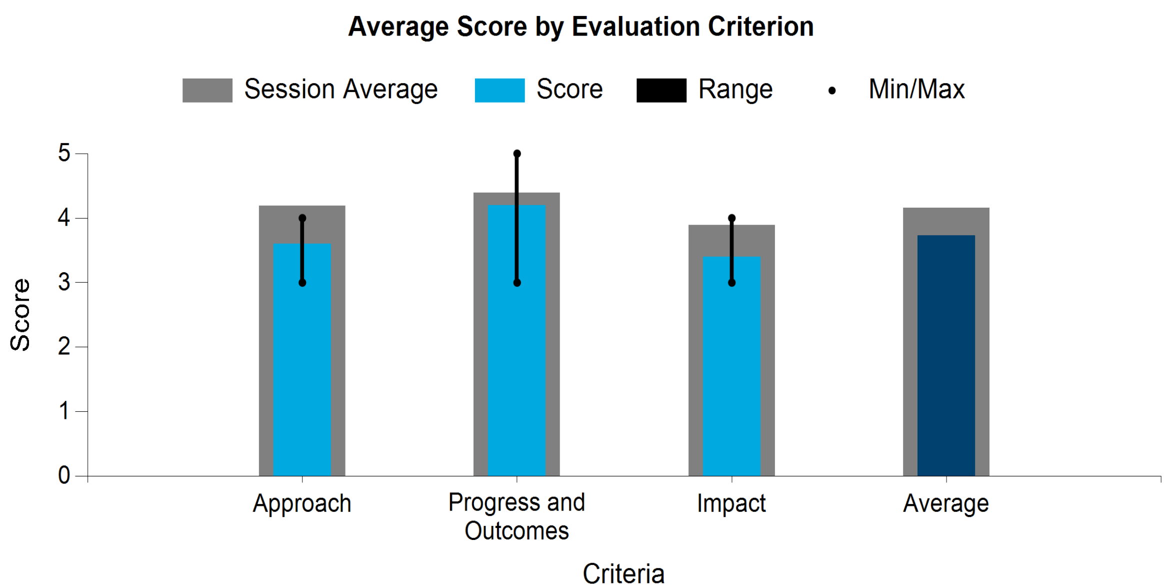
SYNERGISTIC THERMO-MICROBIAL-ELECTROCHEMICAL APPROACH FOR DROP-IN FUEL PRODUCTION FROM WET WASTE

Princeton University

PROJECT DESCRIPTION

WBS:	2.3.4.609
Presenter(s):	Jason Ren
Project Start Date:	10/01/2020
Planned Project End Date:	03/31/2024
Total Funding:	$3,124,665

The overarching goal of this project is to develop a synergistic thermo-microbial-electrochemical process that converts food waste to jet fuel blendstocks and simultaneously treats aqueous wastewater, thereby recovering H_2 and nutrients. The project will utilize HTL to convert food waste into biocrude. The biocrude wastewater will be processed in a microbial-electrochemical process that utilizes microbes and electricity to generate H_2, NH_4^+, and clean water. The H_2 generated from the microbial-electrochemical process will be utilized for hydrotreating/upgrading the biocrude into jet fuel. The outcome of the project will be the continuous operation of a process on 1 ton of wet food waste that encompasses all technologies developed to achieve >50% CCE improvement and/or 25% levelized cost of disposal reduction relative to traditional AD.



COMMENTS

- Lot of work framing the progress against the current baseline, and really helping to showcase the importance of the project.
- Clear focus on the cost of a material versus performance. Quite interesting that base metals for 1% of the cost are performing relatively similarly. This helps to make a big difference in the final selling price.
- Cathode alloys show significant progress beyond what has been demonstrated by other efforts for electrolyzers/electrolysis.
- The project's HTL shows improvement over AD for CCE.

- Project decisions have an eye on commercialization, but does not appear to be pursuing it.
- Team is tackling one of the major issues with HTL in aqueous waste.
- The HTL element of this project does not seem to be pushing the envelope.
- DEI elements were briefly discussed, involving students and PIs underrepresented in STEM. Working to incorporate even though it was not part of the original scope.
- Did not spend time speaking about management/communication plan, but did not appear to be any concern.
- Some of the graphics, particularly the Sankey diagram, are quite instructive. Others are a bit dense and require a bit more explanation than can be had by reading slides.
- Team seems to be coordinating well, but is struggling with a bit of geographic dispersion.
- In this project, the investigators simultaneously convert food waste to jet fuel using a synergistic thermo-microbial-electrochemical process and recycle HTL wastewater by using it as substrate for the HTL process, thereby producing hydrogen and nutrients as byproducts. The project is aimed at improving carbon yield by >50% and reducing waste processing costs by >25%. This is a very interesting and unique project. It not only deals with the generation of energy from food waste through HTL, but goes a step further to find solutions to the problem of disposing of the resulting wastewater from the process. The project is unique in the sense that not so many studies look at the post-treatment/utilization of waste generated from energy generation. Also, the project incorporates a closed-loop circular economy approach where everything generated is still recycled within the same system, and this is highly commendable. Apart from having environmental benefits, it also has economic benefits as it reduces the cost of energy generation. A lot of benefits will accrue from implementing this project on a large scale.
- So far, the project has shown tremendously good progress. In the microbial-electrochemical cell, one day was enough to remove most VFAs and alcohols from the liquefaction wastewater, the CCE of food waste used in the process is more than 50% that of the conventional AD process, and the chemical oxygen demand (COD) removal efficiency is greater than 90%.
- Strengths: It is very impressive that high-purity hydrogen was recovered during the treatment of post-HTL wastewater, and there was also very strong degradation of the organics present in the wastewater. Apart from carrying out laboratory experiments, the researchers go a step further by carrying out TEA and LCA for the project. The project has patents, publications, presentations, and awards, which show how good the project is.
- Question/weaknesses: The researchers stated that two types of post-HTL wastewater (PHW) were tested with the microbial electrolysis cells (slide 12). I want the authors to throw more light on this by stating the two types of PHW that were tested. In the same slide 12, the researchers indicated that the microbial-electrochemical cells will generate hydrogen gas during the treatment of the liquefaction wastewater while removing organic pollutants from the wastewater; however, throughout the PowerPoint presentation, nothing was mentioned about quantifying the organic pollutants present in the wastewater before and after treatment.
- This project seeks to improve the CCE of food waste in an HTL process generating biocrude as an output. A particular strength of this project is that it addresses wastewater arising from HTL. The reduction of COD and N in PHW is an important topic. The LCA presentation of the proposed technology, compared to AD and HTL with upgrading, shows improvements in ecotoxicity, eutrophication, and global warming potential compared to one or both alternatives.

- For applied settings, the process relies on clean food wastes. Should the project seek feedstock from curbside collection of source-separated food wastes, attention to contamination with plastics, as well as potentially other materials, should be taken into account.
- The DEI approach can be strengthened in future phases of this project. The team should proactively seek students between the high school and Ph.D. levels to support this team, and it should organize educational outreach to engage HBCUs in this process in particular. In general, more information on industry engagement and commercialization potential, as well as procedures to ensure communication among project partners, would improve this project.
- The goal of the project was a more holistic approach to HTL of food waste. The researchers used a couple of representative food waste simulations and then performed HTL with the subsequent treatment of the waste streams of the HTL. The focus of the entire process is on higher CCE and reduced energy costs for treatment. A goal of the waste treatment portion of the project was to convert remaining carbon compounds to molecular hydrogen. The authors conclude that microbial electrolysis cell and HTL leads to better CCE than AD of food waste. There was a good emphasis on TEA, which the researchers seemed to use to guide their research as they met various milestones.
- The project appears to be meeting its goals (albeit I cannot really critically evaluate this conclusion because I did not understand the presentation). There are multiple project partners, who had their first in-person meeting as part of the BETO presentations. The speaker claimed to have met various DEI metrics but did not provide details.
- Interesting concept with a compact, modular thermal-microbial-electrolysis cell to treat HTL aqueous wastewater, recovering H_2 and nutrients.
- The research has considered TEA by investigating lower-cost catalysts with base metal to provide lower-cost options to optimize organic waste streams. Organic wastes are sourced from a number of partners to investigate the applicability of this technology to various waste streams. The technology is cost-competitive with AD at facilities above a 50-ton/day limit but has a positive LCA, as natural gas inputs are required for operation (could this system take advantage of local renewable energy to replace natural gas inputs?).
- As more investigations continue, recommended valorization of nutrients recovered through the process that may further reduce costs or reduce LCA due to the offset of fossil-derived nutrient removal and reuse.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the positive and constructive comments from the reviewers. All reviewers commented positively on the value of the project and the progress made to date, and we are grateful for the feedback. The reviewers raised a few questions regarding technologies, DEI, and analyses, and we address them here. Regarding the HTL tasks pushing the technology envelope, we will perform additional HTL pilot runs in Phase 3 to obtain additional biocrude oil and PHW for downstream processes. Using a rotating furnace (in development), we will investigate the mixing effect on HTL performance in terms of conversion efficiency, oil quality, and char formation. We are currently conducting the catalytic hydrotreatment of HTL biocrude oil based on PNNL's work, with the first set of experiments completed. We have also identified the key steps for upgrading HTL biocrude to the jet fuel standard. Regarding organic removal in microbial-electrochemical treatment, we did not get a chance to provide many details in the presentation. Here, we add some results regarding the removal of organics in PHW. More data presentations can be found in our manuscripts. We characterized the COD of PHW from salad dressing PHW and food processing PHW, and in both cases, the COD removal was gradually increased 80%–90% in several days. We also characterized the transformation of different organics during microbial-electrochemical treatment. High-performance liquid chromatography and nuclear magnetic resonance results showed sequential glycerol fermentation to VFAs and subsequent microbial-electrochemical VFA degradation. Regarding the DEI metrics, we strove to recruit and retain students with diverse backgrounds, and our leadership team has a good balance of gender, race, and ethnicity. We have been active in increasing the diversity of our team members. We have multiple female graduate and undergraduate students in the project. Our labs host visitors and open houses about our research to high school students multiple times per year. In addition, the project supports and aligns with the Justice40 Initiative because it aims to collaborate with a school and a food manufacturing company seated in a disadvantaged geographic area in the Champaign-Urbana, Illinois, region. The project takes food waste from a food manufacturer within an identified disadvantaged area. The disadvantaged community will benefit from the reduction in GHG emissions created when this unused food goes to landfills. Regarding the positive LCA and replacing natural gas with renewable energy, we have performed more analysis. The proposed technology has higher electricity requirements compared to AD, which means that the reduction in the environmental impact associated with the use of renewable electricity will be more pronounced for the proposed technology relative to AD. We do acknowledge the limitation of the analysis, as we only considered electricity source without counting other factors such as CH_4 process emissions from AD, chemical uses, and others. We expect that efficiency improvements in the processes studied in this project will result in parity in these LCA measures.

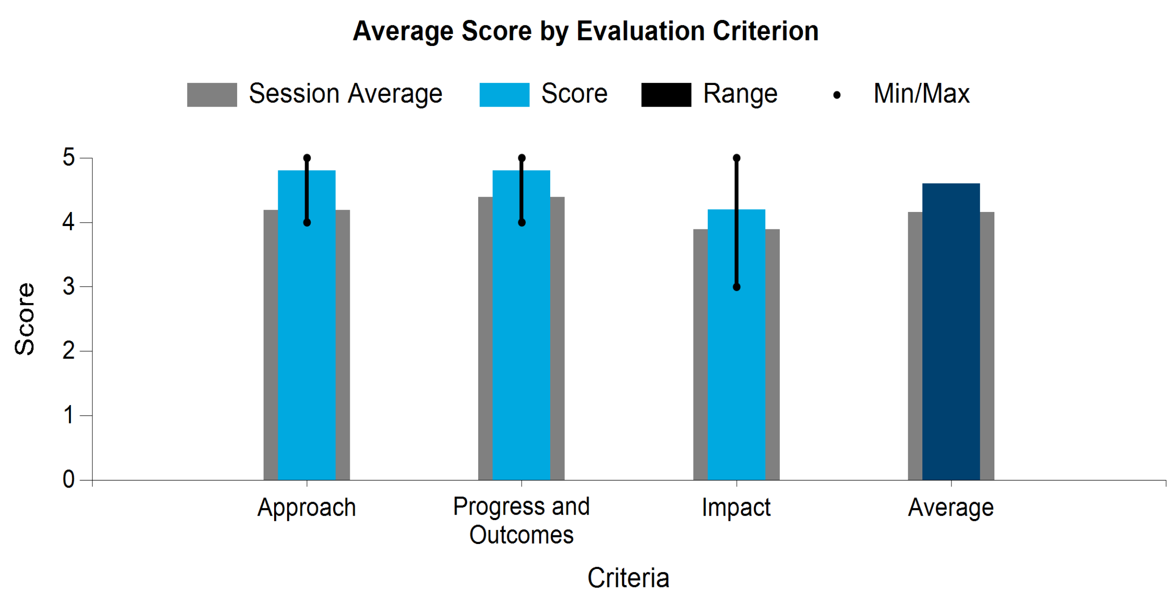
INTEGRATED BIOCHEMICAL AND ELECTROCHEMICAL TECHNOLOGIES TO CONVERT ORGANIC WASTE TO BIOPOWER VIA NORTH AMERICAN RESEARCH AND EDUCATIONAL PARTNERSHIPS

University of Michigan

PROJECT DESCRIPTION

WBS:	2.3.4.611
Presenter(s):	Lutgarde Raskin
Project Start Date:	10/01/2020
Planned Project End Date:	01/31/2027
Total Funding:	$6,790,983

In this project, we aim to reduce the production cost of pipeline-ready biomethane from urban and suburban organic wastes by at least 25% via the demonstration of a pilot-scale system with integrated biochemical and electrochemical technologies, making bioenergy production more market competitive. The system combines three modular components to achieve this goal: A two-phase anaerobic dynamic membrane bioreactor system produces biogas from mixed organic wastes at high yields and production rates; an electrochemical reactor for CO_2 and H_2 delivery purifies the biogas by capturing CO_2 as HCO_3^- and simultaneously produces H_2; and a gas-phase methanogenesis bioreactor converts captured HCO_3^- and H_2 to high-purity CH_4. Each component involves significant innovation compared to the state of the art. A primary challenge of this project is the integration of the three components, which requires diverse technical backgrounds. We address this challenge by establishing strong collaborative programs to facilitate knowledge transfer between research and industry partners, including technical meetings, student co-mentorship and exchange, course development, internship opportunities, and consortium meetings and symposiums. This project will help BETO achieve its Multi-Year Program Plans to "validate proof of performance at integrated pilot, demonstration, and pioneer scale" and "reduce biorefinery capital and operating costs."



COMMENTS

- Very impressed with the early progress and the preparation for piloting at a real WRRF. Impact is as expected for the moment; will be much stronger after the completion of the planned pilot.

- Commercialization potential is present, but is not discussed at this stage. Not expected, as it is still early.
- Motivation is strong to address this challenge because the issue is commercialized in many markets. Marked improvements like this with regard to AD would make the technology more widely commercialized.
- Have done several things to address DEI, including education and outreach.
- The team has made solid progress toward their goals. Have met their target/interim goals on the project. Actually seems to be doing even better.
- I'm assuming that the proposal detailed how these goals would lead to the 25% reduction, but would like to see a brief summary in this presentation to recap.
- Solid management and feedback processes involving numerous stakeholders.
- Doing a lot of co-siting of project meetings to educate beyond the project team.
- Missing a high-level discussion on some of the operating principles of these units. Curious to better understand implementation strategy (retrofit vs. new).
- AD is being run at mesophilic temperatures, making these data more impressive.
- Risk discussion is focused on the integration of unique unit ops. Doing a lot to build trust and relationships between the partners (monthly meetings, work-study program, student exchanges).
- Looking at each of the unit ops as both independent and collective items. As the modeling is done, I would be curious to see these scenarios spelled out.
- Overview/impact:
    - This project is investigating the conversion of organic wastes to biopower using integrated biochemical and electrochemical technologies. Three extremely innovative techniques—a two-phase anaerobic dynamic membrane reactor, an electrochemical reactor, and gas-phase methanogenesis—were applied to improve the hydrolysis process, enhance the efficiency of biogas production, and improve the purification process for methane. The project focused on producing renewable energy from organic wastes at a reduced cost, which is a key consideration in scaling up the techniques applied. Further, the proposed techniques present environmentally friendly ways of converting organic wastes to biomethane, thereby reducing the production of carbon dioxide and the GHGs released into the environment.
    - Considerable progress has been made in this project, and the results obtained speak volumes about the efficiency of the applied techniques, as they have achieved production rates beyond the target values. The researchers have been able to achieve greater than 94% carbon dioxide capture, improved methane and volatile fatty production, and reduced the amount of power consumed during the AD process to less than 12 kWh/kg CO_2.
- Strengths: One component of the project involves the electrochemical conversion of electricity to bioenergy; this presents a highly efficient and easily utilizable method for storing energy when surplus electricity is produced. In addition, the project involves a synergistic collaboration between researchers from different universities who have different areas of expertise. This promotes the cross-fertilization of ideas and improvement in the quality of the output of the project. Another commendable aspect of the project is that it includes a mentoring plan for students through symposiums and conferences. The results

of the project are also incorporated into online courses, bringing about research-led teaching activities. Importantly, the project has made substantial efforts in promoting DEI.

- Question: Though the project involves a collaboration between partners with different areas of expertise, there is a need to provide more clarification on how the techniques from the different partners are interconnected in the project.

- Recommendations: The researchers tested their technique using food waste and sludge as feedstock; it will be great to know if the technique will also provide suitable performance for other types of feedstock. Even though the project involves conducting AD in a mesophilic state, the results obtained are very impressive. This implies that if the researchers make use of thermophilic temperatures, better results will be obtained; however, I can understand that this was not the goal of the project, as they wanted to mimic the rumen conditions. Further, the researchers should try to see how they can retrofit existing AD systems/plants with their techniques.

- The project seeks to improve biomethane production from AD of food waste by addressing recalcitrant (fibrous) fractions of this feedstock. Its research question is clear and well focused. Other strengths include good integration of a multicomponent process, with regular communication and coordination among multiple stakeholders. There is an excellent focus on workforce development, engaging with minority-serving institutions and institutions in Mexico, and offering bioenergy online courses in the context of socially engaged design.

- These researchers are attempting to integrate a handful of novel biotechnologies to convert organic wastes to high-purity methane (RNG). Each individual technology is reasonably novel, and the researchers explicitly admit that integrating these technologies together poses a significant challenge.

- The management of the project seems to be excellent, especially given that there are researchers at the University of Michigan, Northwestern University, and Argonne National Laboratory. There are regularly (monthly) meetings between project personnel, as well as less frequent in-person meetings. I particularly like that the research appears to be quasi-iterative in that process modeling partially drives the experimental design, the results of which (presumably) help improve the modeling effort. The LCA and TEA efforts appear to be ongoing.

- DEI goals are met via collaboration of multiple and diverse partners, grad student exchanges, and the development of online courses.

- I am generally very optimistic about the chances of this project for long-term success. My biggest "criticism" at this phase is basically an acknowledgement that predictions are not facts, and this project is still relatively early in its process and development.

- Research into electrochemical and biology biogas upgrading technologies represents a leading edge of research work with few technology providers that offer cost- or energy-efficient upgrading options. Developments could significantly improve the net performance of biogas derived from all organic streams of waste given the expensive and energy-intensive systems currently in operation, offering beneficial outcomes for the performer and government. But more information is needed about the optimization challenges of the electrochemical reactor for CO_2 and H_2 delivery and gas-phase methanogenesis bioreactors as they move into testing phases.

- High-lignin waste streams significantly impact the ability to digest waste streams without significant upfront sorting, at the expense of additional energy inputs and time (reducing organic waste conversion rates). Is it possible to quantify the benefits not only in improved organic waste conversion but also in streamlining organic waste processes?

- Improving the hydrolysis of lignocellulosic components would improve the applicability of AD to process organic waste streams that are not currently feasible. A breakthrough in this area could greatly impact the amount of bioenergy available from waste by forgoing the energy, time, and expense of sorting out high-lignin streams of waste. Additionally, given the typical high cost of refining biomethane resources into pipeline-quality gas, this research area has the potential to reduce cost across the bioenergy economy spectrum. The goals of this project could impact the initial and final steps of the bioeconomy. It will be exciting to see this research as it moves forward into the pilot-scale phase.

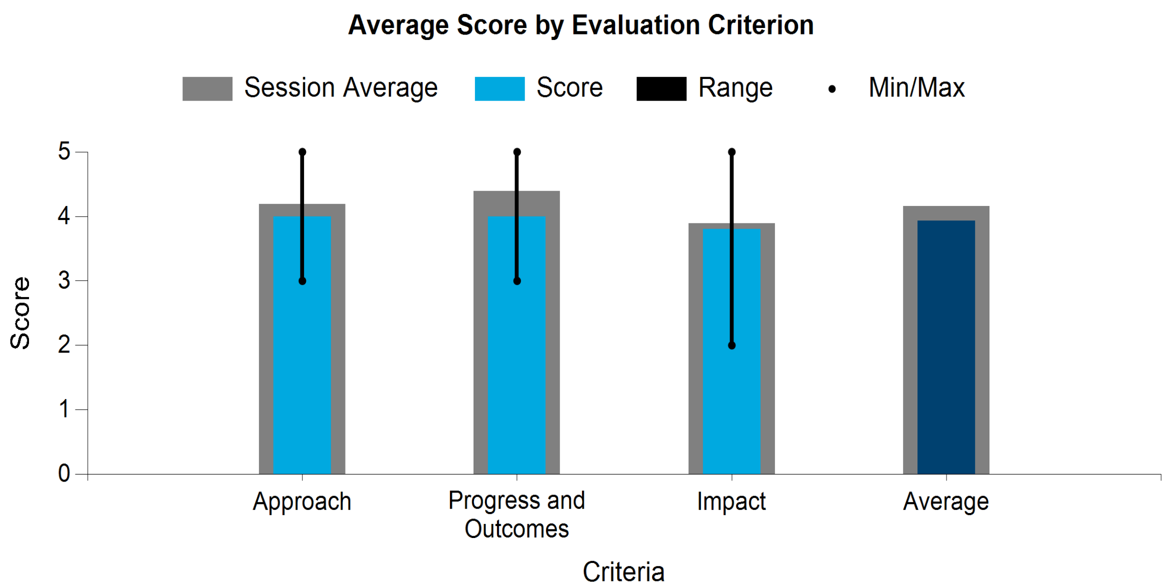
UPGRADING BIOGAS THROUGH IN SITU CONVERSION OF CARBON DIOXIDE TO BIOMETHANE IN ANAEROBIC DIGESTERS

Washington University in St. Louis

PROJECT DESCRIPTION

WBS:	2.4.1.500
Presenter(s):	Zhen He
Project Start Date:	10/01/2021
Planned Project End Date:	04/30/2025
Total Funding:	$2,881,916

This project aims to develop an innovative system for the *in situ* biological conversion of CO_2 to CH_4 through integrating several existing processes/technologies—such as membrane-supplied H_2, thermoelectricity, and microbial-electrochemical systems—in innovative and synergistic ways to ensure both novelty and a high chance of success. At the end of the project, an integrated bench-scale system will be able to produce pipeline-quality RNG containing >97% CH_4 via two steps: biological CO_2 conversion to CH_4 that generates a biogas of >95% CH_4 and gas cleaning that reduces impurities and further enhances the CH_4 content to >97%. Our target CO_2 concentration in the final RNG is <1%. The H_2S content will be kept below 5.7 mg/Nm^3 (or 0.25 grains/110 scf). Advancements in research and development, as well as a holistic understanding of the potential impacts of system deployment across economic and environmental indicators, are critical to the successful transformation from bench-scale to transitional-scale systems (i.e., not yet pilot scale). In this project, a multidisciplinary and multi-institute team is built to jointly advance the proposed technology. The potential technology users/stakeholders will be involved in the early-stage research and will attract more users/stakeholders in its further development. This project will act as a bridge to transform basic research toward further technological development.



COMMENTS

- Not clear on the inclusion of the H_2/CO_2 ratio, as that trend line seems to not be a good fit. Understand that a 4:1 ratio is ideal, but there seems to be very poor process control.
- Great DEI elements.

- The tangential elements around sorbents and thermoelectric materials is not as well tied back as the whole project. I see how it is part of the schematic, but it is not clear where it needs to be to meet project goals. Still seems early on those tasks though.
- Good initial slides to help frame the project, particularly where we as reviewers do not have the full proposals.
- This project is very focused on improving AD efficiency. Clear approach in moving toward a zoned *in situ* methanogenic process.
- Team management seems to have a clear management process and appears to be following it.
- Engagement of commercialization partners could use some more work. Not as clear on the ultimate pathway to the market.
- Production costs of methane seem quite high. Typically, market values are reported in cubic feet (probably worthwhile to include when speaking to commercial partners).
- Overview/impact:
  - This project is investigating innovative methods for upgrading biogas through the *in situ* biological conversion of carbon dioxide to biomethane in anaerobic digesters. The investigators employed an adept technique by applying an external microbial-electrochemical system to infuse hydrogen into the AD system and increase the quantity of methane obtained from carbon dioxide in the AD process. This simultaneously reduces carbon emissions by utilizing CO_2 for upgrading biogas.
  - The project has made significant progress toward addressing the project goals, and it is now moving forward as scheduled in BP2. So far, the investigators have been able to show that the proposed system can upgrade biogas to >90% methane while treating synthetic wastewater, which is a significant contribution; however, the researchers should note that the performance of the system may significantly vary when they use it for treating municipal wastewater.
- Strengths: The project employs a microbial-electrochemical system to provide the hydrogen gas needed for converting carbon dioxide to methane, thereby avoiding the limitations of transferring hydrogen in the liquid state. The project has an excellent team management plan and education outreach program that addresses DEI issues.
- Weaknesses: The title of the project, which states that biogas is being upgraded through the *in situ* conversion of carbon dioxide to methane, belies the actual work done. The project involved external techniques, such as the use of MES to provide hydrogen, and also a biogas purification step for upgrading the biogas to methane. In this study, there is no mention of the quantity of hydrogen that is normally generated in the AD system to serve as a guide for determining the quantity of hydrogen that needs to be infused into the system. Further, the way the results section of this project is presented is discombobulated. The researchers do not clearly state what they have achieved so far in the project.
- Questions: One thing that baffles me is the practicality of providing hydrogen gas into the reactor for increasing methane production by hydrogenotrophic methanogens; won't this disrupt the AD process? Also, at what stage of the AD process was the hydrogen gas added to the system? Was it added throughout the process or just at a particular stage? In addition, the process flow in slide 4 shows that effluent is generated in the MES; what happens to this final effluent from MES? Further, it is noted in the process flow diagram of your proposed system that the heat from methane combustion is supplied to the anaerobic digester. What is the rationale for supplying this heat to the anaerobic digester? This was not clear to me. In slide 6, the investigators state that the project had passed the initial technical verification

step but did not explicitly state what the verification entailed. Last, the researchers should also comment on the feasibility of scaling up this system or incorporating it into the existing AD systems.

- This project proposes a novel, *in situ* method to upgrade biogas and increase methane yield. It has exceptionally strong DEI engagement with students at a range of levels, including outreach activities and HBCU engagement. The project shows that applicability to real-world cases has been thought through and is potentially applicable to a range of feedstocks.
- The presentation provided a nice introduction to the project and its focus. The goal was to produce RNG through a single-stage bioreactor treating organic waste. This was achieved using a gas transferring membrane. Personally, I feel like these gas transferring membranes offer a substantial opportunity for biomethanation, which these researchers are attempting to exploit via a single bioreactor design. My counterpoint (although I agree with Dr. Ren that a single-stage system would be better) is that these membranes would also be attractive for a two-stage system (i.e., stage two would produce the RNG).
- The management of this project appears to be excellent, with multiple project partners serving well-defined roles. There is excellent education and outreach, although an industry partner is still being sought.
- I suggest that the researchers more carefully investigate the ability of gas transferring membranes for biomethanation. There has been a good deal of work on these membranes for oxygen transfer; the researchers could benefit from this work but shift its application to transferring hydrogen rather than oxygen (look up the past publications of Semmens, Nerenberg, and others!). I am particularly optimistic about this technology because I think they should be self-optimizing, meaning that the transfer of hydrogen should be primarily controlled by microbial uptake, thus ensuring the optimal 4:1 hydrogen-to-CO_2 ratio. The researchers have attempted some preliminary optimization of the hydrogen addition, but they only saw increases in the methane content of the biogas; ideally, I'd like to see the researchers continue to increase the hydrogen addition until methane quality reaches a plateau (or decreases).
- This project is still relatively early, but I am very optimistic of its chances for success. LCA and TEA work is planned but is still quite preliminary. The DEI aspects of this work are good, establishing a connection with grade school students and an HBCU. The researchers also claim that 50% of the personnel working on the project are from an underrepresented group, but this is not explained well.
- I'd like to see a more rigorous experiment of hydrogen addition. What is the optimal condition to get highly pure methane? I would like to see a hump-shaped profile.
- Each task is aligned with new and strategic work in biogas upgrading technologies; however, there seems to be the potential for siloed work products, as tasks progress from 1 through 5 with limited industry or potential end-use partners. There is the potential for disjointed work products/separate teams pursuing work apart from one another with current project partners.
- The design of the system setup is unique and may not be applicable in many real-world operational settings. I would recommend that upcoming research reviews typical system design, as there may be significant operational barriers to the deployment of this technology.
- I recommend the inclusion of additional industry partners to secure real-world waste streams for testing and analysis. What is the current LCA and TEA of the progress to date? How has this informed potential improvements? Overall, there are few results available, possibly due to patent processes underway.

PI RESPONSE TO REVIEWER COMMENTS

- We are excited to receive the feedback from the review panel, and we deeply appreciate their efforts and comments. As the reviewers pointed out, this project is still in an early stage. That makes it challenging to address some issues but will allow us to improve or revise toward successful completion of the project. In the following, we are responding to the key questions raised by the reviewers. Because the 4:1 ratio was widely used in the literature, we include it as a factor of study; however, the design of the proposed bioreactor makes it (nearly) impossible to know the precise ratio given that the produced carbon dioxide would be converted within the bioreactor. Therefore, we will focus on monitoring the quality of the produced gas (and residue hydrogen gas) as a means to control the hydrogen gas supply. The reviewer has raised a great point that microbial activities may accelerate or help with the hydrogen supply through gas-permeable membrane. We will conduct more extensive literature analysis and necessary experiments to understand this process. In this project, pure hydrogen gas is used and will be replaced by hydrogen produced from MES (or electrolysis when MES is replaced due to limited hydrogen production). Our unique design allows the reaction of hydrogen with carbon dioxide “outside” the AD zone, thereby minimizing the effects on AD process. It is typical to heat AD to either mesophilic or thermophilic temperature by combustion of the produced biogas. The effluent from MES will be returned to the mainstream treatment, like that of AD effluent treatment. In BP3 we will explore the feasibility of system scale-up. Because AD is a mature technology, the key challenge to scaling up the proposed system will lie in where/how to install membrane units for hydrogen supply. It will be one of our key tasks to involve industry partners (beyond what is in the original proposal) for multiple purposes, such as technology transformation, market discovery, and system development/scale-up.

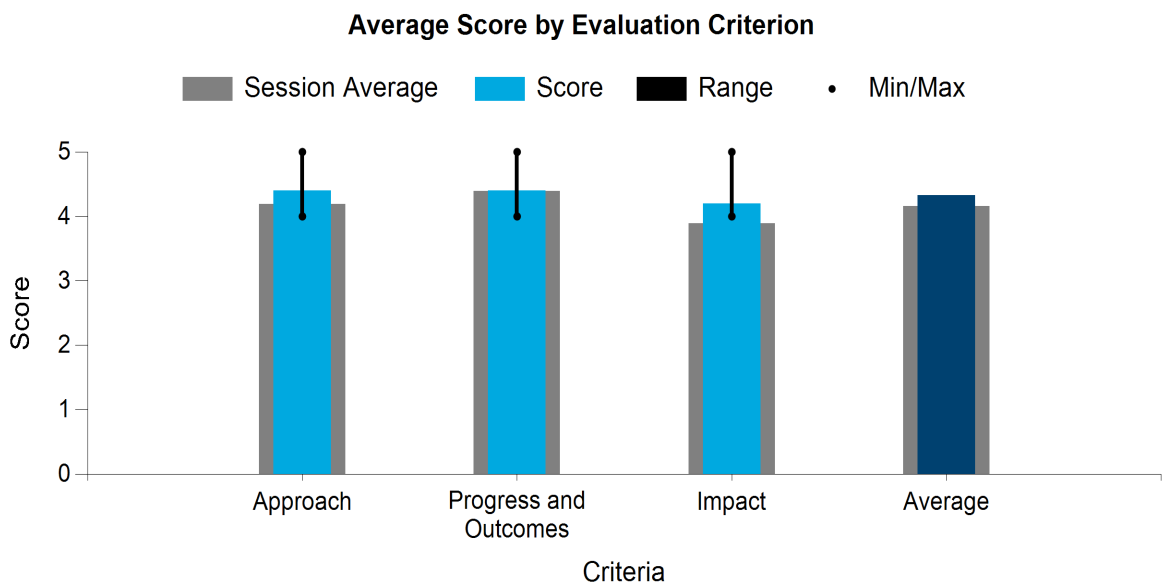
BIOMETHANATION TO UPGRADE BIOGAS TO PIPELINE-GRADE METHANE

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	5.1.3.102
Presenter(s):	Kevin Harrison
Project Start Date:	10/01/2018
Planned Project End Date:	06/30/2023
Total Funding:	$1,500,000

NREL is working closely with DOE, Electrochaea GmbH, and Southern California Gas Company (SoCalGas) to reduce the costs of a biomethanation process capable of megawatt-scale deployment that upgrades organic biogas waste streams to produce pipeline-quality RNG. Biomethanation uses a single-celled methanogenic archaea that converts low-carbon, low-cost hydrogen and waste carbon dioxide to produce renewable methane. The process upgrades the biogenic CO_2—while allowing the CH_4 to pass through—from biogas sources like dairies, wastewater treatment plants, and landfills. NREL and Argonne National Laboratory have completed an LCA using the GREET model to show that the product RNG can be carbon negative even when H_2 production is driven by the existing carbon intensity of California's electricity grid. And, of course, even more carbon negative (−233 kg CO_2e/kWh) when the electricity is produced from low-carbon sources like wind and solar. Leveraging lessons learned from operating SoCalGas' 700-L, 18-bar bioreactor system, NREL is designing and building a flexible research, development, and deployment platform that will enable field trials at biogas and other CO_2 sources. A 16-foot-long trailer will house a 20-L, 18-bar bioreactor, 10-kW electrolyzer, and dosing and thermal systems with only power, biogas, and water feedstocks required by the field locations. The end-of-project goal is to demonstrate pipeline-quality RNG production using real biogas feedstocks.



COMMENTS

- Would be valuable to have the LCOE/TEA because it is also about commercial viability.
- The Low Carbon Fuel Standard does not currently credit CO_2. The 45Q tax credit does provide value. As the LCOE is presented, it will be important to be more transparent about what is/is not included.

- Thank you for including the selling price of RNG in California as a good reference point.
- This project is really tackling a valuable issue. I think the presentation is struggling to convey the steps this project is tackling to lead to commercialization.
- Understand that DEI goals were not part of the original project in 2019. Will be doing a bunch of educational/outreach activity (would have liked to have seen more, particularly for something as well suited to address DEI and remote communities).
- Very excited that so many companies seem willing to invest money in this project. Speaks well about its ultimate commercialization. Seventy percent production of RNG is a big deal. Easy economics to convey.
- As best as I can tell, this most recent phase of the project was to build the mobile unit. Knowing about the supply chain disruptions, it is certainly a feat that this was accomplished during COVID.
- The baseline is other gas separation technologies of biogas feedstocks.
- Methanogen is very robust to impurities, oxygen, and H_2S; easy to inoculate.
- Can do load following with this technology; an important grid technology and for remote applications.
- Overview/impact:
    - The project focused on scaling down the entire hydrogen-biomethanation system into a mobile electrolyzer-bioreactor system to enable faster research in the field, intellectual property development and validation, and improved gas mass transfer. This is all aimed at reducing the cost and de-risking the biomethanation process by supporting on-site renewable energy production from animal waste, landfills, and wastewater treatment by using the CO_2 typically released by these facilities to nearly double pipeline-quality RNG production compared with gas separations systems.
    - The research project has shown considerable progress as the design-build-deployment of the mobile bioreactor system is in the finishing stages, patents have been applied, and papers, publications, and presentations have been made.
- Strengths: The project involves a large group of university researchers, industry partners, and utility partners who have different forms of expertise that are used to improve the quality of the project. The project is environmentally friendly, as it biologically upgrades carbon dioxide.
- Weaknesses: Though the technology is interesting and impressive, one main concern is the level of risk associated with the process. The project seems risky, as leakage of hydrogen gas may lead to casualties, especially when the system is not operated by highly skilled personnel.
- Questions: The researchers mentioned that one advantage of the system they are designing is that the reactors can be made in small sizes to fit the needs of a particular area; however, they only talk in terms of size. The cleanup requirements for gases can vary from place to place; the researchers should throw more light on how they intend to incorporate this in their design.
- This project seeks to improve the efficiency of biomethane production from a variety of feedstocks through the conversion of CO_2 to methane using hydrogen as a fuel source. Among the strengths of the project is the engagement of a range of potential partner utilities in the United States and abroad. Another strength is the demonstration of the scalability of the process in tandem with supply and the development of a mobile R&D platform. The TEA presented makes a strong case for the viability of the project

concept at full scale. Two recommendations for future improvement. First, although the BETO award was prior to the DEI requirement and the project will not be assessed formally on that basis, researchers need to educate themselves more fully on what DEI requirements entail internally to project staff, as well as externally to communities. Specifically, researchers should strengthen their understanding of the importance of diversity in project staffing at senior as well as junior levels, and they should integrate a proactive strategy of engagement among students from the high school through doctoral levels. Further, researchers should pursue community engagement among community and/or nongovernmental organization groups working in waste sustainability and renewable energy. In addition, the concept of excess wind/solar energy storage in biomethane is intriguing but may be concerning to many stakeholders, including policymakers and elected officials, as it entails the conversion of carbon-free energy to a chemical form that emits carbon upon use. This may not be a contradiction from an engineering or business perspective, but it does present a system contradiction at a societal scale.

- The researchers did a nice job of framing the problem and their associated solution. Their partnership with SoCalGas appears to be very strong and very helpful to the success of the project.
- Scientifically, the researchers did a good job of framing their research in terms of the fundamental constraints (i.e., hydrogen addition is mass transfer limited). They did a nice job of explaining their novel use of an "evolved" hydrogenotrophic methanogen (i.e., not a genetically modified organism). They do a nice job of recognizing the limitations of their work (i.e., the focus on hydrogen sulfide as a limitation). One issue appears to be their ability to add hydrogen at the optimal molar ratio; this was shown to be successful but not explained very well (possibly for confidentiality reasons?).
- The DEI aspects of this project were weak, albeit the project was initiated prior to 2020, so there were no specific DEI requirements.
- This project seems closer to commercialization than many of the other projects that I have seen so far.
- An increase in the production of RNG to 60%–70% would increase the feasibility of ever-smaller organic resource facilities participating in RNG projects and accessing the incentives available to such projects. This project provides a clear path toward commercialization and the potential for significant impact and outcomes.
- Once tested in Maine, it would be ideal to evaluate and mitigate issues related to the transportation and deployment of these mobile units nationwide. Industry and research partners assisting with this project are well poised to evaluate such issues to ensure operability and safety of the unit.
- This mobile unit technology seems ideal for deployment in remote areas with an available renewable energy source and a biogas resource (e.g., landfills, wastewater) yet unreliable or poor quality electricity. Such communities (e.g., West Virginia, desert Southwest, Alaska) could benefit from increased RNG resources while forgoing the emissions of degraded organic waste streams and transportations cost to secure delivery of fossil fuels to remote areas. Utilities and their customers would benefit from increased grid stability and additional renewable energy.

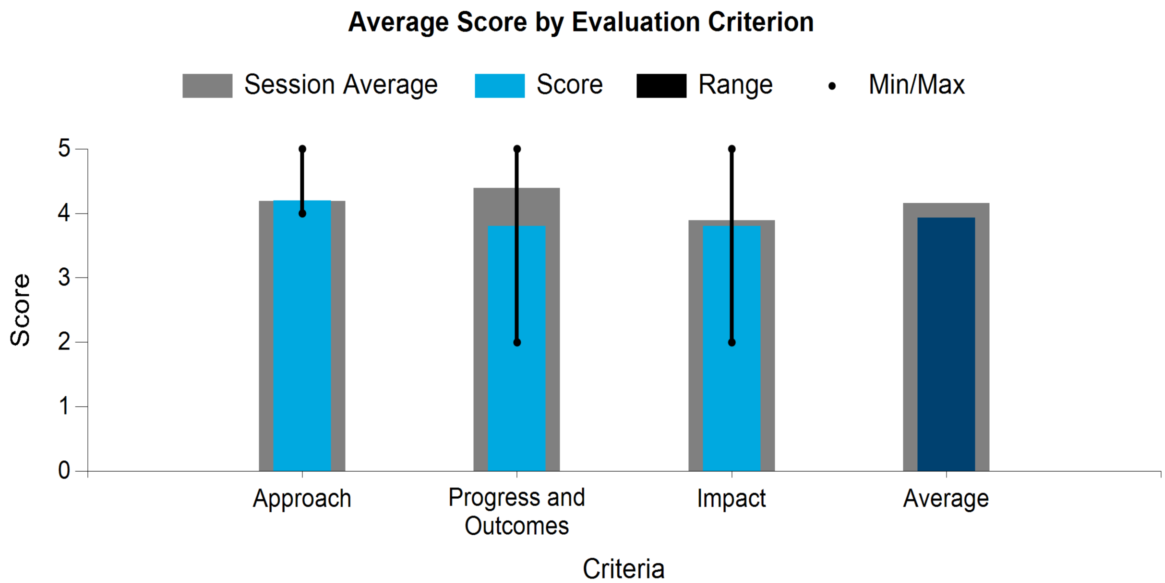
PI RESPONSE TO REVIEWER COMMENTS

- Thank you to all the reviewers for their thoughtful and constructive feedback. While most comments were positive, especially regarding industry involvement and pathway to commercialization, one minor theme about risk and gas cleanup was identified. The mobile electrolyzer-bioreactor research apparatus being designed and built under this project will provide an opportunity to conduct research in the field at various biogas or carbon dioxide sources. The NREL team acknowledges that the mobile system carries some risk of not having all the required gas cleanup technologies when first deployed to handle every biogas source; however, the team is building in flexibility to add or remove subsystems as needed. In other words, if one of the biogas sites to be visited ends up being a landfill, requiring additional input gas cleanup for siloxanes, for example, the team will take extra measures to ensure that gas cleanup technologies are integrated to address typical impurities prior to the site visit.

MAXIMIZING BIORENEWABLE ENERGY FROM WET WASTES

University of Illinois at Urbana-Champaign

WBS:	5.1.3.201
Presenter(s):	Lance Schideman
Project Start Date:	10/01/2018
Planned Project End Date:	06/30/2023
Total Funding:	$1,981,397



COMMENTS

- Was able to clearly see the effect of temperature on the productivity of the AD organisms (seasonality). Not much of an issue because the effective solids retention time is increased in that situation. How clean is the ammonia coming out of the cloth filter anaerobic membrane reactor (CFAnMBR)? Wondering if the additional step of electrolysis is worthwhile. Ammonia is also a liquid as opposed to H_2, which is a gas. The H_2 market is not as well developed nationally as NH_3.

- Overview/impact:

  - The researchers investigated techniques for maximizing biorenewable energy from wet wastes (sewage sludge) using an integrated system that comprises novel cloth filter anaerobic membrane bioreactors (CFAnMBRs), ammonia ion exchange, and ammonia electrolysis to hydrogen gas. The aforesaid techniques were used in improving the efficiency of conventional anaerobic membrane bioreactors (AnMBRs), which have limitations such as low gas flux and high membrane fouling. Applying the techniques used in this project in wastewater treatment plants will help to reduce their energy costs, as there will be no need for aeration (which usually consumes a lot of energy) at the treatment plants.

  - Quite a lot of progress has been made in this work. The researchers were able to achieve about 80%–90% removal of COD from the influent waste stream, which is about twice the COD removal efficiency of conventional AnMBRs. The production of hydrogen from ammonia helped to improve the fuel energy output of the AnMBR by 22%.

- Strength: Rather than stripping ammonia and releasing it to the environment, the project involves ammonia ion exchange and electrolysis to produce hydrogen gas, which makes the project eco-friendly. The project also has a very good management plan.

- Weaknesses: One main goal of this research was to increase the net energy yield from municipal wastewater treatment; however, the researchers need to note that energy in wastewater may be lower than the energy invested in energy recovery, as in most cases the wastewater is highly dilute, especially during the wet/rainy season. Further, the researchers should also comment on the feasibility of scaling up this system or incorporating it into the existing treatment systems. In the same vein, the researchers indicated in slide 20 that the overall distributed low-energy wastewater treatment (D-LEWT) process is net energy positive. The researchers should note that the lab-scale operations and performance of the system may significantly differ from the full scale. Therefore, a bench- or full-scale assessment is needed to establish if the proposed system is viable. Also, the researchers propose a technique that involves the addition of coagulants or adsorbents to AnMBR, and I am wondering if they have considered the implications of adding chemicals to the system, as this may have a significant impact on the final product and AD process. Moving forward, the researchers should also consider the toxic shock of the AD process, which is usually common from raw wastewater. Last, in reporting the progress made in the project on slide 21, the researchers indicate that chemical and material consumption in the project increases climate impacts; however, they fail to provide any research data to back up such a claim.

- The project seeks to improve municipal wastewater treatment through the use of membrane bioreactors as well as the conversion of ammonia to hydrogen. The issue of membrane fouling was addressed through the use of a cloth filter membrane. Optimizations achieved lower treatment costs and the potential to commoditize hydrogen as an income source; however, this led to the overall net energy positivity of the approach.

- The project showed strong partner engagement, including a potential host community in Urbana-Champaign, Illinois. In future work, the project team should seek to include a broader range of stakeholders in education and outreach, including local organizations engaged in waste policy. Further, the project should work with Black, Indigenous, and other disproportionately underrepresented groups in STEM to engage and build an understanding of the benefits of this approach to the wastewater treatment industry.

- The goal of this project is to reduce energy usage during the mainstream treatment of municipal wastewater by replacing conventional activated sludge (CAS) with a novel AnMBR design. The investigators proposed to remove ammonia from the wastewater via electrolysis to generate hydrogen gas; the ammonia removal process was augmented by using an ion-exchange process (using clinoptilolite as the ion-exchange medium). The project was well managed, and the results were disseminated to the various stakeholders.

- Treatment efficiency was generally good as far as COD removal, although the investigators were careful to avoid performance comparisons with CAS processes. This treatment process appears to involve lower energy usage compared to CAS, but without a performance comparison…this does not necessarily appear to be a fair comparison. That is, there appears to be a trade-off between process performance and energy usage; in that case, there are other lower energy process designs (e.g., a trickling filter) that are also lower energy users that produce lower effluent quality. The investigators also did not seem to have a solution for the dissolved methane in the treated effluent, which is particularly problematic because this was cited in the previous BETO review process. Finally, a benefit identified by the LCA was the reduced potential due to eutrophication, but this LCA did not seem to incorporate phosphorus removal, which is the more common cause of eutrophication in inland waters. In addition, the LCA compared the proposed treatment scheme versus a CAS process that was not intended to perform complete nitrogen removal; again, this is an unfair comparison, particularly given that a total nitrogen removal process is typically believed to require less energy than a CAS process (i.e., nitrate is used as the terminal electron acceptor for microbial respiration, thus reducing the oxygen demand by the process).

- Generally speaking, this is really high-quality research, although I think that the researchers are trying to "spin" the work to generate a commercially ready process per the BETO requirements. That is, many people recognize that CAS is a highly energy-intensive process, and these same people have suggested mainstream anaerobic treatment. With this in mind, rigorous and fair-minded LCAs and TEAs could be incredibly valuable because they would identify the specific situations in which mainstream anaerobic treatment would be preferred over conventional aerobic wastewater treatment processes.
- The project demonstrates clear improvement of anaerobic membrane bioreactors and makes additional improvements in the conversion of ammonia (which can inhibit AD) to hydrogen gas by electrolysis. This area of research targets 1%–3% of national energy consumption in order to move WRRFs toward a position of neutral or net-positive energy generation.
- The application of technologies could potentially be deployed at small facilities with a limited budget, in all making a large impact on the creation of bioenergy from smaller organic sources.
- AnMBRs have had limits to their deployment due to the issues discussed by the project leads. Although research targets WRRFs, applicability to other organic waste streams seems to provide an even larger target for further beneficial outcomes for the performer and the government.

PI RESPONSE TO REVIEWER COMMENTS

- Response to Reviewer 1: Ammonia in the CFAnMBR permeate is typically 25–35 mg N/L. This ammonia must be removed from the wastewater prior to discharge, and we have selected an ion-exchange process to do that. Regenerating the ion-exchange media results in an ammonia-laden brine regenerant solution, which is not well suited for fertilizer applications because it is not concentrated enough (~0.1% N) and the salt concentration is too high. Ammonia could potentially be sparged out of this brine solution to provide gaseous ammonia, and the gaseous ammonia could be compressed into liquid (anhydrous) ammonia, which is a viable commercial fertilizer; however, this project was designed to investigate a more novel route to utilize the ammonia brine for hydrogen production by electrolysis. It is possible that H_2 production from ammonia is not the most economic method of removing ammonia from the wastewater stream and that production of a concentrated NH_3 product is more economic. Considering the relatively high-energy and chemical inputs for the ion-exchange/electrolysis step, the University of Illinois group is also pursuing funding sources to research other low-energy, low-chemical-use processes for treating the ammonia-rich permeate (e.g., biological nutrient reduction). The team will continue to work with Aqua-Aerobics on the potential commercialization of the technology for the application of AnMBR and share the final project findings with the company to discuss strategies for achieving this. The team is also working with other cloth filter manufacturers who may be interested in commercialization for this application. The recipient acknowledges that the DEI plan for this project was underdeveloped, as this was not originally included in the scope of the work requested by DOE at the time of this award. The team has since submitted additional proposals with a DEI document with measurable milestones to improve work in this area. The Illinois Sustainable Technology Center is leveraging the DEI resources available to the University of Illinois, which have helped support hiring diverse staff at senior, junior, and student levels. A number of minority-serving institutions in Illinois have been identified for potential collaboration in the greater Chicago area for future work. The applicant does feel that the goals of the project support the goals of the Council on Environmental Quality, which includes environmental justice, and could produce lower-cost, energy-positive wastewater treatment for rural and economically disadvantaged communities, which typically have fewer municipal resources for wastewater treatment. The reviewer mentions the difficulty in overhauling or retrofitting existing large

WRRFs. We agree this is an important target for the development of this technology and have included some information on this in our 2021 BETO Project Peer Review presentation. Basically, we have proposed that existing tankage for aeration and sedimentation can be covered with flexible tops and converted to anaerobic bioreactors with plastic media similar to integrated fixed-film activated sludge processes. Then a cloth filter can be added to the effluent of the converted tankage. Thus, if we can get the hydraulic retention time of the AnMBR process to roughly match the current aerobic treatment processes, a relatively low-cost retrofit option can potentially be achieved that will greatly increase the net energy production of existing WRRFs.

- Response to Reviewer 2: While municipal wastewater is relatively low strength (400–600 mg COD/L), AnMBR helps decouple the hydraulic retention time and solids retention time to provide conditions sufficient for AD to proceed with short hydraulic retention times. By increasing the membrane flux and lowering cleaning energy, the CFAnMBR increases the share of organics treated anaerobically (i.e., increasing net energy produced as biogas) and lowers the energy inputs by reducing or eliminating aeration. Energy balance showing net-energy-positive process was based on our CFAnMBR pilot performance over 2 years, not bench-scale work. The chemicals currently used in the coagulation step are commonly used in coagulation processes used in the WRRF industry for improving effluent quality and are not known to induce toxicity under normal operating conditions. The LCA has incorporated the effect of ferric chloride on reducing phosphorus and its effect on eutrophication potential, and it will continue to explore other effects of the coagulation step on operational parameters. Increased GHG emissions from material and chemical consumption were based on the pilot-scale operation of the CFAnMBR and ion-exchange system, their respective chemical inputs, and the indirect GHG emissions embedded in the production of those materials. This evaluation was performed in the LCA step using widely accepted emissions estimates for these materials. The main GHG contribution is for NaOH, which is used consumptively in the process because electrolysis requires a high pH, and the ammonia removed in this process is a base that must be replaced to maintain a high pH.

- Response to Reviewer 3: The recipient is currently working on the dissemination of the project results to industry and academic sectors through journal articles and conference presentations, including a presentation at the annual Anaerobic Digestion Conference in spring 2022 and presenting at a regional meeting for wastewater operators. The team will consider future work with local or state organizations that work in waste management policy. See response to Reviewer 1 for additional comments regarding DEI and working with historically underrepresented groups.

- Response to Reviewer 4: The TEA/LCA comparisons for the baseline CAS and the proposed D-LEWT process scenarios were developed in CapdetWorks wastewater modeling software such that all the processes achieved 90% COD removal, which the CFAnMBR pilot was able to achieve with a sufficiently high coagulant dosing rate. The reviewer is correct in that the CAS and D-LEWT processes are not comparable in terms of total nitrogen removal; however, this is why the CAS + denitrification scenario was also modeled to more accurately compare the two processes when both are designed to meet the same effluent water quality goals. A separate TEA/LCA scenario has been modeled for the case in which endogenous COD is used for denitrification; however, this scenario was not included in order to simplify the Project Peer Review presentation and comply with the time limits. This scenario was excluded because its results generally fall between the limiting cases of CAS and CAS + tertiary denitrification. In our work, we are trying to match the costs of CAS, which is the predominant current WRRF process, while trying to achieve the better effluent water quality associated CAS + denitrification, which is expected to become prevalent as discharge regulations become more stringent. The reviewer noted that "a total nitrogen removal process is typically believed to require less energy than a CAS process (i.e., nitrate is used as the terminal electron acceptor for microbial respiration), thus reducing the oxygen demand by the process)." There is significant literature showing that plants providing advanced nutrient removal typically use 30%–50% more energy (e.g., Burton, F. L. 1996. "Water & Wastewater Industries: Characteristics & Energy Management Opportunities," CR-10691, Electric Power Research

Institute). Although nitrate may be used as an electron acceptor, it generally requires aeration to first convert ammonia to nitrate, such that there is not a net reduction in the oxygen demand for using nitrate. The LCA slide discussing eutrophication potential may not have been clear, as the differences in eutrophication potential between the five scenarios was only due to lower phosphorus removal due to the coagulation step in the D-LEWT process. The finalized TEA/LCA due at project end will consider all the operational parameters of the pilot-scale system and refine the TEA/LCA for other scenarios for a more comprehensive comparison that addresses the reviewer suggestions. The University of Illinois team intends to begin work on dissolved methane recovery later this year, using external funding from U.S. Army partners and future DOE grants for WRRF decarbonization. Discussions with several commercial degassing equipment manufacturers have determined that vacuum degassing over packed beds is the most promising technology, which will be tested at the pilot scale using permeate from the CFAnMBR.

- Response to Reviewer 5: The recipient agrees that future research and collaborations should include the market potential for higher-strength organic waste streams (e.g., industrial wastewater, food and beverage, agricultural wastewater).

A CATALYTIC PROCESS TO CONVERT MUNICIPAL SOLID WASTE COMPONENTS TO ENERGY

Worcester Polytechnic Institute

PROJECT DESCRIPTION

WBS:	5.1.3.202
Presenter(s):	Mike Timko
Project Start Date:	10/01/2018
Planned Project End Date:	06/30/2023
Total Funding:	$2,497,821

Biofuels and bioenergy have the potential to reduce GHG emissions, improve energy security, and reduce energy price volatility (https://doi.org/10.1016/j.eneco.2005.11.003). Unfortunately, despite significant progress in the past 20 years, the conversion of biomass into transportation fuels is not yet directly competitive with fossil fuels (https://doi.org/10.1016/B978-0-12-407909-0.00030-4). In fact, biomass conversion costs have steadily decreased in the past 10 years, as indicated by successive cost estimates published by NREL, while biomass feedstock costs have remained nearly unchanged (https://doi.org/10.2172/1013269; https://doi.org/10.2172/982937). Reducing the costs of biomass production, transportation, and storage has proven more difficult. As suggested in DOE's Billion-Ton Report (https://www.energy.gov/eere/bioenergy/2016-billion-ton-report), a potential solution to biomass production costs is to use waste feeds that would otherwise require a tipping fee for disposal. MSW, including food waste and green waste (e.g., yard waste), is especially attractive as a feed for bioenergy production. Depending on location and tipping fees, the conversion of MSW to energy diverts it from landfills, where its AD leads to GHG emissions, and the generation of MSW coincides with population centers.

Food waste constitutes approximately 15% of the total mass of MSW. Water constitutes approximately 50% of the total mass of food waste, effectively reducing its energy content relative to other organic components of MSW. Its high water content and variable composition make conversion using pyrolysis and gasification unattractive energetically, as these require energy-intensive drying and result in significant char and tar formation. The HTL process is a great fit for the conversion of waste feedstocks with high water content. This project is designed to tackle the main challenges associated with converting the combined food and green waste feed to fuel product, namely diesel.

The main project objective is to generate bench- and pilot-scale experimental data and models to de-risk the commercialization of a process to convert a combined stream consisting of the food waste and green waste components of MSW into an energy-dense bio-oil and refined lignin stream. Green waste is fed to a solvent-based fractionation process that produces furans from the cellulose and hemicellulose fractions and lignin. The lignin is co-fed with food waste to an HTL process for the production of an energy-dense biocrude. The biocrude undergoes catalytic hydrodeoxygenation and denitrogenating to improve its fuel properties. The component processes are being investigated at the bench scale, and the data are used for operating a continuous HTL system constructed at Mainstream Engineering. Finally, the economics and LCA of the carbon emissions from the overall process will be continuously assessed using standard metrics of energy return on investment and LCOE. The project is split into eight tasks based on the individual expertise with milestones for each task. The main products of the technology are upgraded HTL biocrude and a furan stream to be sold as chemicals. Byproducts will include a gas purge stream, consisting primarily of carbon dioxide; a char stream, with many potential applications; and an aqueous phase containing water-soluble organic compounds produced in the HTL process. The catalytic upgrading process is designed to minimize carbon loss to the aqueous phase, since aqueous-phase carbon represents energy loss and the contaminated aqueous phase must be treated prior to discharge, thereby increasing costs and decreasing overall efficiency. The catalytic hydrogenation step further improves HTL bio-oil properties, specifically heating value, by rejecting oxygen and nitrogen.

The main target markets are the U.S. chemical market and the U.S. diesel fuel market for the upgraded bio-oil product. These markets represent billion-dollar opportunities in both transportation and stationary heat and power. The feedstock of MSW is around 250 million tons per year in the United States. Utilizing the organic fraction (~40%) would significantly divert waste from landfills while providing an inexpensive and renewable feedstock for fuel production. The proposed technology could produce 10%–15% of the annual domestic gasoline usage (assuming 100% material efficiency) or 3%–5% with 25% efficiency.

To date, the team has successfully fractionated two different real green waste streams into lignin-rich and carbohydrate-rich fractions for lignin products and biofuel feedstocks, with the carbohydrate fraction having less than 10% lignin. The team is now finalizing solvent recovery experiments.

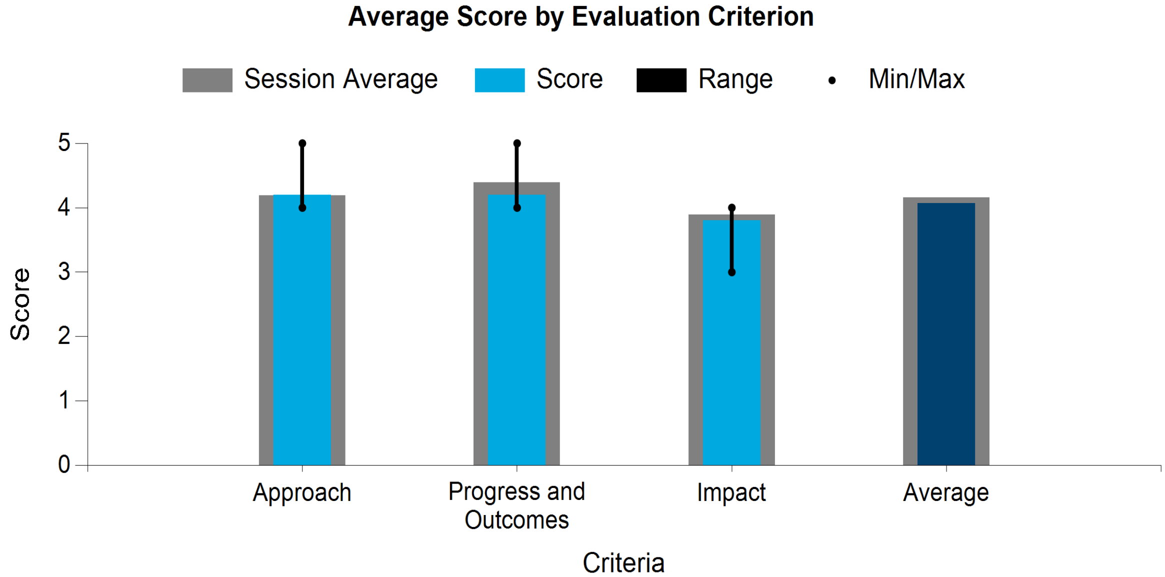
The team has evaluated HTL of many different feeds, including green waste, lignin, food waste, and their mixtures. Food wastes available in cafeterias provide the best HTL performance of these, with energy recovery exceeding 60 wt %. The team has studied interactions between co-fed components in molecular detail, identifying sources of synergy when food waste and green waste are co-fed. The team has developed machine-learning and physics-based models to predict biocrude yields and nitrogen fate.

Catalysts are used to minimize carbon loss to the aqueous phase. The team has evaluated four generations of catalysts to achieve this goal: (1) $CeZrO_x$, (2) inexpensive oxides, (3) Ni-impregnated oxides, and (4) hydroxyapatite. Of these, hydroxyapatite is the most effective at boosting biocrude yields while minimizing costs.

The hydrotreating step required to convert biocrude to diesel fuel can be performed using industrial CoMo or NiMo catalysts. The team has studied Mo_2C as a potential disruptive catalyst to minimize H_2 consumption in the hydrotreating step. Mo_2C is an effective catalyst for hydrodeoxygenation to preserve the carbon content of the biocrude. Conversion to the oxide form remains a challenge.

Continuous HTL tests have been performed with various food waste streams. The team has now completed 45 of 100 hours required for continuous testing. Performance in continuous tests is comparable to that observed in the batch. The team has gained useful experience in formatting real waste streams to ensure pumpability.

Economic and environmental analysis have been performed, with the finding that a 75% food waste and 25% lignin co-feed stream to the HTL process is optimal. This arrangement leads to an MFSP of $2.74/GGE, a 50% reduction relative to the starting point. The energy return on investment is 1.73, which is an acceptable value for a fuel product. The team is actively engaged in patenting these technologies, and the PI recently cofounded a company for commercialization purposes.



COMMENTS

- Hydroxyapatite (catalyst) research for HTL is showing real promise and improvement over standard practice. Clear value in increasing the oil yield from existing feedstocks.
- Curious about the catalyst life and resiliency. Project team is leaning heavily on its low cost and acceptable lifetime/resiliency.
- Less clear of the impact/value of lignin separation because it looks like its oil yields are in the middle. Seems its value is not in HTL yield but in the co-solvent enhanced lignin fractionation (CELF) fraction itself. Lignin separation does increase the yield of bio-oil. The CELF process is more valuable because of the furfural/hydroxymethylfurfural recovery.
- Would also be interested in the resiliency of this process—e.g., what happens if a plastic bag ends up in the stream? If these numbers are real, it seems like just commercializing the CELF process would be valuable on its own.
- Analysis work is generating interesting data and serving as an independent sounding board for the national lab work.
- The biocrude upgrading task appears to be less progressed than many other tasks.
- The team has incorporated DEI activities in real time. Nice inclusion of undergraduates from nontraditional STEM individuals.
- The team recognizes that the state of the industry has moved beyond what is in the FOA, and it is still seeking to push the technology forward.
- The team has spun out River Otter Renewables to commercialize the technology. Positive development that River Otter Renewables is looking to license the technology. Still a lot of bent on the academic literature; it's going to take a lot to commercialize (see PNNL's ongoing difficulties). I'm not saying that this team wouldn't have more success, just noting that investor appetite for this kind of a project has been less than ideal.

- Initial phase of the project was delayed by the pandemic but appears to be back on schedule.
- While the 100-hour run time seems to be within reach, unclear about the learning from the intermediate run times. Could one of the earlier runs be bumped up? Is there some value in marginally adding about 10 hours at a time? Should be looking at longer continuous run time, perhaps not 100 hours.
- The project team is talking but doesn't seem to be coordinating as well as ideal.
- Overview/impact/progress:
    - The researchers investigated a novel, innovative, and widely applicable technique for effectively managing the organic fraction of MSW. The researchers combined green waste fractionation with HTL and catalytic upgrading to produce energy-dense liquid products from MSW. A lot of ingenuity is shown in this project, as the researchers applied the novel technique to a wide array of substrates, including food waste from hospitals and green waste from industries, showing that the technique is widely applicable, as any type of waste can be properly degraded.
    - The project is highly impactful to the urban environment, as it will help curb the menace involved with the indiscriminate disposal of MSW, especially the organic fraction of the waste. It helps in reducing overdependence on landfills, as it serves as a way of treating/managing solid waste while generating renewable energy from the waste. A lot of versatility is shown in the project, as high-quality fertilizer is obtained as one of the end products of the process. Also, the process is designed in such a way that there is phase water/oil separation, and thus the process water can be recycled. The patents, awards, conferences, and publications that have been obtained with this project speak volumes about the originality of the project.
    - The researchers have made tremendous progress toward achieving the goals of the project. Despite the challenges and delays in the project, it is still on track, as most goals have been met. The researchers have been able to produce lignin-rich (>90% lignin) and lignin-free (45 hours time on stream) and obtained greater than 45% energy recovery from food waste.
- Strengths: The researchers show a lot of inventiveness in this technique for converting MSW to biofuel by combining waste fractionation with HTL and catalytic upgrading. Also, the project involves collaboration between researchers from different universities and industry partners who have different kinds of expertise that are being fused together. In addition, there is a logical flow of tasks, as the work from one principal investigator feeds/fits into those of other principal investigators. Another major commendation for this project is the incorporation of scenario-based models.
- Weaknesses: In this study, nothing was shown about the characteristics of the feedstocks used in the process. The researchers should note that the feedstock type/characteristics have a significant effect on the catalysts used and process performance. The researchers should therefore conduct a sensitivity analysis between the catalysts and feedstock type/characteristics. After this sensitivity analysis, the researchers should determine the optimum conditions of the process before moving forward to scaling up the system. Further, the researchers should consider assessing the economic viability/feasibility of using catalysts on a full scale but testing different models. The researchers should also comment on how they plan to handle MSW contaminated with non-biodegradable materials such as plastics, etc. I am worried this may limit the scaling up or commercialization of the system.
- The project investigates the use of HTL to convert food and yard wastes into two products: biocrude and refined lignin. The project appears well managed and is making progress. Among operational strengths is attention to the modularization of HTL components and the minimization of transportation.

- In their next presentation, the researchers should more explicitly address the markets and end uses for lignin.
- The researchers define food and yard waste as abundant and inexpensive; however, they should carefully consider food waste sources and potential for significant contamination with film plastics, as well as plastic containers and packaging (glass, metal, and other contaminants are less of an issue in source-separated organics collection). The researchers used institutional kitchen waste as the test feedstock, but most food waste generated is from residential or food service establishments and may not have the same level of purity. If this process can accept and convert plastic contaminants, then researchers should specify maximum levels and other feedstock requirements. Being able to manage plastic-contaminated biogenic feedstocks will greatly improve the acceptability of this method of treating versus what many small and regional compost operators and the public prefer to do with well-separated food and yard waste: make compost to enrich soils and promote food sovereignty (regardless of energy return on investment [EROI] or other bioenergy metrics commonly applied to compare projects).
- This project is focusing on a catalytic form of HTL to convert MSW to a usable energy source.
- This project has very much benefitted from the TEA in which the researchers have considered various different catalysts with the goal of increasing biocrude yield, increasing char reduction, and reducing the cost per GHG equivalent. The project also has a legitimate effort in DEI, although this was not a requirement. The investigators have also been very successful in promoting their work, both via academic publications and other routes of publicizing their work. The management of the project appears to be excellent (a lot of data sharing) through regular meetings (online and in person) with all project personnel.
- The project is making substantial progress toward the identification of chemical and thermal processing to create biocrude from high-lignin wastes, which would further reduce needs for diverting such wastes to compost facilities or high-energy drying for gasification. Benchmarks exploring new catalysts and treatment options are continuing, with the future development of other catalysts for processing identified chemical contaminants in the remaining project time. Research has established fast, efficient, and adaptable pretreatment possibilities for lignin-containing wastes that are currently difficult to convert to energy, all while creating valuable coproducts for sale and environmental co-benefits.
- Shipping container size of technology could enable the development of completed technology at a lower cost for quick deployment, with a clear path for potential commercialization. Lignin is a large barrier to sorting and processing waste; its beneficial use will provide significant impact and outcomes.

PI RESPONSE TO REVIEWER COMMENTS

- The team appreciates the reviewers' thoughtful comments. The project has not been without its challenges. BETO's consistent support throughout, especially during the pandemic, was critical to our accomplishments. In exciting news, we are happy to report that the company commercializing this technology, River Otter Renewables, has nearly finalized licensing key patents that stem from this BETO-funded work and is in advanced discussions with an early-stage investor and a state incubator. The town of Stow, located in central Massachusetts, is enthusiastically supporting these efforts, especially as the extent of its PFAS contamination problems become increasingly evident. The reviewer comment that the bulk of this project has tended toward the academic is accurate, and seeing the rapid transition to potential commercial deployment is evidence that targeted science can yield tangible results. Responding to every comment is not possible. We pick several recurring or important themes instead.
- Reviewers identified catalyst lifetime as an area for future attention. We agree with this assessment. Initially, we deployed catalysts in the same reactor as the HTL process. Since our early work, we have moved to using two separate reactors, one for HTL and one for catalytic conversion. The two-reactor

system shows promise for extending catalyst lifetime, with an achievable known limit of 200 h based on catalyst endurance testing. While 200 h is less than is typically considered necessary for industrial applications, our focus on inexpensive catalysts allows us to operate economically with catalysts that last less than 200 h. Batch experiments that simulate the two-reactor system have yielded promising results. This summer, we plan to test the catalytic step in a dedicated packed bed reactor. Early results obtained on a collaborator's reactor were promising.

- The relative value of CELF and HTL. The reviewer is correct: Much of the economic value of the process is driven by the furfural products of CELF; however, much of the waste reduction value is driven by HTL. The two technologies are a good fit for one another, especially since the lignin product obtained from the CELF process needs a better end use than combustion to offset heating.
- Biocrude yield must be sensitive to feedstock composition, and the relationship between the two should be studied. The team recognized this early in the project and built a machine-learning model to predict biocrude yields from feedstock composition. That model was published in 2022 and has already been cited 15 times. We are now working on developing a similar model for catalytic HTL. This is a more difficult challenge since the catalyst adds a degree of freedom to the analysis. Ideally, a future study will systematically test a handful of representative catalysts for several different feeds to test the hypotheses that our machine-learning model can generate.
- The fate of plastics should be examined. The waste streams evaluated in this project contained microplastic contaminants, as do all food waste streams. Any yield we report includes those microplastics. For macroplastics, future work can be performed to add different amounts of different types of plastics to a food waste stream to determine the effect on biocrude yield. At low levels (<10 wt %, approximately), plastics are expected to improve biocrude yield, though more severe conditions may be required than we've found optimal for waste streams lacking plastics. In fact, new studies are reporting synergistic interactions between biomass and plastic during HTL. The origin and amount of these synergies is worthy of study in a future BETO project.

DEVELOP AN EFFICIENT AND COST-EFFECTIVE NOVEL ANAEROBIC DIGESTION SYSTEM PRODUCING HIGH-PURITY METHANE FROM DIVERSE WASTE BIOMASS

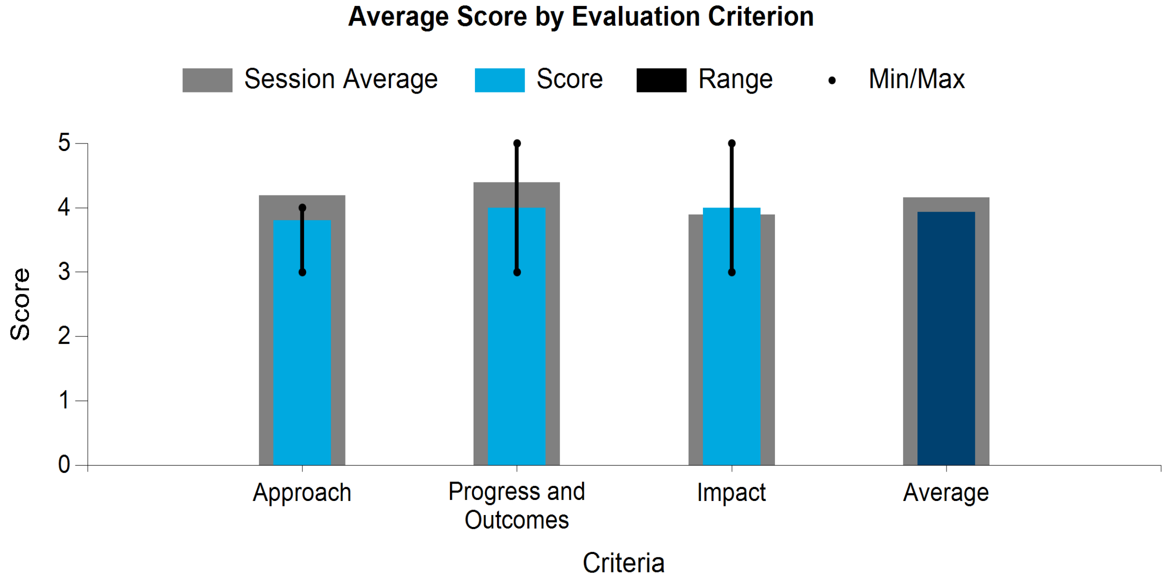
Washington State University

PROJECT DESCRIPTION

WBS:	5.1.3.204
Presenter(s):	Shulin Chen
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2023
Total Funding:	$2,792,893

The lack of cost-effective AD technology is a major hurdle for wide allocations of this technology for converting organic wastes to RNG. This project aims at developing a novel AD system to increase methane yield, productivity, and purity through process intensification. This system takes the synergistic advantages of innovative process engineering and a high-performing microorganism to (1) overcome the recalcitrance of waste biomass through hydrothermal pretreatment, (2) enhance biological conversion rates by using hyperthermophilic microbial communities, (3) achieve *in situ* purification of biogas through methanogenesis under pressure, and (4) relieve inhibition by recovering ammonia as a fertilizer. This novel system is expected to have a near-term commercialization potential by significantly reducing the cost of biogas-based RNG production. The project team includes Washington State University, PNNL, Regenis LLC, and DVO Inc. The active participation of the industry partners makes it possible to use existing AD systems as baseline technology and accelerate technology transfer and commercialization of the novel technology.

The project is expected to produce significant impacts. The proposed novel AD system offers a new platform to DOE's technology portfolio for the production of RNG from different types of organic wastes. The project results will lead to critical data for advancing the technology from TRL 3 to TRL 5, decreasing the risk factor in commercializing the technology. The progress of the project to date has proven the merit of the concept. The project has passed the go/no-go evaluation. Success in this project will remove several key technical barriers and lead to economic development opportunities by creating value from the immense amount of waste biomass. The project also benefits the federal government, as this effort aligns well with the priorities of several governmental agencies, especially those of BETO.



COMMENTS

- The team seems to be addressing the key elements of commercialization.
- Working with two large AD installers is really critical to getting feedback. Have thought through retrofitting and implementation. Actually seem to be underselling the project's performance, which is refreshing.
- Active engagement of DVO throughout the project.
- The team has been able to model quite low EROI, which should make for large market demand. That said, unfortunately, folks are not necessarily looking for solutions, so you will have to go to them, as opposed to them coming to you.
- Not quite clear why the volume and productivity decreased over the life of this project. Have been able to decrease the volume of reactors; I figure that ultimately reduces the capital expenses without dramatically compromising the productivity of the process.
- Clear improvement in EROI and levelized cost of disposal.
- Was the solid retention time also impacted along with the hydraulic retention time?
- Met the overall project metrics as well as the lesser goals that rolled up into these.
- No elements of DEI outreach.
- Project is only producing biogas, which aligns less with the current focus of BETO on SAF and other difficult-to-electrify transportation.
- Certainly a valuable project in the BETO portfolio.
- Interesting thought on high pressure to force more CO_2 into solution and increase the concentration of methane in the biogas.
- Overview/impact:

- This project aimed at developing an efficient and cost-effective novel AD system producing high-purity methane from diverse waste biomass. This project investigated the use of an intensified versatile AD process comprising a hyperthermophilic anaerobic acidification process for the rapid conversion of organic wastes to VFA and a thermophilic anaerobic methanogenesis process for expedient transformation of VFAs to high-purity methane.
- The project has made appropriate progress toward addressing the project goals. It passed the go/no-go evaluation of reducing the LCOE and EROI by 25% of the baseline technology. The project reached all six milestones scheduled for BP1, and only three more milestones remain for BP2.

- Strengths: The researchers did a great job of combining biological and hyperthermal processes without derailing the metabolism of the microorganisms in the AD system. Also, the researchers applied avant-garde molecular biology techniques, such as proteomics and florescence-activated flow cytometry. The project is being carried out using collaboration between academia and industry, thereby providing a means through which the expertise from these two sectors can be leveraged. Further, the industry partners involved in this project are well known for their expertise in designing and building anaerobic digesters.
- Weaknesses: In the process of using hyperthermophilic anaerobic acidification to convert biomass to VFAs, it is expected that other products will be generated from the acidification process. In the flow diagram (slide 3), the researchers do not indicate/mention these products and how they were managed. Further, the researchers suggest the use of hyperthermophilic process; however, I am worried about the costs of operating this energy-intensive system, and this may limit the scaling up or use of the system. It would be great if the researchers could conduct an energy balance and LCA of the system. In slide 13, the researchers present gas production and composition; however, fluctuations can be observed in the gas production, with daily gas production dropping to 0 liters on days 2/25 and 2/26. I am wondering if the researchers could consider repeating the experiments to determine the optimum process conditions of the system before moving to the pilot scale. The researchers should also consider describing the type of organic wastes used in the study, their mixing ratios, and characteristics. This is because the performance of the AD process depends on the characteristics of the feedstock. The waste streams used in the process are manure, biosolids, and food waste; the researchers need to provide more clarity on which type of manure was used and if the results of the project are applicable to other waste materials.
- Recommendations: In the future, I suggest that all the presenters provide a Gantt chart in their PowerPoint presentations tracking the progress of their work against the planned milestones.
- This project is of potential application to the management of manure waste through improved treatment of recalcitrant (fibrous) fractions in feedstock to enhance methane production, with ammonium-derived nitrogen as a recoverable side product. Strengths include building on existing baseline technology, including industry partnership, as well as looking holistically at the whole process. Applicants should build DEI goals into future research through outreach to HBCUs and other institutions serving students unrepresented in agricultural engineering applications, as well as mentoring such students through steps that include job training and higher education. Applicants should continue industry stakeholder engagement to assess feasibility of the modifications to widely used baseline tech in real-world applications.
- The goal of the research was to develop an AD process that could generate a high-methane-content biogas from diverse wastes. The investigators seemed to focus on animal manure as its feedstock, which led to pertinent issues of poor conversion efficiencies of fibrous material and of ammonia inhibition. Three primary activities were to reduce the reactor size, concentrate the feedstock, and alleviate inhibition. The first stage of the process was a high temperature (>60°C) operated at a low pH (5–6). A hydrothermal treatment process was also used. Finally, a thermophilic AD process (T = 50°C, pH = 6.5–

8) was used to generate high-methane (>80%) biogas. The purpose of the first bioreactor was to optimize the hydrolysis of fibrous material, which is believed to be a rate-limiting step. Research goals were generally achieved in that treatment performance, and the methane content was >80% in the biogas.

- The project seemed to lack a rigorous TEA, which I think would be especially helpful. The paradigm of the proposed process design seems to be these unit operations should achieve a goal, which is very different than a rigorous analysis of pertinent variables to optimize the system's performance with respect to carbon conversion, COD reduction, methane content of the biogas, etc. It would be particularly interesting to see how a TEA would rank this process design to compare to other process designs that could achieve similar treatment goals.
- Could industry partnerships be expanded to ensure a diversity of feedstocks and differing AD digester types? Typically, the AD systems employed by the industry partner are of the plug flow variety, which are not conducive to the digestion of diverse feedstocks. Concerned this is a technology gap that impacts the future deployment of this research to all types of digesters.
- Results indicate clear progress toward goals, significantly exceeding targets; however, in order to secure beneficial outcomes for AD, the project needs to diversify the deployment of research to other common AD technologies (lagoon, complete mix, etc.). Refinement of microbial communities offers a path forward toward shared improvements to digest wastes across other AD technologies, yet more information is needed on how hyperthermophilic microbiomes have specific applicability toward diverse waste (food wastes, WRRF) streams.
- Overall, the project is advancing toward the stated goals; however, without more information, it is currently unclear how the results apply toward other AD technologies and specific wastes outside of food waste in concert toward its stated goal of applicability to diverse wastes.

PI RESPONSE TO REVIEWER COMMENTS

- The research team sincerely thanks the reviewers for both their positive and constructive comments for improvements. The responses presented here cover only the constructive comments. The working volume of the anaerobic acidification reactor was reduced to test the effect of reduced hydraulic residence time. As a result, the total volume of gas production was reduced, but the unit volumetric productivity did not. The team has made DEI efforts in training to include female students in the research. More efforts will be made during the results dissemination phase of the project. More specifically, the project team will recruit underrepresented students for the summer of 2024 to work on the pilot system evaluation. The project goal is to produce pure methane that can be compressed for vehicle uses, although not for aviation. Other products from the acidification process will not be recovered. It is not economic to utilize these products because of their relatively small quantity. The research team has conducted an energy balance analysis as a part of the LCOE and EROI calculations. The detailed analysis was not presented due to the time limitation. The research team is continuing the optimization of the bench-scale system. The research team does have the data on the manure/waste characterization. The research team has a Gantt chart for the project schedule and will use it to track the progress. The research team will proactively engage industrial stakeholders during the next phase of the technology scale-up and results dissemination. Although a preliminary TEA was conducted based on the results of the project to date, a more rigorous analysis will be further conducted based on the performance data of the pilot system during the next phase of the research to answer the questions that the reviewer asked.

RENEWABLE NATURAL GAS FROM CARBONACEOUS WASTES VIA PHASE-TRANSITION CO_2/O_2 SORBENT-ENHANCED CHEMICAL LOOPING GASIFICATION

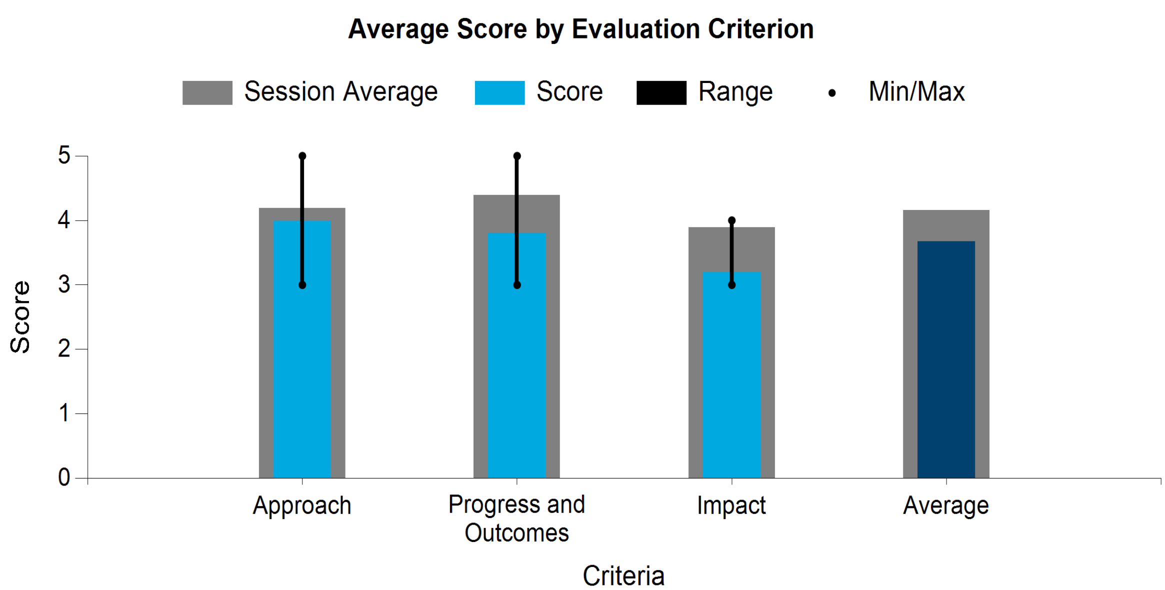
North Carolina State University

PROJECT DESCRIPTION

WBS:	5.1.3.205
Presenter(s):	Fanxing Li
Project Start Date:	10/01/2019
Planned Project End Date:	05/31/2024
Total Funding:	$3,135,560

This project aims to develop and demonstrate a sorption-enhanced chemical looping gasification (SE-CLG) technology that combines biomass gasification, air separation, and syngas conditioning/cleaning into a single circulating fluidized bed (CFB) gasifier. The resulting syngas, with a high H_2:CO ratio, would be ideal for RNG production. This intensified gasification process is facilitated by our recent discovery of unique CO_2 and O_2 phase-transition sorbents (PTSs), which allows dual functionality of air separation and CO_2 capture. As such, it enables sorption-enhanced gasification to produce syngas with a high H_2:CO ratio.

During the first six quarters of this project, the team has successfully demonstrated the functionality and stability of the multifunctional PTSs. Near complete conversions of various tar model compounds and woody biomass particles were achieved in lab-scale reactors, producing syngas with high H_2:CO ratios ideal for methanation reaction. Various sorbents were designed and optimized, showing excellent cyclic stability in the presence of biomass waste ash and under a fluidization environment. A 5-kWh CFB cold model was also designed, constructed, and operated, showing desirable solids circulation rates and stable performance. A hot unit design is subsequently finalized, which will be constructed and demonstrated in Phase II of the project.



COMMENTS

- The team involves an HBCU, which is a great way to incorporate DEI elements and communication into the project.

- Still very early in this project.
- Not clear about the commercialization or the involvement of commercial partners, although the team does appear to be engaged in outreach to these parties.
- Interest from commercial partners in the technology is important and merits more mention. Will be curious to see how the interest plays out.
- Gasification does not tend to be the most common way to address wood waste, so it will be interesting to see the ultimate LCOE and economic metrics.
- Does it matter which part of the wood waste is used? Good that they seem to be pretty agnostic to the construction and demolition waste. Have started doing some characterization of the feedstock.
- Process intensification is a great way to address numerous unit operations and avoid integration.
- Early work shows promise in terms of what the PTS catalyst is supposed to do.
- Project goals are set to show significant improvement in LCOE.
- Have been stepping through the project phases in increasing risk (so sequentially) to minimize challenges.
- Did not discuss risk and contingency plans.
- Have received a quote for the hot reactor, awaiting on a second quote from a different vendor before purchasing.
- Not making fuels and products that are difficult to electrify. Challenge is going to be a lot due to the office's priority shifting away from biogas/natural gas.
- Tested ash at values beyond what you would see in real operation.
- Overview/impact:
    - The researchers assessed the generation of RNG from carbonaceous wastes via phase-transition CO_2/O_2 sorbent-enhanced chemical looping gasification. The researchers applied a novel technique comprising a multifunctional integrated system where mixed oxide-based PTSs are used for biomass gasification with integrated air separation and CO_2 sorption.
    - The project objectives fully align well with the BETO goals, as it serves as a means of generating renewable energy while reducing the release of GHGs into the environment. It is also aimed at reducing the LCOE and increasing the EROI.
    - So far, the project seems to have moderate progress, and a lot still has to be done to develop and validate the equipment that needs to be built for the project.
- Strengths: In this project, the removal of CO_2 occurred through *in situ* capture; thus, there is no need for extra expenses on post-treatment and scrubbing for the removal of CO_2. The presentation shows that the PTS is working properly, and the reactor shows very good performance. Further, the fact that the project involves connections between different experts from different universities and a blended approach to the project makes it worthwhile. Also, the application of different thermogravimetric and mass sorption techniques shows how high the technological expertise of the researchers on this project is. In addition, the buildup of a novel dual fluidized bed gasifier cold model speaks volumes about the ingenuity of the researchers.

- Weaknesses: The project seems to have a lot of phases that are not blended together. Also, the researchers do not provide adequate clarity on how many aspects of the project were conducted. Further, the researchers seem not to have a clear project team communication and management plan. Last, I am wondering if the researchers have considered the limitations of scaling up this system, especially those related to the presence of impurities in the feedstock or feedstock quality.

- Questions: There are many boggling questions with regard to the overall approach for the project. In the first stage of the process, why is torrefaction used as a pretreatment step? Are there other processes that could be looked at for the pretreatment of the biomass? Also, one thing that is not clear is how the authors plan to validate a 35% reduction in LCOE. Further, I am wondering if the researchers could provide more clarification on how the isothermal thermogravimetric analysis test was used to preliminarily test the efficiency of the concept in the project. Another thing that still remains unclear to me is what informed the design of the cold fluidized bed gasifier. It will be good if the researchers could clearly state how the prior experiments they conducted influenced the design of the fluidized bed gasifier. One weakness observed is the catalytic activity for tar removal from the process; can't the tar be recovered and used for the generation of biofuel? I understand that this may be outside the scope of the research study.

- This project addresses the gasification of multiple biomass feedstocks. Among its strengths, it seeks to optimize the efficiency of syngas production and tar removal in a single step. The management and progress on the project appear sound. Further progress will be enhanced by more regular engagement with program partners at other universities and a greater level of engagement with potential use cases through consultation with industry and locality partners. The project also needs to integrate attention to DEI in all stages of project staffing, working proactively with students from the high school through Ph.D. levels in outreach, education, and inclusion on long-term aspects of this project.

- This project was strongly focused on applying fundamental thermodynamics to develop multifunctional mixed-oxide-based PTSs. While I am very pleased that the foundation of this work is in thermodynamics, this poses a particular challenge for this reviewer as far as my ability to understand the technical aspects of this project.

- The management of this project appears to be excellent, with monthly Zoom meetings and numerous in-person meetings with local-ish collaborators. In the future, I urge them to consider a larger, in-person meeting of all the collaborators.

- There is a strong industrial collaborator, and an HBCU (i.e., DEI participant) is involved. The fact that this HBCU is relatively close to North Carolina State University, I believe, increases the chances for impact as far as DEI (i.e., the students at North Carolina A&T are more likely to have a prominent role). The researchers at Yale are responsible for the TEA and LCA

- This project is still early, having yet to reach its first go/no-go milestone. Despite this, there are already substantial results for the speaker to share. Admittedly, though, the scores for "Progress and Outcomes" and "Impact" are likely a little low, simply as an artifact of this project still being relatively new.

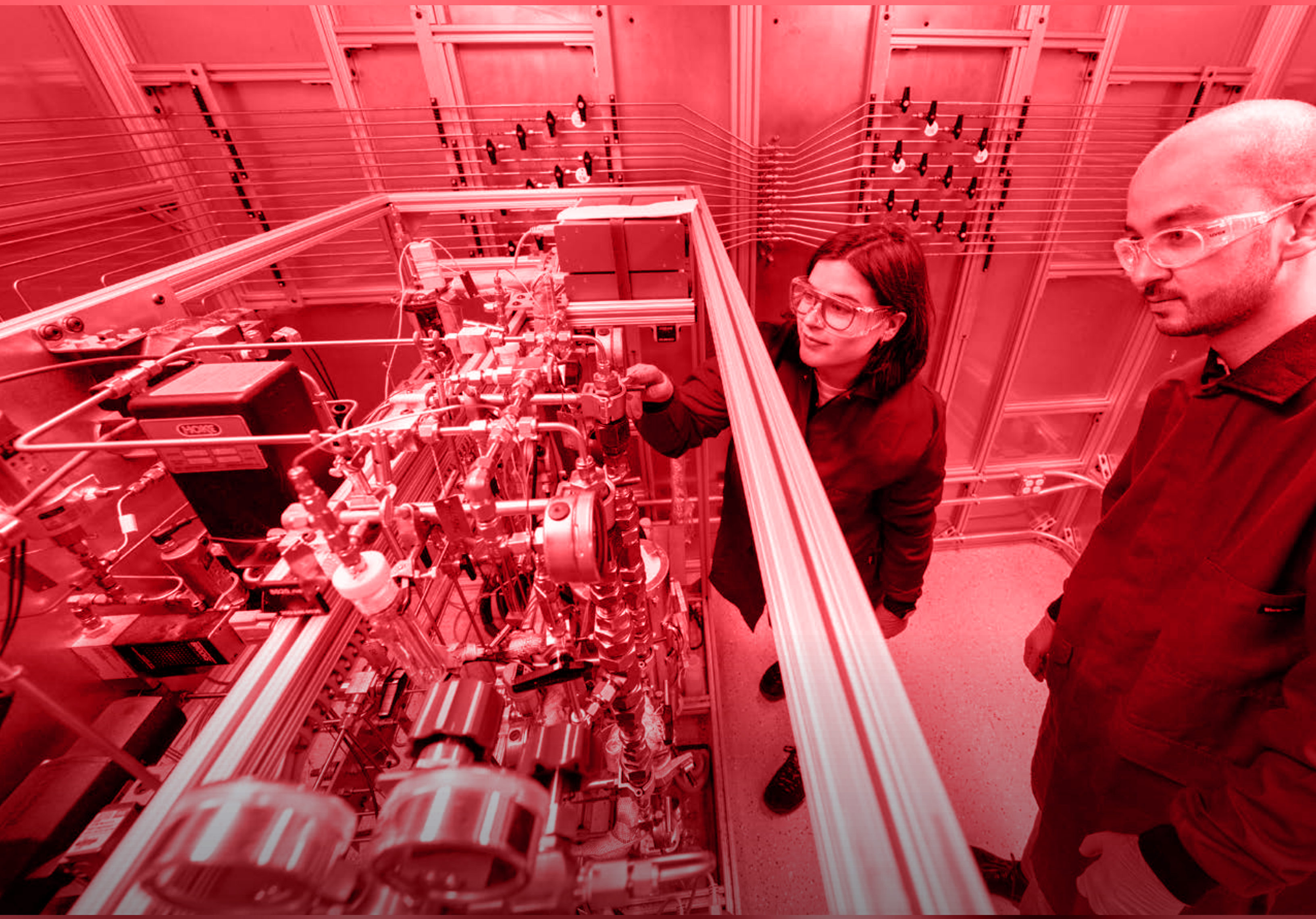
- Offers a path to managing construction and demolition wastes, as well as woody biomass, difficult waste streams to mitigate.

- The team indicates active management by selecting members to de-risk forecast issues. Clear diagrams show how each member's work interfaces toward the whole of the project. Interested to hear more about industry partners and the role they fill in creating a circular economy. Concerned about cost inflation of the reactor; how does this compare with existing technologies' TEA? To ensure beneficial outcomes to the performer and government, to what extent are lab wastes applicable to real-world waste streams?

Would significant contamination of streams (chicken waste and/or grit in pine and metals/plastics in construction and demolition waste) negate advances of the research?

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for recognizing the originality of the suggested method and the progress we have made so far while acknowledging that this project is still "relatively new." We are also glad to hear the reviewers acknowledging our DEI efforts in terms of involving an HBCU and their encouragement on furthering our efforts. We agree with the reviewers' concerns over our target product (RNG) but respectfully submit that this target product was required by the original FOA. We also note that the SE-CLG technology we are developing has already shown promise to produce concentrated H_2 or H_2-enriched syngas with varying H_2:CO ratios. The latter can be converted into jet fuels or methanol using commercial technologies. Therefore, SE-CLG can be a platform technology for a variety of renewable products beyond RNG. The feasibility of the SE-CLG and PTS concept was demonstrated through isothermal thermogravimetric analysis, and the preliminary efficiency estimations were based on lab-scale fluidized bed and packed bed data. The design basis for the cold model was established using kinetic measurements from thermogravimetric analysis and lab-scale bubbling fluidized bed experiments. The SE-CLG technology effectively addresses tar, an undesirable biomass gasification byproduct, by converting almost all of it into hydrogen-enriched syngas. In terms of the scalability of SE-CLG and the effect of feedstock impurity, the adopted CFB design offers scalability for commercial-scale applications, and careful attention has been given to impurity considerations. We have tested contaminants at levels well exceeding those in the anticipated industrial operations, and we will continue to assess their impacts during the CFB studies in BP2. We also understand one of the reviewer's comments over "a lot still has to be done" for "the equipment that needs to be built" but respectfully note that the construction and demonstration of the CFB equipment will occur in BP2 according to the statement of project objectives, and currently we are still in BP1. The project progress is fully consistent with the originally proposed objectives, and in several areas, it has exceeded the milestone performance targets. The BP1 work, which focuses on proof of concept, sorbent development, reactor design, and cold model studies, is crucial to de-risk the subsequent BP2 equipment construction and demonstration work. The project will validate the reduction in the levelized cost of electricity through a detailed TEA in BP2, incorporating operational results from the hot CFB unit, preliminary design of the commercial reactor, and vendor-provided cost estimates. Reactor cost inflation will be considered in the TEA, ensuring a comprehensive evaluation of the technology's competitiveness against conventional gasification. In terms of project management and outreach, the project team actively collaborates with industry partners, including a catalyst producer and a large chemical company, while intensifying outreach efforts and engagement with HBCUs. The risk and mitigation aspects were comprehensively considered and addressed in slide 5 of the Project Peer Review presentation.



SYSTEMS DEVELOPMENT AND INTEGRATION: EMERGING AND SUPPORTING TECHNOLOGIES

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Systems Development and Integration – Emerging and Supporting Technologies (SDI-EAST) Technology Area is one of 12 technology areas reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 26 presentations were reviewed in the SDI-EAST session by five external experts from industry and academia. For information about the structure, strategy, and implementation of the SDI-EAST Technology Area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks (energy.gov/eere/bioenergy/systems-development-integration-emerging-and-supporting-technologies).

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $57.8 million, which represents approximately 10% of the BETO portfolio reviewed during the 2023 Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Robert Natelson as the SDI-EAST Technology Area review lead, with contractor support from Remy Biron of Boston Government Services. In this capacity, Robert Natelson was responsible for all aspects of review planning and implementation.

SYSTEMS DEVELOPMENT AND INTEGRATION – EMERGING AND SUPPORTING TECHNOLOGIES REVIEW PANEL

Name	Affiliation
Gene Petersen*	Retired
Corey Leclerc	New Mexico Institute of Mining and Technology
Marie-Odile Fortier	University of Nevada, Las Vegas
Rishi Shukla	Archer Daniels Midland Company
Amit Goyal	DNV

* Lead Reviewer

SYSTEMS DEVELOPMENT AND INTEGRATION – EMERGING AND SUPPORTING TECHNOLOGIES REVIEW PANEL SUMMARY REPORT

Prepared by the Systems Development and Integration – Emerging and Supporting Technologies Review Panel

INTRODUCTION

The SDI component of the BETO program deals with technologies that are on track to evolve into demonstration-level systems or are involved in supporting demonstration or commercialization efforts. As such, they have developed a strategy that looks at this process from an industry point of view. The SDI component is addressing the potential for taking technology beyond the R&D stage into actual implementation and readiness for commercialization. Its span of projects and focus on catalyzing the development and commercialization of promising bioenergy technologies are pivotal to the continued growth of the bioenergy sector.

Their mission is well defined, including their contribution to the Sustainable Aviation Fuel (SAF) Grand Challenge, which, along with other federal agencies, is to enable industry to produce 35 billion gallons/year by 2050 with a near-term milestone of 3 billion gallons by 2030. As part of this larger effort, BETO has a target goal of having four projects undertake a demonstration-level effort in producing SAF. To get there, they have included several projects in their portfolio that have the potential to achieve this. In addition, they have kept the door open to newer technologies through funding some emerging technologies that have promise. In SDI-EAST, the program has sought industry and stakeholders via workshops and the inclusion of industry participants in funding opportunity announcement (FOA) reviews. The critical paths have changed over the years, and the SDI program has sought to fill these gaps with opportunities for the R&D community to participate via FOAs. The latest FOAs are getting more precise, so the mission, goals, and targets are getting clearer. To develop the program, almost every project had industry or stakeholder input. In addition, they have filled gaps with annual operating plan (AOP) efforts for crosscutting and enabling technologies. Another strategy tool that was employed was the use of road maps that outline the technology development needed and opportunities for public-private partnerships. The current emphasis in the new Multi-Year Program Plan focuses on reducing carbon intensity and increasing carbon dioxide (CO_2) reduction in areas beyond light-duty fuels. These have driven some program priorities that are reflected in the selection of projects.

The program includes a diverse set of projects, including all pathways—pyrolysis, hydrothermal liquefaction (HTL), upgrading of waste greases and oils, gasification/Fischer-Tropsch, blending, syngas/landfill gas upgrading, aqueous phase, and ethanol conversion unique approaches. Feedstock handling, modeling efforts, and bioproducts reflect the breadth and depth of the program. More importantly, these programs have also mandated high greenhouse gas (GHG) reduction potential and lower cost targets. Stakeholder input in feedstock selection (ethanol, pyrolysis, greases, bio-based solid feedstock handling), market readiness levels, specifications for product/testing, and validation is well documented. Industry-led efforts and participation with academia and nonprofits are good indicators of a well-balanced program. AOP crosscutting and enabling programs have made significant progress. The modeling efforts, the study of marine fuels, and developing coprocessing with refinery streams have all achieved desired results and, more importantly, shared information/tools with the larger community. DOE’s initiative to determine how biomass can play a role in marine/rail fuels is new and well directed.

The transportation sector produces significant levels of GHGs. Although BETO has previously looked at light-duty vehicle fuels, they have now broadened their efforts to other very important impact areas that are hard to decarbonize, such as SAF, marine fuels, rail fuels, and other heavy-duty-use fuels. The focus on reducing carbon emissions has put a different spin on some priorities and emphases of R&D within the SDI program.

The current market for light-duty fuels continues to be impacted by electrification, so the SDI program's efforts at finding new directions for bio-based fuels is appropriate.

The effects of the recent pandemic became a bit apparent in some projects. Staffing became an issue for some. BETO may need to be sensitive to deadlines and milestones where this situation occurs and consider extending deliverables as appropriate.

STRATEGY IMPLEMENTATION AND PROGRESS

The industrial-like approach involves increasingly more efforts at due diligence for achieving technology readiness levels (TRLs) and the validation of each step in the progression toward the completion of milestones within each project. Independent analyses of progress along a project's timeline are being effectively implemented. The granularity of technology development in production or system development is much more aligned with industrial technology development and the road to implementation and possibly commercialization. Not all technology development is a linear or smooth path. The requirements for projects in this SDI area include the identification of risks and mitigation strategies, clear performance objectives, and where the system development has an impact on meeting BETO's strategic goals and intermediate performance milestones. These areas are all actively managed by BETO staff through quarterly reports and site visits, where possible and feasible. The program is to be lauded for bringing in expertise beyond their program capabilities to help evaluate progress on projects such as ICF as an independent engineer.

One other salient point of the SDI program is the participation of national laboratories in appropriate areas. These include independent analyses of the potential development of fuel decarbonization efforts in areas such as marine and rail fuels, as well as helping develop tools for enabling system development or establishing analytical criteria that can be used to compare competing technologies.

While yield is very important, a process that is stable and reproducible may allow for a little loss in yield. This is particularly true for commodity products such as fuels; hence, figures of merit or minimum benchmarks should be used to assess the integration of unit operations and allow for the development of proof of the overall system. Then improvements in individual unit operations can be addressed as needed. Some projects hit targets by changing reactor conditions, but that comes at a cost and should be reflected in techno-economic analysis (TEA). But as long as there is more value in the product than the cost of producing it with some margin for profit, the technology can be successfully developed.

The TEA/life cycle analysis (LCA) modeling for each project is appropriate, though there could be a better correlation between LCA related to reducing carbon intensity and emissions and the components of LCA. How the SDI programs supports and pushes the role of LCA in a project will be important to the overall success of the BETO efforts. In this vein, it is a concern that Fischer-Tropsch has not worked in the past and whether it will work with current efforts.

When assessing impacts, the projects should probably address only the market penetration potential of their technology, not the whole market as is typically shown. Process viability and stability is more important than achieving maximum yields or optimum performance. Several projects used technologies that are typically not economically viable. It would be great to see this addressed early on. An example is the use of supercritical anything for a fuel-producing process.

Greases as a source of fuel have long been envisioned. It is worthwhile to see some efforts in assessing this potential. There are existing commercial facilities that produce biodiesel from oils, and if greases can be brought into the supply mix, it would be good for meeting BETO's goals and help deal with an existing waste management issue.

The program has funded three projects on high-value bioproducts under the SDI-EAST portfolio that enable SAF economics. This aligns with most BETO SDI FOAs that allow using up to 50% of carbon for valuable product production other than SAF. The projects showcased the production of different bioproducts using waste streams and have made significant progress in terms of better understating the process conditions and underlying science. One important feature for bioproducts, however, is to meet the required product specifications that are generally more stringent in terms of purity compared to a fuel. On this, the projects seem to lack clear identification of the minimum specifications required to qualify as bioproducts. One initiative that presented on graphite products for battery applications has recently started and made good progress with clear plans for testing, scale-up, and stakeholder engagement. There are some specific comments on a couple of projects. One involves the recovery of methoxyphenol and other compounds from fast pyrolysis waste streams; it is a derivative of a past DOE-funded program (MEGABIO), and, so far, it has demonstrated a mixture of products, with several distillation cuts with no effective separation, and no clear strategy on the future separation of products to meet required specifications. Even the names of compounds have not been identified. Second, lignin-to-carbon-fiber and/or asphalt additive projects also require a fair benchmark for comparison. These projects may also be better suited under the conversion or bioproducts portfolio wherein the product specification criterion is more rigorous.

Several projects do not look economically feasible, so it would be good to discuss that aspect early on or throughout the project. The TEA/LCA modeling for each project is appropriate, though there could be a better emphasis on early-stage TEA/LCA work to guide the project outcomes. Several projects lacked results on LCA or TEA and had it scheduled for the last budget periods. The wood-heating projects do not seem to address the social justice aspects that were highlighted in the introduction of this part of the program and that give more credence to these efforts to be included in BETO.

For the woodstove projects, the idea that people from lower socioeconomic backgrounds use wood heat most often was important, but several solutions seemed to be for high-end heaters that those people could not afford. One presenter mentioned that high end was how you get it on the market, and that you can then sell it to lower-income people, which was reasonable but not obvious. It is almost like a diversity, equity, and inclusion (DEI) component specific to wood heaters. Another issue involved in these efforts is the availability of electricity and internet, which low-income people may not have, especially internet.

RECOMMENDATIONS

The following recommendations are not listed in any sort of prioritized order and represent items that should provide increased viability of the SDI component of BETO.

Recommendation 1: The SDI program should interact more with the Conversion Technologies and Renewable Carbon Resources programs to enable more acceleration of technologies across the BETO portfolio of projects.

Similar to the previous 2021 Peer Review recommendations, a recommendation to the program is to foster greater interaction between BETO programs. One example can be drawn from the CO_2 utilization area. A task was described in this BETO technology area about how to tie TEA and LCA together. It is evident that some emerging technologies do both, but they have not really done the effort to tie them together, as was done in the CO_2 utilization area. This may be a future direction the SDI program could take to enhance the viability of demonstrating that a process system is viable. The interface with the Feedstock-Conversion Interface Consortium (FCIC) and technology developed there should be a resource all system development projects should follow or be exposed to if it is not already ongoing. Also, the SDI program could look to pluck some projects from the bioconversion and thermochemical areas into further development in SDI. A question is whether the SDI program should invest in more emerging technologies or focus on using the portfolio they have to scale up to demonstration projects to achieve their strategic goal.

Recommendation 2: BETO should consider increasing resources for the marine fuels effort.

Marine fuels projects have progressed really well. BETO should consider a higher level of support for the testing and implementation of marine biofuel technologies. The level of support divided between four national labs really limits the availability of resources for progress in the time committed. Marine biofuels should have a higher level of support than currently provided to deliver on the goals for carbon intensity reduction and GHG reduction.

Recommendation 3: The SDI program should encourage projects to have even more transparency with TEA/LCA efforts.

Projects were sometimes loath to show the estimates drawn from TEAs relative to costs, etc. Some LCAs were a bit spotty in providing meaningful data. Some projects cannot seem to get out of the TRL 3–4 stages, where they feel they need to maximize performance. They just need to define a figure of merit that allows them to proceed with process integration, and they can come back to the individual process steps to improve them, if needed. The lack of a requirement of preliminary, and, later in the projects, complete LCA and TEA is a missed opportunity for quantitative checkpoints in the decarbonization and commercialization potential of the technologies and pathways studied by program-funded projects. Some projects showed sensitivity analyses based on their TEAs. Such analyses should be part of any emerging technology system to show directions for reducing operating expenditures (OpEx).

Recommendation 4: BETO should have greater interaction with the DOE Hydrogen and Fuel Cell Technologies Office due to the importance of hydrogen use in reducing biofuel carbon intensities.

Several emerging projects employ hydrogen, and greater interaction with the DOE hydrogen (H_2) program may be warranted, particularly with regard to reducing the carbon intensity of processes using steam methane reforming.

Recommendation 5: DEI efforts may be better strengthened through better inclusion of DEI tasks with overall project tasks.

Not all the projects that require a DEI component have truly incorporated these values into their approach and could benefit from clearer expectations in the FOAs to meet these goals. This could be guidance for project teams to include budget items dedicated to these efforts in their proposals, to weave inclusion and equity into key components of their projects like their approach to industry involvement, and to include diversity and equity in their discussions of risk management.

Another example of this are the projects supporting wood-burning stoves and associated technologies. Clarity with the U.S. Environmental Protection Agency (EPA) on regulations would help the industry progress and meet the strong social justice aspect of the projects. The majority of the focus on achieved improvements should be on households living at or below the poverty line. A higher degree of support on projects with a strong social or environmental justice clause would benefit society and deliver on air quality improvements. A discussion of how their solution will be attractive to lower-income groups would be helpful. It would also be helpful to better understand the validation process. This could be done project-by-project or just more generally. Some groups spend more than a year validating, which seems like a long time. Resources for efforts in improving wood-burning stove technology are beneficial.

Recommendation 6: BETO needs to listen to industry more to understand the metrics needed to off-ramp a technology to industry.

The program may benefit from having criteria that lead to the termination of a project and when industry can take over. BETO is not in the business of picking winners, and it may be that BETO believes industry can determine what they want to pursue, but there may be value in defining criteria when BETO support is no longer warranted.

SYSTEMS DEVELOPMENT AND INTEGRATION – EMERGING AND SUPPORTING TECHNOLOGIES PROGRAMMATIC RESPONSE

INTRODUCTION

The SDI-EAST team would like to thank the review panel for providing their time and expertise throughout the 2023 Project Peer Review process, including the critical and helpful interaction with the presenters, the Review Panel Summary Report, and the valuable project comments. We appreciate the review panel's comments noting the clear strategy for supporting near-term, demonstration-scale projects (around 50 dry metric tons of biomass per day; corresponding to around 1 million gallons of biofuel per year) of integrated technologies while also supporting novel unit operations at the pilot scale (around 1 dry metric ton biomass per day; corresponding to around 20,000 gallons of biofuel per year). We appreciate that the review panel observed the emphasis on reducing GHG emissions. The review panel noted that the portfolio includes industry-led projects but also national laboratory-led enabling activities. The SDI program strives for technology demonstration but also appreciates the expertise at the national laboratories to reduce universal technical uncertainties.

The review panel commented that the SDI program should be cognizant that sometimes maximizing a certain parameter may not be the best target for a pilot/demonstration project, but rather at this stage it is important to demonstrate process stability. Without minimizing this important comment, some additional background may place this in better context. Typically, a scope for a project, as written on the negotiated statement of project objectives, will include ambitious metrics for the project to reach at the end of the intermediate budget periods. For an active project presenting at the Project Peer Review, these ambitious metrics are often presented in detail. But, also, most FOAs include requirements for continuous operational runs (100–500 hours continuous for the pilot scale; 500–1,000 hours continuous for the demonstration scale). These continuous runs usually occur at the end of a project and thus may not have been discussed for many projects at the Project Peer Review unless they are sunsetting. The SDI program will keep in mind the importance of these continuous tests to demonstrate process stability.

Following are the SDI program's responses to the review panel's recommendations. Again, we appreciate the effort and are listening and responding.

Recommendation 1: The SDI program should interact more with the Conversion Technologies and Renewable Carbon Resources programs to enable more acceleration of technologies across the BETO portfolio of projects.

BETO, including the SDI program area, has recently instituted efforts to create more engagement between the various BETO programs, including with the Carbon Conversion and Renewable Carbon Resources programs. A recent adjustment in BETO's personnel activities is assigning liaisons where a technology manager from a separate program joins another program's regular weekly update meetings. We are also instituting quarterly meetings for more interfacing to share program highlights. One potential impact of these more frequent interactions is better recognition of project progress across different TRLs and across the pathway from feedstock logistics and preprocessing to conversion, scale-up, and integration.

The SDI program is also working with the FCIC to facilitate conversations between the FCIC and the pilot and demonstration projects in SDI's portfolio. The FCIC is jointly managed by the Renewable Carbon Resources, Carbon Conversion, and SDI programs. The FCIC is actively conducting R&D in feedstock variability, materials handling, preprocessing, materials of construction, and feedstock impacts for both low-temperature (biochemical) conversion and high-temperature (thermochemical) conversion. SDI's pilot and demonstration projects benefit from hearing the latest research on the impact of feedstock variability on preprocessing and conversion. Sometimes pilot or demonstration projects make simplifications about feedstock quality, or dismiss potential challenges at the feedstock-conversion interface, or, at least, do not have the bandwidth or resources to consider these challenges; thus, more communication sooner, across the BETO platforms, is critical.

Recommendation 2: BETO should consider increasing resources for the marine fuels effort.

BETO's second-highest fuel priority is marine fuels. The SDI program funds some laboratory and private recipient R&D in the marine fuels space and plans to increase marine funding in the future. The SDI program also supports DOE's role as a co-lead of Mission Innovation's Zero-Emission Shipping mission, which seeks to introduce commercially viable zero-emissions fuels for oceangoing vessels by 2030.

Recommendation 3: The SDI program should encourage projects to have even more transparency with TEA/LCA efforts.

The SDI program will work to include more language in future FOAs, pending appropriations, requiring transparency of TEA assumptions. The SDI-EAST review panel did not see many projects selected under FOAs where LCA was required. The SDI's Fiscal Year (FY) 2016 FOA required LCA to ensure that the projects were developing pathways producing advanced or cellulosic biofuels with more than 50% or 60% GHG reductions, respectively, that would meet the requirements of the Renewable Fuel Standard. On the other hand, the SDI's FY 2017, FY 2018, and FY 2019 FOAs did not have strict requirements for LCA. For example, the SDI's FY 2017 FOA only required applicants to report the GHG estimate in the application, but no LCA work was required as part of the project scope. The SDI's FY 2018 FOA required applicants to report the GHG estimate in the application, and the GHG reduction had to be at least 50%, but no further LCA work was required in the project scope. The SDI's FY 2019 FOA required applicants to report the GHG estimate in the application and conduct LCA in the project scope, but the FOA did not require any quantifiable metric for GHG reduction. The SDI's FY 2020 FOA had a requirement for LCA to show that the project was developing a pathway producing fuel with at least 60% GHG reductions. The SDI's FY 2021 FOA then reverted to more transparent efforts, requiring projects to develop pathways producing fuels with at least 70% GHG reduction, and moreover requiring projects to include special deliverables in the project scope whereby the project will release a public final technical report describing how the technology would contribute to BETO's 2030 goal of $2.50/gallon gasoline equivalent (GGE) minimum fuel selling price (MFSP) with at least a 70% reduction in GHG relative to petroleum-derived fuels.

Recommendation 4: BETO should have greater interaction with the DOE Hydrogen and Fuel Cell Technologies Office due to the importance of hydrogen use in reducing biofuel carbon intensities.

The SDI program acknowledges that, thanks in part to DOE leadership, massive improvements are underway in the hydrogen sector. These activities include the Hydrogen Shot to reduce the cost of clean hydrogen by 80% to $1/kg by 2031; the H2@Scale initiative to convene stakeholders across the hydrogen production and use supply chain; and the development of Regional Clean Hydrogen Hubs, led by the DOE Office of Clean Energy Demonstrations with $7 billion in funding. Because these activities are still nascent, it is difficult to identify the right interfaces where SDI projects would have meaningful interaction. It is noted that BETO has historically shared expertise around the bioenergy state of industry with H2@Scale to ensure that the hydrogen community is aware of the need for clean hydrogen utilization in biofuels production. The SDI program will seek to maintain communication with the DOE Hydrogen and Fuel Cell Technologies Office. Coincidentally, a BETO program manager has recently started a temporary detail as the deputy director of the DOE Hydrogen and Fuel Cell Technologies Office. Closer interaction among the offices is anticipated.

Recommendation 5: DEI efforts may be better strengthened through better inclusion of DEI tasks with overall project tasks.

The inclusion of DEI considerations is relatively new for DOE and BETO/SDI. Only one year of FOA awards, from FY 2021, were required to include DEI tasks in their projects. The SDI-EAST review panel saw only the start of efforts for DEI incorporation into SDI projects. As the projects from the FY 2021 FOA progress, DEI activities should become clearer and targeted. There have also been ongoing working groups at the DOE Office of Energy Efficiency and Renewable Energy level to ensure better integration of DEI efforts into FOAs.

Recommendation 6: BETO needs to listen to industry more to understand the metrics needed to off-ramp a technology to industry.

This is an excellent recommendation, especially considering the need to accelerate scale-up efforts to meet the goals of the SAF Grand Challenge and the Zero-Emission Shipping mission. Recently, BETO announced a request for information to understand the maritime industry's current alternative fuels trajectory, the driving forces behind it, and key barriers to achieving the transition to zero-emissions fuels. The SDI program will continue to consider opportunities where requests for information or workshops would be a reasonable approach.

On another note, the SDI program is supporting a new AOP led by the Data, Modeling, and Analysis Technology Area team to develop a SAF state-of-the-industry report. Better understanding of the metrics of the current SAF industry, which uses hydroprocessed esters and fatty acids (HEFA) technology, is one way that the SDI can understand the paths for commercializing SAF and other fuels.

IMPROVED BIOMASS FEEDSTOCK MATERIALS HANDLING AND FEEDING ENGINEERING DATA SETS, DESIGN METHODS, AND MODELING/SIMULATION TOOLS

Forest Concepts LLC

PROJECT DESCRIPTION

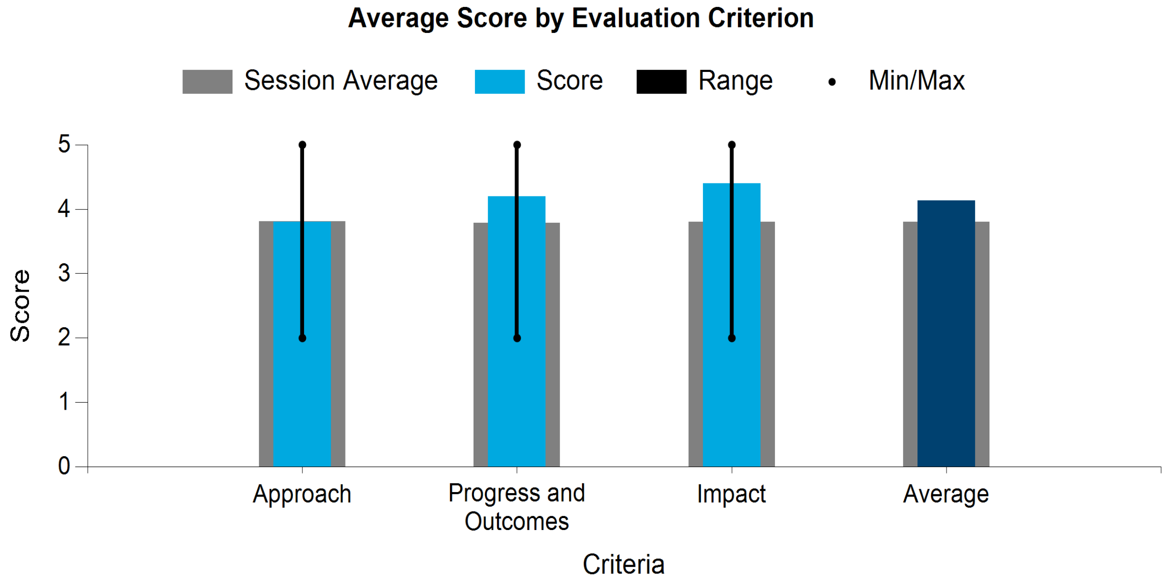
WBS:	3.1.1.002
Presenter(s):	Christopher Lanning
Project Start Date:	06/01/2018
Planned Project End Date:	04/30/2023
Total Funding:	$1,849,411

The overarching objective of this project is to contribute to the design and operation of reliable, cost-effective, continuous feeding of biomass feedstocks into a reactor of an integrated biorefinery.

The overarching goal comprises two subgoals: (1) develop and validate a comprehensive computational model to predict the mechanical and rheological behavior of biomass flow to enable the systematic and reliable design of biomass handling/conveying system, and (2) engineer and improve laboratory protocols and equipment to generate property-driven response curves for specific biomass feedstock species and formats accounting for their dependence on biomass physical properties including particle size distribution, true density, bulk density, and moisture content and external mechanical properties including temperature and pressure.

The project team includes Forest Concepts and Pennsylvania State University. Forest Concepts leads the design and construction of new laboratory methods and equipment. Penn State leads the development and adaptation of bulk flow models to the problem of biomass materials and equipment.

New equipment developed include a 250-mm cubical triaxial tester (CTT) to provide biomass mechanical property data and a large gas pycnometer to quantify biomass particle density to ensure that simulations are populated with biomass-specific data. New analysis software developed include an application for CTT and pycnometer data reduction and analysis, a biomass materials database, and finite element method-based simulations. Biomass materials used in the project include milled wood chips and corn stover.



COMMENTS

- Approach: The project's approach aligns with the metrics defined under Topic Area 4, DE-FOA-0001689. Particle sizes from 1 mm to 6 mm for two different types of biomass were tested. The focus is on tool development, repeatability, and the move from conventional materials (such as soil); limited pilot-scale testing; and an improved modeling tool. The project leverages other projects for data that are under DOE's purview. The team has worked closely with Purdue and Idaho National Laboratory. Stakeholder engagement is by a variety of sample testing for industry clients.

- Progress and outcomes: A new CTT tool scale-up allowing for the measurement of material behavior in three orthogonal directions, adopted for biomass materials; and a gas pycnometer to measure solid densities (true particle density) using air as the pressure medium for larger particle sizes up to 30 mm. Data were presented for two biomass types; the experiment versus simulation difference was less than 15% for two hopper wall angles. Budget Period 3 added a new task—integrated biorefinery projects were also modeled.

- Impact: One key piece for all biomass technologies is understanding biomass feeding processes. This is not well understood. The project has provided new tools to study the physical and mechanical properties of wood chips for applications in hoppers, valves, and conveyors. Results: five potential licenses for new lab equipment; six additional materials studies for others using tools built during this program; and workshop and knowledge sharing. This is a 5-year project with nondestructive testing under 10 minutes for low temperature, a significant achievement in tool development.

- The project has developed a modeling approach using data from newly purchased equipment to improve the prediction of biomass flow in industrial equipment. Anyone who has used biomass knows that it is a much different solid than many others that have been an issue previously in industry.

- The team has used mechanical measurements from new equipment to inform a model on how biomass will flow. They demonstrated some successful examples of how their technology can be used with a thorough discussion of why the method they are using is needed and what the shortcomings are of using physical properties.

- The technology can either be used as a user facility-type opportunity for those in need of understanding their handling systems or the company can sell units for companies to use in-house. This project fills a hole that will greatly help solve a tough problem with solids handling. They have presented at trade meetings and put considerable effort into contacting potential stakeholders.
- This is a project that has great relevance to the processing of biomass. The success of the project is evident by the interest from potential users and stakeholders.
- The need for new equipment and analytics was proven to be valuable. The effort will be proven at TRL 6 and up by others. This proof of concept is a valuable addition to the overall processing of biomass for fuels and chemicals. They have been partners with several other BETO projects, which attests to the value of their efforts. It was not made clear the costs for using their unique technology and what bearing that has on the overall TEA of processes.
- The project team is developing new equipment and modeling tools to determine the bulk flow properties of biomass feedstock handling and feeding, with pilot-scale validation, to fill this data gap in the biomass industry. The project team has presented their progress at an industry forum and presented webinars for major test plants as well, thus keeping industry informed. Patenting and peer-reviewed publications are in progress; however, it is unclear how the model tool itself will be disseminated, such as whether it will be open source, and how the team is ensuring that its design will be compatible with the needs and expectations of operators and other users. The approach is thorough, and the outcomes of the project have the potential to be widely adopted by various types of biomass processing plants. The project team has made timely progress in all R&D efforts of the grant, with a budget extension that is primarily to leverage this project's data collection to benefit other ongoing DOE-funded projects.
- The project would have applicability in coproducts as well. The model has very large error bars (Slide 17), so there are concerns about the applicability of the model to real-world situations; all work done so far is on lab and pilot equipment. Even after the model output, however, the changes in finished equipment are limited, and the sample application is very limited in the study.

PI RESPONSE TO REVIEWER COMMENTS

- Thanks to each reviewer for the countless hours devoted to assimilating and evaluating the various projects. We highly value your thorough review and thoughtful comments. A first-of-its-kind biomass-scale CTT and associated gas pycnometer were wholly designed and built by the project team under this project to provide data sets for existing bulk materials flowability models used in other industries. The driving need for the improved flow modeling and equipment is widely recognized throughout the industry, as pointed out by the reviewers and confirmed in our extensive industry interactions. While the current design of the equipment is now available to academia and industry customers, we will continue to revise and streamline the entire data collection, reduction, and modeling process based on industry feedback and ongoing in-house use of the technology. We are working on a standard format for the dissemination of various model coefficients and related material characteristics so that the data sets generated by the project team and other users of the equipment may be comparable. Once a material is fully characterized, the resulting mathematical material model is applicable to all scales of equipment. One reviewer expressed concern about the large spread of material property data around the mean values. The presented data sets have large statistical error bars, but experience with biomass materials suggests that variance is more a confirmation of the natural range of variance of the material rather than experimental error; thus, (1) mean values are useful to understand relative differences between different species, sizes, etc., but (2) the range is vital to engineering robust handling systems because the span must be accommodated for reliable flow. Simulations need to be conducted with high, median, and low values to predict the effect of natural variance on the variance of instantaneous flow or nonflow. Mean values are rarely used for engineering design with biological materials in other industries. For example, the structural wood industry uses strength ratings at the second standard deviation such that roughly 95% of the beams will have actual bearing capacity larger than the design capacity. Similar techniques should be applied to the results and applications from these tests.

VIRTUAL ENGINEERING OF LOW-TEMPERATURE CONVERSION

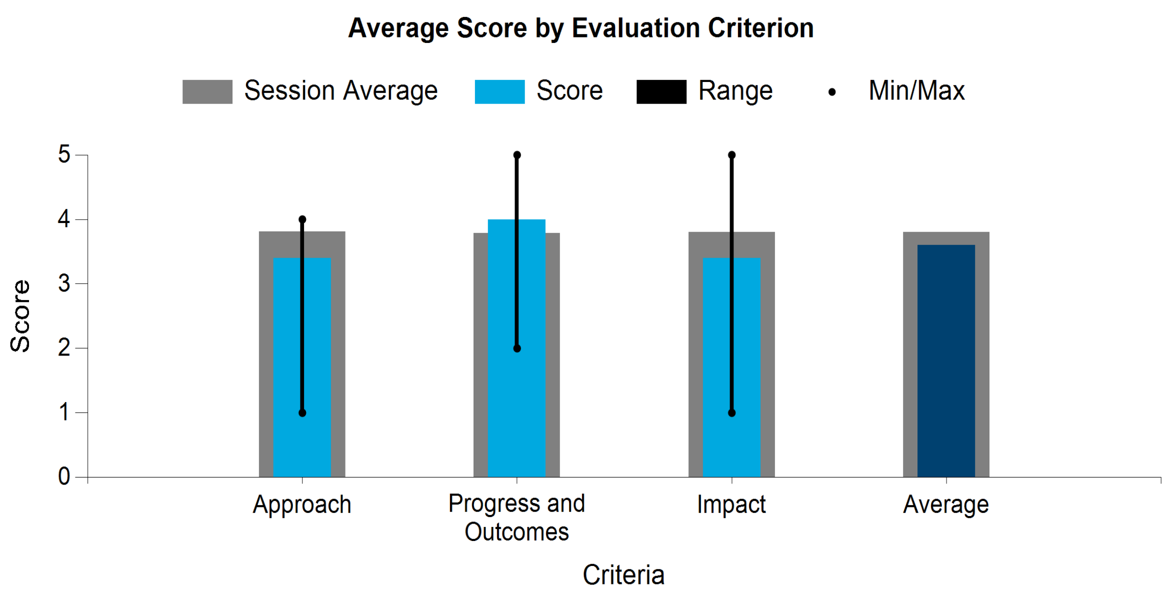
National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	3.1.1.010
Presenter(s):	Ethan Young
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2023
Total Funding:	$835,000

In this work, we present the development of an overarching software framework and supporting multiphysics models to simulate the end-to-end process of biomass conversion. This virtual engineering software is designed with the goal of accelerating R&D and reducing risk for market-relevant biomass conversion processes. We currently support multiple models, computing paradigms, and fidelities representing the steps of feedstock pretreatment, enzymatic hydrolysis, and bioconversion. Although this virtual engineering approach was developed to support a biomass workflow, we have designed each component in a way that allows us to easily support new domains, unit models, and feedstocks.

We begin by presenting the user-facing aspects of the virtual engineering software and highlight how simulated elements are defined and linked by virtual engineering functions. We then present an overview of the high-fidelity computational fluid dynamics (CFD) models developed to support our target domain before segueing into our efforts to develop accurate and fast surrogate models, capturing the salient outcomes from the CFD simulations in a significantly less computationally demanding manner. We then present how virtual engineering calculations interface with a commercial TEA software, Aspen Plus. We conclude by presenting virtual engineering case studies that leverage these methods and discuss how our methods can be extended to support a wide variety of accelerated biofuel commercialization pathways in the future.



COMMENTS

- Approach: The project is funded under AOP lab call Advanced Development and Optimization; it focuses on modeling/hardware co-development to improve biomass processing/handling inside the plant. The approach is to validate, using parallel models on each identified step, and showcase integrated results. The project team and level of engagement from each subject matter expert seems appropriate. The project management team roles are well defined in the presentation and explained during the presentation.

- The project's goal is to incorporate detailed unit operation simulations into plant-wide simulations to give more accurate process simulations. They have used cellulose extraction, conversion to sugar, and sugar conversion as an example. Because many of the more detailed unit operations take days to simulate, a model reduction process that uses artificial intelligence will be used to incorporate detailed simulation data into a simpler-to-run model.

- The team has put together a model that incorporates unit operation simulations into plant-wide simulations. They have determined improved ways to reduce the model that takes less time than a Monte Carlo simulation.

- The resulting simulations work for a very narrow set of inputs even for a narrow set of unit operations. This project holds so much potential if another layer of programming could be used to either make the results more general or to speed up the reduction of the model. This project could automate what we already do in designing chemical plants. It is just not there yet.

- This project meets one of the strategies for BETO to meet their goals. They have gone beyond the normal use of Aspen to make a more robust virtual engineering package with CFD. Results show relatively low error compared to experimental data.

- As a whole, this effort is the kind of work a national laboratory can do because it is more of an unbiased entity. The national lab effort avoids the purely academic side of such modeling because they are joined at the hip with the experimental side of the business. The proof of value will be in those who will attempt to use it. The team did not address this issue other than to say that it is an open-source software.

- This capability could benefit several projects in the SDI portfolio in undertaking their work, and that potential should be pursued.

- The project is developing proof-of-concept virtual engineering software that is domain-agnostic and connects mathematical models of unit operations to predict the outcomes of biomass pretreatment, hydrolysis, and bioconversion, with a focus on reducing computational time for users while providing reliable modeling results through surrogate modeling components. The users would need to enter three to five inputs for each of the three steps, which are based on the most sensitive or driving variables that are mostly within an operator's control. The model includes input parameter limits so that it will only perform within the ranges that have been validated through the software. Validation against published data shows an acceptable error percentage. Optimization capabilities are also incorporated. The approach appears solid and considers the needs of the industry, but it is unclear how the model will be disseminated or promoted to users beyond being accessible on GitHub or whether future user needs are being solicited via an advisory board, survey instrument, or otherwise to further improve the implementation potential. Because the goal is to provide accelerated development and reduce risk for market-relevant biomass conversion processes, the development of this open-source model has high potential for impact to industry if it genuinely fits the needs of operators (and if operators are aware of its existence). The project is now within its last year and has met its goals at this stage within the scope of the software development, and it could now benefit from considering outreach and feedback with industry.

- The model is only as good as the input provided to it for development. It seems the model is not continuously updated based on feedstock variability, etc. How applicable would this model be to different sources of feedstock and affected by operating conditions? I am concerned that they have simplified a set of computational models to satisfy the Python solver. The model's connection with Aspen is unclear to this reviewer. It seems the model is stand-alone, without the interplay with Aspen, and several key parameters (particle size, biomass type, etc.) are hard-coded and not available for the user to change. No confidence of the model prediction is provided.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you to the reviewers for their detailed analysis; it was a pleasure discussing the virtual engineering project with you, and we were pleased to see that the merits of a computational, system-wide approach were well received. The reviewers generally identified two critical areas for future work: the dissemination and adoption of the methods we have developed and the generalization of these tools to new pathways, models, and inputs, which we will elaborate on here. We agree that this cross-platform enabling software is only as useful as our ability to get it in front of end users to see how they interact with the tools and what missing features we could collaborate on to provide. In FY 2022, we wrote and successfully delivered a milestone demonstrating an overview of the virtual engineering capability to groups from both academia and industry. These sessions were helpful in terms of informing us which directions we should pursue more heavily (e.g., more development of Aspen techno-economic integration) but fell short of providing us with real-world users and future developers. To remedy this, we have proposed to host webinars and training sessions as part of the work during this project's continuation. Enabling new users to download, install, and run our methods would significantly reduce the barrier to entry for creating Notebooks tailored to the unique needs of their workflows and models. With regard to any perceived narrowness of our allowable inputs and models, we understand that demonstrating virtual engineering tools using explicit case studies risks giving the impression that only the chosen variables are mutable and/or that only a single, rigid workflow is supported. Generally speaking, the virtual engineering elements that link different unit operations do not presuppose any programming framework, data structure, or computational complexity and make it very easy to construct collections of widgets to solicit user input for new values, e.g., the particle size in the pretreatment model. Adjusting the value of a variable outside the confidence interval of a model or simulation may lead to unpredictable results, but we attempt to preempt this by enforcing conservative limits during input validation. Further, we have proposed integrating the initial training of surrogate models and adding the ability to augment those training sets with subsequent high-fidelity simulation evaluations as part of this project's continuation. The ability to automatically inject an Aspen model with calculations from an external physics model is the focus of our end-of-project milestone, which will be described in a manuscript in the near future.

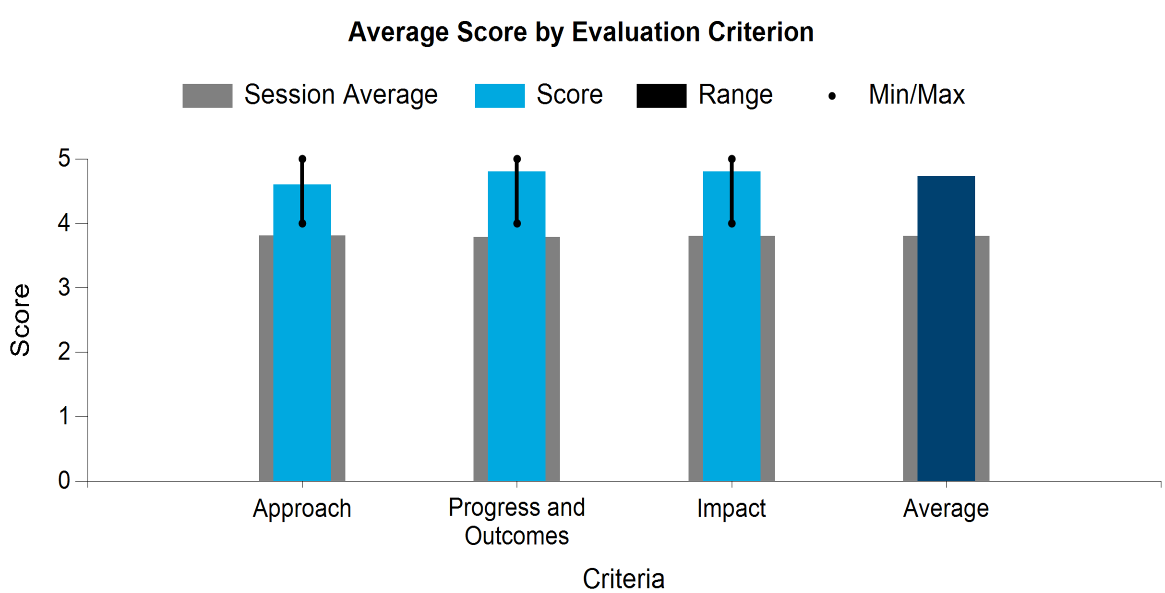
ADVANCING THE DEVELOPMENT OF BIOFUELS FOR THE MARITIME SECTOR—ORNL, NREL, PNNL, ANL

Oak Ridge National Laboratory

PROJECT DESCRIPTION

WBS:	3.1.4.014
Presenter(s):	Michael Kass
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$5,216,787.45

This project seeks to understand the efficacy of biofuel use in the marine sector as a means to reduce carbon intensity and GHG emissions. The research team includes Oak Ridge National Laboratory (ORNL), Argonne National Laboratory (ANL), the National Renewable Energy Laboratory (NREL), and Pacific Northwest National Laboratory (PNNL), and it is year 2 of a 3-year study. The major research thrusts are to conduct a techno-economic feasibility study/LCA and gage the technical feasibility of biofuels. Promising pathways include the use of bio-intermediates (pyrolysis oils and HTL oils). These efforts demonstrate solid pathways toward GHG reduction in the maritime sector. Challenges exist in the forms of resource competition and lack of information, especially engine test results. Progress can be summarized as (1) the team has established a framework and methodology for TEA studies based on feedstock type and production pathways, (2) GHG emissions reduction potential has been determined for many biofuels and production pathways, (3) HTL oils have demonstrated stable blends with heavy fuel oil, and (4) the compatibility and combustion quality of bio-intermediates is suitable for blends up to 15%. The research team periodically disseminates information to the stakeholder community via a number of channels. One measure of interest is the expanding membership in the project advisory committee and industry requests for information and participation from team members.



COMMENTS

- Approach: The project approach aligns with metrics defined under the lab call. Technical: Identify pathways that can meet marine fuel blending requirements; several pyrolysis and HTL pathways are considered. A ranking of schemes was conducted to downselect or find suitability of blends, especially with regard to spot ASTM tests. Project management: Elaborate national lab participation on blends, TEA, and LCA, with feedback from several industry partners. Opportunity lies in two-stroke engines. Key goal: Blends with very-low-sulfur fuel oil.

- Progress and outcomes: The team has made significant progress on identifying catalytic fast pyrolysis (CFP) and HTL oils with mitigating strategies for upgrade and blending. The TEA/LCA results clearly show that most HTL routes and a few CFP routes show promise. There is a lack of clarity in the industry for decarbonization or adoption/selection of fuels. In this regard, the consortium has definitely engaged the right partners from industry, regulatory, adoption/standards, and guidance.
- Impact: The project has not only achieved results, it has also advanced the cumulative knowledge for the fragmented approach due to the variety of biocrudes and risks involved in adoption. The TEA/LCA results serve as guidance for GHG impacts, costs, and the stability/reliability of fuel oil blends. Further, all major pathways (except a few Fischer-Tropsch diesel results are sparse) have been considered and included. Fuel properties have not been neglected, resulting in a narrow band of biofuels that might be acceptable. The consortium is led by national labs and can leverage (benefit from) some other projects that have looked at upgrading biocrudes for refinery processing. It seems the budget is sparse relative to the achievements and potential impact this project can make. I hope this study will continue and find the required support.
- A collection of national labs have combined their capabilities to address problems with marine fuels. They have received buy-in from a range of companies, including some shipping companies that can help inform them of the nuances of fueling maritime vessels and the role biofuels can play.
- The presentation described an analysis of asphaltene precipitation and how they were able to determine which biofuels would cause asphaltenes to precipitate.
- A significant amount of LCA and TEA were completed for various fuels, showing that some are competitive.
- This seems like an excellent hole for the labs to fill. The labs have a lot of the necessary equipment to test biofuels for maritime applications, which is likely not common for a university consortium or independent testing lab. The labs are an excellent fit here and have made excellent progress.
- This is an appropriate project for DOE laboratories. They can provide an unbiased assessment of the potential for processed biomass fuels to impact the maritime market. They have made significant progress and have addressed many concerns from the 2021 review comments. A question that probably needs to be addressed is when is there a logical point at which to let industry take it over? This group may want to define their desired ideal outcome, so they can plan toward that. There should be some measures of performance that would encourage shipping companies to start contracting out fuel supplies from companies like Ensyn or others.
- This project involves four national labs and funding at $2 million annually. The expertise at each lab is being used toward investigating the potential opportunities for marine biofuels. The project appropriately incorporates LCA and TEA throughout the tasks instead of using these analyses as one-time checkpoints at the very end of a project. There is active engagement of industry and related stakeholders; 20 entities are represented across energy companies, shipping and engine companies, industry experts, biofuel companies, shipping terminals, nonprofit organizations, and governmental organizations, while new partnerships and initiatives are still being generated. The results of this project are being disseminated on a timely basis, across peer-reviewed publications and industry presentations, and detailed parametric LCA models have already been incorporated into the latest release of ANL's respected Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) platform. The project has also

identified challenges such as the precipitation of asphaltenes, which will require mild hydrotreatment of heavy oils, and studied the stability of fuel blends at the laboratory scale. This is a well-designed project that has made commendable progress and shows high potential for a significant impact to the marine biofuels industry.

- The project is quite well formulated with relevant industry stakeholders. The presentation covered all relevant FOA goals, and the reviewer did not find any technical concerns with the project. The reviewer suggests looking at longer-term stability testing for asphaltene precipitation in the blends.

PI RESPONSE TO REVIEWER COMMENTS

- Response to Reviewer 1: Thank you for the positive and encouraging comments. The specific lab roles related to blend testing, TEA, and LCA are as follows: ORNL has acquired and has access to several residual fuel oils. These fuels have served as the basis for blend stability testing. ORNL, along with PNNL and NREL, perform blend stability experiments; PNNL is focused on HTL oils, NREL is focused on pyrolysis oils, while ORNL evaluates blend stability from the PNNL and NREL oils as well as commercial oils. ORNL is also planning on conducting aging studies with industry input. All LCA work is conducted by ANL. TEA work is conducted by both PNNL and NREL. PNNL has primarily focused on HTL oil pathways, while NREL is looking into pyrolysis oil pathways and other biofuels (methanol, lignin ethanol oil, biodiesel, etc.). With regard to the concern on the budget level, the research team is actively looking at opportunities to leverage with the U.S. Department of Transportation, U.S. Department of State, and industry.

- Response to Reviewer 2: Thank you for the encouraging comments.

- Response to Reviewer 3: We have had several internal discussions regarding industry transfer. Based on the feedback and input from our external advisory board, there are several fuel-specific metrics that include successfully demonstrating long-term (4 months) blend stability aging studies. The other key metric is successful operation in engine performance studies before realistically considering industry adoption. Our ideal outcome would be to identify and confirm an economic, sustainable, and scalable pathway toward biofuel use as a blend with residual fuel oil (in the near term), with the eventual implementation of a zero-carbon fuel option.

- Response to Reviewer 4: Thank you for the positive comments.

- Response to Reviewer 5: Based on this reviewer's comment along with input from our external advisory board, the research team is pursuing long-term stability tests based on standard sedimentation tests and gel permeation chromatography. Another planned set of experiments includes operating selected blends in a closed-loop circulation system where the fuel is periodically sampled to determine blend stability and potential degradation over an extended period of continuous operation.

INTEGRATED SEPARATIONS TO IMPROVE BIOCRUDE RECOVERY FOR BIOFUELS AND BIOPRODUCTS

Research Triangle Institute

PROJECT DESCRIPTION

WBS:	3.4.3.305
Presenter(s):	Dave Dayton
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2025
Total Funding:	$4,612,503

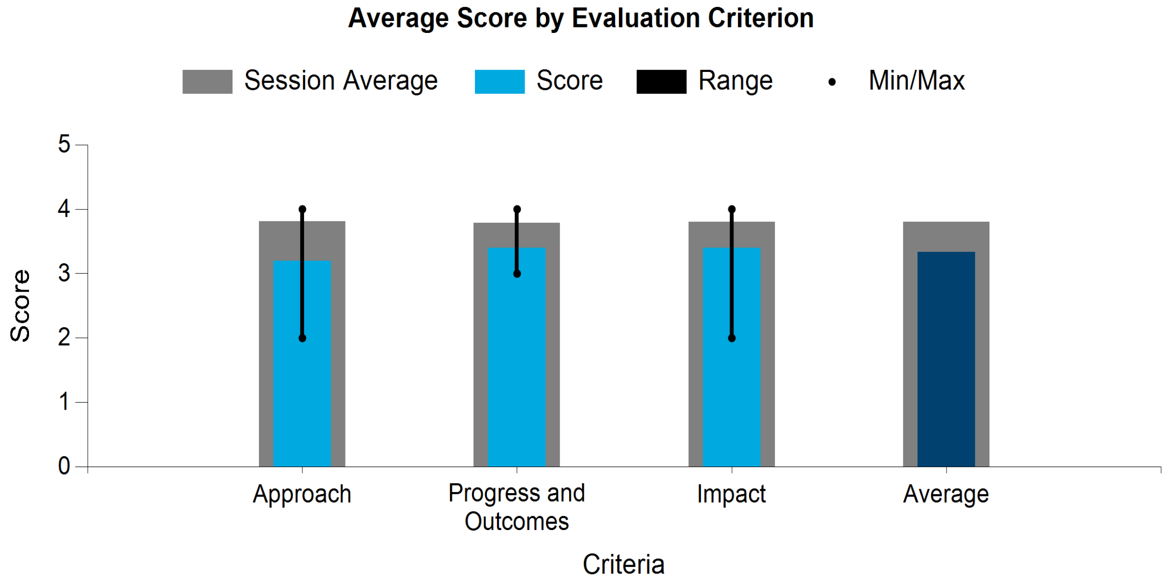
Research Triangle Institute (RTI) International has been developing an advanced biofuels technology that integrates catalytic biomass pyrolysis and hydrotreating to produce advanced hydrocarbon biofuels and high-value chemicals. Current efforts are geared toward key technical challenges, such as improving the carbon efficiency of the integrated process by optimizing the biomass thermochemical conversion step to simultaneously maximize both biocrude intermediate yield and quality. Other efforts include developing strategies for bioproduct recovery and efficient upgrading of biocrude to bio-blendstocks.

RTI continues to focus on optimizing the operation of our 1-ton-per-day (1-TPD) catalytic biomass pyrolysis unit and process conditions (temperature, flow rates, catalyst-to-biomass ratio, and feedstock properties) to increase biocrude yields. Capturing biomass pyrolysis vapors requires separating solids at pyrolysis temperatures, quenching the pyrolysis products that have a broad molecular weight distribution and boiling range, capturing the condensation aerosols, and separating biocrude from water.

Cost-competitive advanced biofuel technology strongly depends on yield, but recovering bioproducts before upgrading intermediates to biofuel provides a higher-value revenue stream to improve the overall process economics in an integrated biorefinery approach. The inherent functionalized nature of biomass offers a unique opportunity for the production of bio-based oxygen-containing chemicals that are not easily synthesized from petroleum feedstocks; therefore, the deoxygenation of catalytic biomass pyrolysis vapors to produce a low-oxygen-content biocrude may be a missed opportunity for bioproducts.

Technical issues across the entire value chain—from feedstock, through conversion, to biofuels and bioproducts—are being addressed with the goal of demonstrating the integration of separations with CFP to enhance biomass conversion efficiency. Ecostrat, with more than 20 years of experience sourcing and supplying more than 5 million tons of wood fiber and organic feedstock in markets across North America, is evaluating biomass supply chain logistics to optimize biorefinery size and location as a function of sustainable, cost-competitive feedstock resource availability, market dynamics, and regional infrastructure.

RTI will focus on the scale-up and integration of separation processes in the 1-TPD biomass pyrolysis unit to (1) improve the separation of solids from the vapor product stream, (2) enhance the rapid quenching and collection of pyrolysis vapors, (3) separate highly oxygenated bioproducts from the liquid intermediates, and (4) recover the remainder for upgrading into advanced biofuel. Coprocessing strategies for upgrading biocrude fractions with petroleum intermediates into finished fuels that meet ASTM specifications will be explored, while biocrude fractionation will support recovering high-value market-compatible bioproducts.



COMMENTS

- Approach: The project approach aligns with the metrics defined under Topic Area 1, DE-FOA-0002203.
    - Technical: Integrated separations to showcase methoxyphenol and other products, recovery, and its impact on the economics of biofuels as byproduct credits.
    - Project management: No slides on management approach. Partner list provided on Slide 16 with roles.
- Progress and outcomes:
    - Builds on several other projects for CFP awarded to this organization.
    - Verification completed.
    - Budget Period 2 work biomass resourcing and procurement.
    - A market study on methoxy phenols and their uses.
    - A 7-gallon-per-day laboratory-scale separation unit.
    - Claims 75% recovery, 90% purity (to what?), no residual losses.
    - What was the yield of methoxyphenols in prior work? What is the required purity? How does it compare with commercial products in terms of acceptable level of trace impurities? Seven different distillation cuts are shown on Slide 8—each has five different components. Even highly concentrated/purified cuts have 5% to 20% individual concentration of molecules. Unfortunately, such product mixtures do not qualify as bioproducts. Are there any precedents cited for such a product mix/sales, or has anyone shown interest in further purifying it? What are the plans to improve this to the desired >90% or commercial benchmark? What is the basis of assuming cost/price for such a fraction for TEA?

- Impact:
  - The project builds on several funded programs on CFP. The organization has high capabilities and partners to support the program; however, the presented results do not reflect that a particular set of bioproduct/s with desired properties is produced even at lab quantities. Anticipated yields with this degree of separation seem too low to make an impact on economics, and rather can be detrimental due to the number of separation steps needed. No clear benchmarks for product specification or approaches to improve purity have been identified.
  - As a reviewer, I felt a bit lost in the number of funded programs at this institute. It was not clear if the intended goals of this particular project are being achieved, even with a great deal of experience and benefit of data from other programs. I am also not sure if this project has different results from past funded programs, such as MEGABIO, and I request a comparison of past versus new results for bioproducts. A more careful go/no-go review is recommended.
- This process aims to include pilot-scale separation for a fast pyrolysis system. A goal is to remove some stream to act as a chemical building block. This builds on previous work by the principal investigator (PI). The initial verification has been completed.
- A significant amount of supply chain analysis was completed. It is not clear why this is the place for supply chain analysis. If it does fit in, it was never stated how it does so at this point, given the number of projects the PI is working on.
- The unit operations are operational. It is not clear what the value of the supply chain analysis was to this project. It is also not clear that the methoxyphenols are the best chemical building block to extract from the process. The actual separation design seems like the most valuable accomplishment for this project, though it was not discussed as in depth as the supply chain or methoxy phenols.
- It is not clear why the results of the verification Step 1 were not included in the original presentation instead of in the additional slides. Those results showed the project was on track. Otherwise, this project is on schedule, and preliminary results demonstrate that it will be possible to coproduce a product stream and fuels. The selection of one type of coproduction stream is sensible, and focusing on that one stream will be good. The team probably needs to see what value that stream has. Good partner with Ecostrat. They are targeting the appropriate TRLs. There is an old saying that “there is a world of difference between a valuable mix of chemicals and a mix of valuable chemicals.” They need to continue to address this issue.
- This project aims to improve solids separation from the gaseous stream for the rapid collection of pyrolysis vapors and to assess the potential for the collection of coproducts along the pathway. Methoxyphenols, which are precursors to flame retardants, can be recovered through separation from the biocrude generated via pyrolysis. This increases the commercialization potential for the system. The project team is investigating approaches to improve (nearly double) the carbon routed to biofuels from the same input amount of biomass. The project is in its second budget period and involves a multitude of industry partners.
- Challenges with their scheme will limit the purification of methoxyphenols. The process team should consider molecular distillation as opposed to distillation on the recovery step.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for taking the time to evaluate our project and providing constructive suggestions for improvement as the project continues into the next phase. Over the past 15 years, we have been developing catalytic biomass pyrolysis technology to produce biofuels and bioproducts with support from DOE/BETO in several different projects. Throughout these projects, we have installed and commissioned a 1-TPD catalytic biomass pyrolysis unit (April 2013), a pilot-scale hydroprocessing unit (January 2015), and a laboratory-scale separation unit (January 2019). Only minor process modifications have been made since the commissioning of the 1-TPD unit; however, after years of operation, issues with biocrude recovery have been identified, and the scale of the laboratory separations does not match well with the 1-TPD unit. Therefore, the primary goal of this project is to scale up the separation unit operations and integrate them into the 1-TPD unit. This will improve biocrude recovery, reduce the effort to effectively fractionate biocrude for upgrading, and facilitate the recovery of bioproducts. Catalyst fines and char often carry over past the primary cyclone and condense with higher-molecular-weight pyrolysis products, resulting in a loss of 15%–25% biocrude unless the solids can be separated after condensation (which is impractical). Therefore, one separation unit operation being considered is a hot gas filter for particulate removal prior to biocrude condensation. Downstream of the primary quench, we are also considering liquid-liquid extraction units that were proven in the laboratory-scale separation unit to fractionate biocrude into low-oxygen-content organic feedstock for more efficient hydrotreating and high-oxygen-content liquids with potential for isolating bioproducts. The basis for the separation unit operations in this project are the results from our previous projects, and the methoxyphenol recovery from biocrude is specifically based on the laboratory-scale separation unit developed in our MEGABIO project (DE-EE0007730). The results collected during our previous projects will be reproduced in this second budget period to inform the intermediate verification and define the basis for the go/no-go decision point to move ahead with the design modifications in the 1-TPD unit. The purpose of scaling up the separation unit operations and integrating them into the 1-TPD unit is to increase the yield of the collected biocrude and separate it into fractions to facilitate methoxyphenol recovery and cohydroprocessing with refinery intermediates. Biocrude yield has the largest impact on the modeled process economics, but the recovery of higher-value bioproducts also has a significant impact, as demonstrated in our previous projects. The experimental results from this project will be input into the process model that forms the basis of the TEA; however, the commercial potential of this proposed pathway is directly related to the scale of the modeled integrated biorefinery. Clearly, the economics are favored by economies of scale, but there is a practical limit to the size of the integrated biorefinery defined by the cost and availability of the biomass feedstock that can be delivered to the plant. Consequently, we are partnering with Ecostrat to perform a supply chain analysis at selected sites in the southeast and the northwest to determine the optimum scale of an integrated biorefinery while considering the existing demand for regional biomass resources and existing infrastructure.

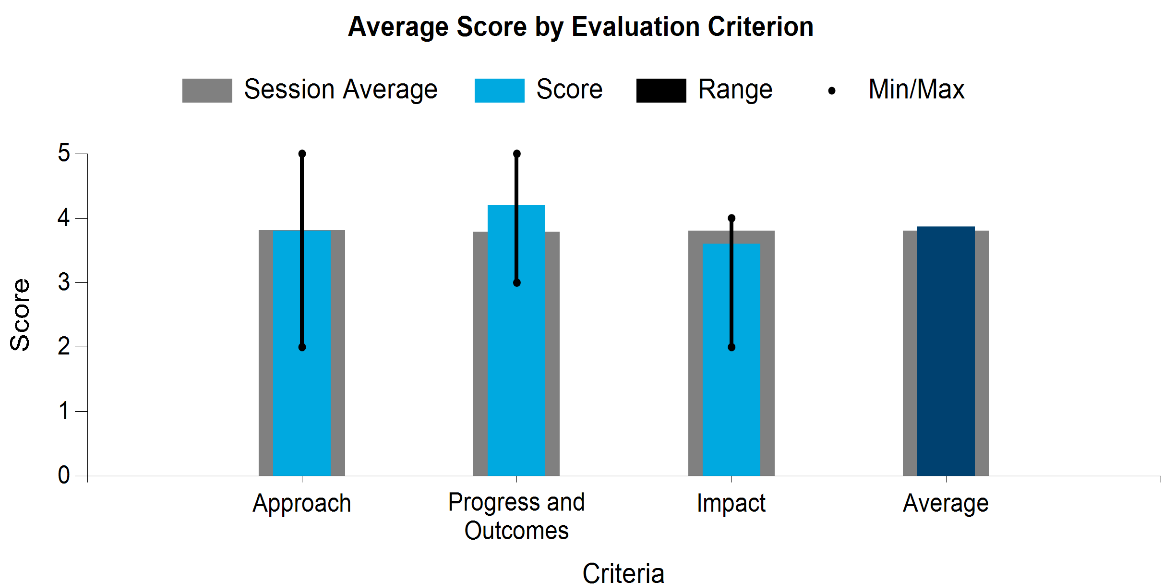
BIO-OIL COPROCESSING WITH REFINERY STREAMS—PNNL, NREL, LANL

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	3.4.3.306
Presenter(s):	Asanga Padmaperuma; Huamin Wang; Karthikeyan Ramasamy; Katarina Younkin; Michele R Jensen; Reinhard Seiser
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2023
Total Funding:	$5,056,000

The objective of this three-laboratory project is to accelerate the adoption of coprocessing biomass-derived feedstocks with petroleum streams in current refineries by developing and broadly disseminating foundational data for processing renewable intermediates and offering coprocessing strategies. It will enable using U.S. refineries that in 2020 had a capacity of 8.8 million barrels/day for hydrotreating and a capacity of 5.6 million barrels/day for fluid catalytic cracking (FCC). Three critical challenges were identified by the project's industry advisory board: (1) a critical operability risk comprising process stability around catalyst deactivation; (2) a regulatory risk comprising the need to rapidly measure biogenic carbon and oxygenates in processed streams; and (3) a significant knowledge risk centered on the lack of coprocessing data, including feedstock compositions and contaminants, product compositions, the reaction kinetics of unique biocompounds, and associated TEA/LCA. The outcomes of addressing the three challenges are: (1) preventing catalyst deactivation by reducing alkali species through hot gas filtering (FCC) and reducing nitrogen compounds by pretreatment (hydrotreating/hydrocracking); (2) developed methods for inexpensive/rapid biocarbon analysis through 14C and delta 13C analysis methods; and (3) provided detailed compositions on bio-oil feeds and coprocessing products, including contaminants, operational data including biocarbon yields, an improved kinetic reactor model for hydrotreating, and associated TEA/LCA.



COMMENTS

- Approach: The project approach aligns with the metrics defined under the lab call.

- Technical: This is a multipronged approach to increase the use of bio-derived crudes for processing in existing refineries: FCC; hydrotreating/hydrocracking; and fats, oils, and greases (FOGs)—biocrudes from different sources. Track contaminants and biogenic carbon.
- Project management: The project includes elaborate national lab participation on blends, upgrading, and the analysis and tracking process. It includes several industry partners/feedback and a few prominent catalyst suppliers/advisors.

- Progress and outcomes:
  - The coprocessing goals expanded new catalysts, feeds, and improved models.
  - The CFP oil coprocessing *in situ* and *ex situ* showed the impact of O on storage and stability.
  - Yields for coprocessed bio-oils with vacuum gas oil (VGO) in FCC were comparable, with a 5% blend.
  - The product has 1%–2.5% O_2.
  - Catalyst deactivation was observed with all bio-oils; the mitigation strategy is a guard bed in addition to upgrading bio-oil.
  - Liquid scintillation counter C14 tracking was improved for several types of colored or raw bio-oils.
- Impact: The project has made considerable progress and showcased the tracking of biogenic carbon using multiple methods—5% blends for all approaches, mitigation strategies for catalyst deactivation, or modifications to reactor models. This directly enables the integration of large quantities of bio-derived feedstocks in current refinery operations. It is unclear how much the quantities were processed—what statistical data, quality control has been done so far? Any insights on this might be helpful for adoption and reliability. The program has clearly achieved its goals per the timeline. The complex network of task owners has been effectively managed to attain the desired outcomes. There is interaction with a lot of minority groups via workshops, webinars, and sharing knowledge.

- The goal of this project is to fill in missing information in which petroleum refiners need to have more confidence, including biofuels in their processes as a first step at bringing biofuels to market. The group of several labs is able to do varied studies on the effects of adding biofuels to refinery-type applications.

- The presentation mentions a few success stories, including a study on adding bio-oils to VGO. The group has also received a significant amount of input from industry partners.

- It is good to see the labs take a role in this important function, though I would expect that the refiners would have a consortium to study different related problems to integrating biofuels. It seems that industry stakeholders would be careful to tell the labs what they truly need to avoid giving away trade secrets. It would be interesting to hear how open and specific the refiners are in describing problems they need addressed.

- The project has made appropriate progress toward the project's goals. The project has provided BETO with information that can be used to justify the incorporation of processed biomass into refinery streams. There are several projects in BETO's portfolio that address the incorporation of processed biomass into refinery streams. The program probably should do a bit more to integrate these projects into something oil refineries can look at. The one reviewer comment on 75% incorporation into oil refinery streams is ambitious, but changing 100-year-old technology would require shutdown economics, and that is not feasible right now. The team has good partnerships in industry. The project does a good job with DEI.

- This project is assessing how existing petroleum refineries could integrate drop-in bio-intermediates, like biocrude from the HTL of biomass, for coprocessing into finished fuels. This has the potential to reduce the scale-up needs of the biofuels industry through sharing the existing infrastructure, and it might possibly reduce the carbon footprint of petroleum-based fuels; however, depending on whether the fraction of biocrude to petroleum crude ultimately coprocessed at scale is relatively small, this may provide greater assistance to the petroleum industry than to the bioenergy industry, or regardless of the fraction, both industries may overlap in their separate accounting of the biogenic carbon throughout processing and in finished fuels. The project team has been tracking biogenic carbon in products, though, to ensure a process that incorporates a high proportion of biogenic carbon in the fuel products. It would be interesting to simultaneously track or model the reductions in fossil fuels going through a refinery. The project's DEI efforts uniquely include an energy justice analysis, which is commendable for a 3-year project that involves shared infrastructure with fossil fuels. Still, it is unclear how this analysis is performed and how the results may be used in future implementation decisions. Since the last DOE Project Peer Review, 2 years ago, the project team has published 14 papers in peer-reviewed journals. Because the DEI efforts also involve the recruitment of underrepresented students, it would be useful to report the number of papers that involved these students as coauthors and other metrics to assess the success of these efforts.

- The project is quite well presented, however, not all refineries are the same, and the differences in processing ability will impact the incorporation of bio-oil. The method developed to track the incorporation of biogenic oil is significant and novel.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for highlighting some strengths of our program, such as the multipronged approach and the wide national lab and industry participation. This program at the national laboratories has evaluated various effects of introducing biomass-derived liquid feedstocks into refinery streams by coprocessing. We have collaborations with large and small refiners, learning about each of their needs and the types of available processing equipment. This has encouraged the study of different next-generation feeds (CFP, fast pyrolysis, and HTL bio-oils) in different coprocessing units (FCC, hydrotreaters, and hydrocrackers). Industry partners have also provided valuable feedback and have expressed appreciation for receiving fundamental data, such as experimental and modeling results, and compositional data of feeds and products. According to refiners' remarks, there exists a collective interest within the industry to integrate bio-derived feedstocks into refineries, aiming for the efficient production of sustainable fuels. To de-risk the adoption, both emerging feedstocks and refinery capabilities will need to adjust, with support from the foundational study. We agree that the future bio-economy will both involve building new biorefineries as well as transitioning petroleum refineries to increase the biofuel portion of their operations. Even fuels produced at biorefineries are often sent to existing large-scale refineries for upgrading and blending. Therefore, the tracking of biocarbon throughout both processes is an important component of evaluating the progress toward incorporating biogenic fuels, which is one of the major objectives of our program. We will continue to provide innovative opportunities to increase DEI through multiple internship opportunities and collaborations with minority-serving institutions. Regarding the stability of various CFP oils, we find good repeatability of pressure-drop increase in our heated nozzle as an indication of bio-oil instability, and we provide this feedback to suppliers and refiners. While various measurement methods show some oxygen content in the product, speciation by gas chromatography-mass spectrometry shows that the expected oxygenates in the product from FCC coprocessing might be less than 1%, mainly consisting of phenols, furans, and ketones. Catalyst mitigation is an important topic for coprocessing in hydrotreaters, employing fixed-bed catalysts, while the catalysts in FCC coprocessing are less impacted due to their continuous replacement during operation. In our laboratory studies, we have coprocessed liter quantities of CFP oils and HTL biocrudes with tens of liters of petroleum feeds. At present, industrial refineries have been coprocessing FOGs, whereas for the above-mentioned next-generation bio-oils, they are currently assessing data regarding their impacts on refinery operation and performance, such as from our program, as well as their availability through large-scale production.

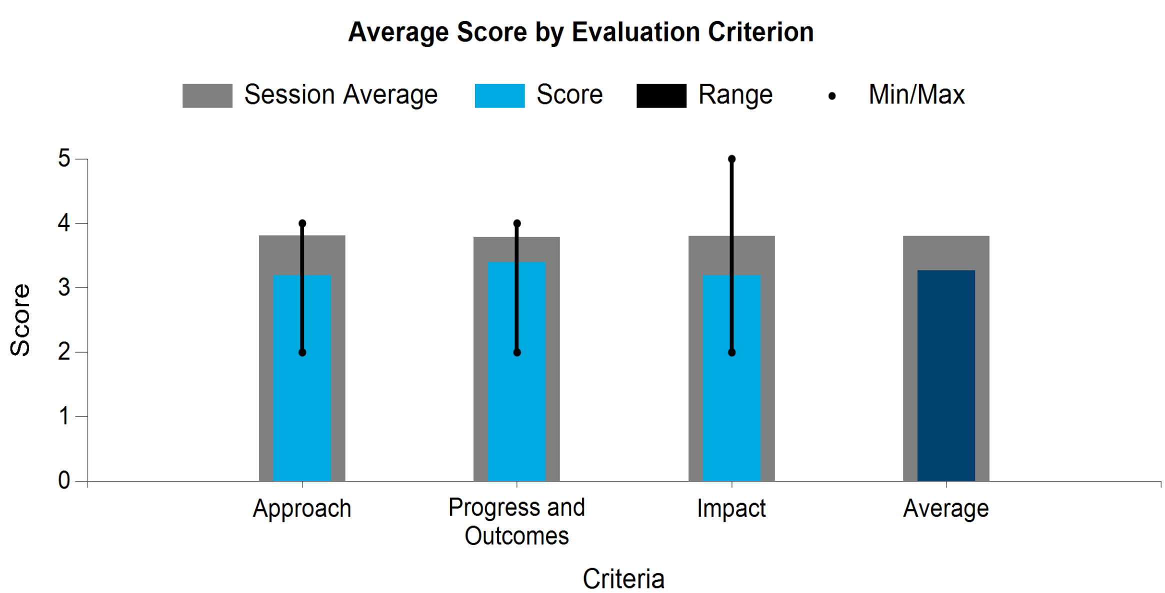
MICROCHANNEL REACTOR FOR ETHANOL TO N-BUTENE CONVERSION

Oregon State University

PROJECT DESCRIPTION

WBS:	3.4.3.504
Presenter(s):	Brian Paul
Project Start Date:	10/01/2020
Planned Project End Date:	06/30/2024
Total Funding:	$5,000,000

Oregon State University (OSU) is partnering with PNNL and LanzaTech to develop a new process technology with the potential for reduced capital and operating costs for an alcohol-to-jet (ATJ) process technology that is currently being commercialized by LanzaTech. Employing new catalyst technology developed at PNNL, ethanol is first converted into n-butene-rich olefins with >90% conversion and >80% selectivity. Olefins are then oligomerized, hydrotreated, and fractionated into jet blendstock. Energy savings are realized by coupling the severely endothermic ethanol dehydration with exothermic C-C bond formation. Further process intensification and modularity is achieved by integration into a microchannel reactor platform. Advances in additive manufacturing methods enable catalyst scaffolds to be integrated directly within reactor channels during fabrication, further reducing capital expenditures (CapEx). The project is now working to demonstrate a one-eighth-scale system prior to a full-scale demonstration of 0.15 ml/min. Single-channel reactors have been demonstrated, and a kinetics model has been developed and used to design “numbered-up” reactors for demonstration-scale evaluation. Three reactor design and manufacturing strategies have been developed that are capable of supporting system-level cost targets set by TEA, two of which have the potential to reduce reactor equipment cost by as much as 50% using advanced additive manufacturing methods.



COMMENTS

- Approach: The project approach aligns with the metrics defined under Topic Area 1, DE-FOA-0002203.

- Technical: This project focuses on ethanol conversion to olefins with an emphasis on butene using microchannel reactors. It showcases advantages in rapid scale-up, leveraging additive manufacturing as the low-cost fabrication process.
- Project management: Although there were no clear slides on this, PNNL and OSU seem to have managed the project progress well.

Progress and outcomes:

- Validation with 90% conversion and >55% selectivity to C3 and above olefins.
- Single-channel reactor 80% ethanol conversion and 80% selectivity to butene-rich olefins with required productivity/yield to meet TEA requirements.
- Clear approaches on catalyst reactor scale-up, cost estimates, and methodology have been presented.
- Details of single-channel reactor show, Slide 7, approximately 60% butene and overall olefins as 80%. Propene and ethylene are not C4 compounds; what other compounds are claimed as C4?
- Advance reactor single-channel performance initial results are presented and look promising but need improvement.

Impact: If successful (the project has 2 more years), at a small scale, the project has shown considerable progress, but it lacks performance criterion. The rate of production, selectivity, and conversion results are promising and can certainly make a meaningful impact if reactor scale-up costs can be managed by improved manufacturing methods. Past work on microchannel results have shown scale-up challenges. It is unclear what the catalyst deactivation rate is at low space velocities. Some decline can be observed at 100 hours time on stream (TOS) (Slide 7); more data are required to estimate regeneration process, downtime, and costs.

- The proposal is going to use microchannel reactors to convert ethanol to butane due to their scalability. This is the first step in an ethanol-to-jet fuel process. The team consists of OSU, PNNL, and LanzaTech.

  The process has been scaled up from a bench-scale reactor to a large version using Fecralloy foam with a catalyst wash-coated on it. In this system, the butane selectivity is less than 65%, but the total olefin selectivity is 80%. A modular design for a microchannel reactor has been proposed.

  The initial run converted 10 g of ethanol per hour with a space velocity on the order of a few reciprocal hours. The microchannel reactor will operate at a similar space velocity. This is slow given the advantage of microchannel reactors is the higher output. It would be great to see what the pressure drop in the microchannel reactor is, though at such a low flow rate, it may be small. Also, it is not clear how the reactor will be maintained at 350°C–450°C. It will be difficult to keep all the channels at these temperatures uniformly as well as to start the reactor.

- Microchannel reactors have been looked at for many years. There have always been limitations in what they can achieve. This project has demonstrated at the single-channel level sufficient performance to look at scaling opportunities. The catalytic process is relatively straightforward and appears to be adaptable to scaling. The project needs to continue to look at interface issues and particularly in continuous operation. There is concern about the multichannel reactor—not that it will not work, but first-of-a-kind units usually have some hiccups. They should be mindful of quality control on the manufacture. The team is very well poised to establish whether this can or will work in an actual operational environment. They will either know it works, or they will find it is too challenging. They should be able to get an answer.

- This project investigates a pathway from ethanol to butene-rich olefins to jet-/diesel-fuel-range hydrocarbon chains in a microchannel reactor. Although the modularity of the microchannel reactors serves a useful purpose in scale-up, it is unclear how (1) removing deposits of solids, (2) clearing channels clogged by heavy oils, (3) regular maintenance on the reactors, or (4) troubleshooting problems occurring in one or more of a large set of microchannel reactors would be handled in reactors with these dimensions; however, bench-scale reactor evaluation results are favorable from the experiments performed thus far. The design of the catalyst as a coating on a removable foam insert into a microchannel reactor mitigates my initial concerns about catalyst recovery for regeneration; however, for adaptation of this design to continuous-flow conditions, this system appears to greatly increase the friction and may require more pumping energy, which would increase the carbon footprint and costs of the produced fuel. The model validation using experimental results appears insufficient for a conclusive fit because each condition has only three data points to fit. Additional experimental testing would be required to more robustly assess the ability of the model to predict conversion or selectivity based on input rates of ethanol. The cost analysis performed is also incomplete at this time because it covers only CapEx; it is unknown whether operational costs completely dwarf the costs of the raw materials, for instance. The results of an energy balance at both the bench scale and the projected commercial scale would be particularly interesting given the unique geometry of the reactors. This could answer a research question about the optimal point in balancing between increasing the surface-to-volume ratio for higher catalytic conversion and decreasing the surface-to-volume ratio to decrease pumping energy needs against frictional forces or higher energy use in maintenance steps. The project is close to its midpoint and will be exploring scalability, life cycle costs, and life cycle GHG emissions within the next 2 years. This will provide more clarity on whether these concerns are valid or would be overcome through continued process design.

- The best results are obtained at very low weight hourly space velocities. I wonder what the advantage is of microchannel versus packed bed at this low velocity. The CapEx of foam are still quite high.

PI RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their insightful comments, and we appreciate the acknowledgement of the merits of this BETO program. In response to questions about what compounds are claimed for selectivity calculations, the “olefins” include the selectivity to all the olefins produced, including ethylene, propylene, and butylene. The selectivity to the predominant olefin produced, n-butene, is separately indicated.

- Regarding the questions related to performance criterion and the need for continuous operation, the performance criteria are (1) achieve >80% total olefins and >80% conversion for a single-channel reactor; (2) demonstrate a scaled microchannel system to convert 0.15 standard liter per minute of ethanol for 500 hours TOS for full-scale demonstration; (3) within capital and operating cost targets.

- On the comment relative to scale-up challenges associated with microchannel reactors, we agree that the scale-up of microchannels is challenging, but we contend that the scale-up of any system can be challenging. First, we note that two companies have successfully deployed microchannel process technology as spinoffs of PNNL (Velocys and STARS Technology Corporation). Further, in this project, we are concerned with only gas phase conversion; thus, there are no solids or liquids reacting or being produced when in the microchannel reactors (liquids will condense out downstream after gas-liquid separation). Beyond this, we have demonstrated that the catalyst can be regenerated *in situ* upon mild oxidation and that separate catalyst inserts can be removed and replaced where necessary. Therefore, even if there are byproduct issues, we expect that many of the same approaches that work, for example, in a 10,000-tube shell-and-tube reactor, having 1-inch-diameter tubes with 1/16-inch extrudates, will apply here, including (1) heating under inert gas to remove heavy oils, (2) hydrogen stripping to remove heavy oils and deposits, and (3) regenerating in air to burn out deposits. In extreme cases, an appropriate solvent or washing solution can be pumped through the reactor. Finally, these units are modular, so different units can be replaced when necessary without affecting the whole reactor system.

- Relative to the comments on catalyst deactivation, the reviewer is correct to point out how there is a small amount of deactivation observed over 100 hours; however, the catalyst has been shown to be fully regenerable, so the processing system will be designed and operated in a manner to periodically regenerate the catalyst. Recently, PNNL successfully performed an 800-hour TOS catalyst test with the catalyst being regenerated every 100 hours. We did not have time to discuss these details regarding the catalyst within the review.

- Regarding the comments relative to the reactor design, we have run numerical simulations with approximately 100% increased throughput (weight hourly space velocity 3.0) and were still able to reach the target conversion and selectivity, suggesting higher throughput is possible. Further, the pressure drop through the reactor is only partially related to the flow through the porous catalyst layer, which is small (with simulations estimating it as approximately 20 Pa). Significant pressure drop is associated with the "feed-nozzles," to ensure even flow distribution between plates, which is a design variable that can be adjusted. Also, simulations show that the overall heat balance of the reactor is sufficiently maintained by transferring heat from exothermic reactions at the end of the reactor bed upstream to endothermic reactions via partition walls (plates) between catalyst inserts. Therefore, the entire reactor energy balance is maintained by the inlet temperature of the reaction mixture, which will be maintained via preheat. Detailed protocols will be developed for startup and shutdown of the reactor, depending on several parameters, with heat distribution being only one of the several phenomena.

- Regarding the questions related to model validation, we are confident that model validation using experimental results is robust and meaningful because the "fit" is not a blind polynomial fit but rather a fit to an extensive mathematical model (set of partial and ordinary equations encompassing all transport phenomena and reaction kinetics). Therefore, the model is based on first principles with no empirical correlations or factorial parameters. The accuracy of the reaction rate constants estimated from the least-square optimization hinges on the number of experiment points used in the modeling. Every point on the graph represents an average of three independent measurements, enabling us to calculate the estimated parameters' variances. We are confident that experimental points on the graph are assuming a monotonous rise without unexpected excursions between recorded points.

- Regarding the comments on finding the optimal surface-to-volume point to balance catalytic conversion, pumping energy, and maintenance cost, this is an interesting comment. We agree. Our mathematical model represents a design tool that is helpful in informing an independent cost model built around the full reactor scale, connecting the technical details mentioned and the overall net present value of the business.

- In response to the comments on the need for quality control in reactor manufacturing, we agree that the precision in manufacturing is critical for successful reactor operations overall, including even flow distribution between reactor beds and layers. To address this, test articles have been fabricated by the reactor vendor to evaluate the effect of tolerances on reactor design. Further, fluidic testing will be performed to verify fluid flow distribution across multiple channels of reactor shells prior to catalyst loading.

- Regarding the comments on the cost of the reactor inserts, this is why we are pursuing two alternative advanced reactor designs that are leveraging the ability for additive manufacturing to deliver more complex structures at lower overall cost.
- Regarding the factors driving economic evaluations, raw material costs have been found to dominate production costs as follows: 87% ethanol; 13% catalysts and chemicals, energy, and other utilities, and fixed costs.
- Regarding questions on the advantages of microchannel reactors over packed-bed reactors, microchannel reactors provide the potential to reduce business risk for scale-up over packed-bed reactors. Significantly less precommercial investment is required to demonstrate scaling by piloting a single module. By numbering up, the first prototype module can be used for production, reducing the time needed for return on investment. With conventional scaling, greater time and investment are required across the conventional bench, pilot, demo, and commercial development pipelines. These advantages are enabled in part by the intensification of microchannel reactors over conventional packed-bed reactors. In a practical (not ideal) packed-bed reactor, the catalyst carrier particles are randomly packed throughout the packed-bed volume, resulting in slight variations of voidage space (especially along the reactor walls). These variations of voidage space (even if small) quickly give rise to significant variations in temperature and flow distribution. In contrast, microchannel reactors contain an engineered porous catalyst carrier media, providing better flow conditions and thermal uniformity, enabling intensification.

INTEGRATED REACTIVE CATALYTIC FAST PYROLYSIS SYSTEM FOR ADVANCED HYDROCARBON BIOFUELS

Research Triangle Institute

PROJECT DESCRIPTION

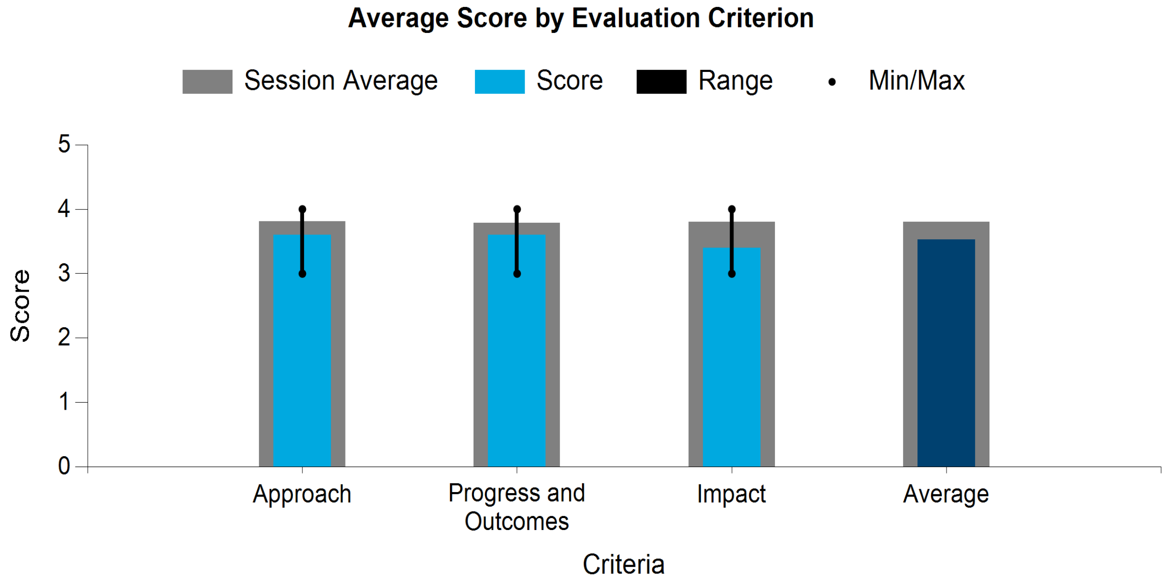
WBS:	3.5.1.204
Presenter(s):	Dave Dayton
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2024
Total Funding:	$2,945,831

The development of a cost-competitive technology for advanced biofuel is largely dependent on product yields. The key technical challenge associated with direct biomass liquefaction technologies is maximizing the carbon efficiency of the integrated process by optimizing the biomass thermochemical conversion step to simultaneously maximize biocrude intermediate yield and quality. Biocrude quality is often simply defined by the oxygen content of the liquid intermediate. Catalysts in the thermochemical conversion step are applied to enhance the deoxygenation of the pyrolysis vapors to produce a low-oxygen-content, thermally stable biocrude intermediate that can be effectively and efficiently upgraded into advanced hydrocarbon biofuels. Unfortunately, the oxygen content in biocrude is inversely proportional to yield in catalytic biomass pyrolysis, so, ideally, the catalyst should promote deoxygenation of the pyrolysis vapors while minimizing carbon loss to light gases, char, and coke.

RTI International has been developing a novel direct biomass liquefaction technology, referred to as reactive catalytic fast pyrolysis (RCFP), and incorporates atmospheric pressure hydrogen and an *in situ* catalyst provided by our partners at Haldor Topsoe. Hydrogen in the pyrolysis reactor improves biocrude yield by reducing char and coke formation and improves biocrude quality by eliminating reactive oxygenates. Catalyst screening in a lab-scale bubbling fluidized-bed reactor system was used to identify a suitable RCFP catalyst for enhanced hydrodeoxygenation (HDO) while optimizing process conditions (H_2 partial pressure, temperature, and space time) and improving carbon efficiency.

A focus of this project is to design, fabricate, and operate a reactor system that can continuously regenerate and reduce the RCFP catalyst to maintain steady-state HDO activity while meeting the hydrogen demand of the RCFP process. With this scaled-up system, enough low-oxygen-content RCFP biocrude can be produced to support extensive upgrading studies.

The outcome of the project is to improve the technical feasibility of the integrated RCFP/upgrading process by producing 100 gallons of a renewable blendstock that meets ASTM D975 specifications. The project goal is to scale up the RCFP technology and meet or exceed the carbon efficiencies measured in laboratory experiments. TEA, based on experimental results, will substantiate the economic viability of a fully integrated process design to produce a finished diesel blendstock that can sell for $3/GGE with 50% GHG emissions reduction potential through robust system optimization and integration.



COMMENTS

- Approach: The project approach aligns with metrics defined under Topic Area 4, DE-FOA-0002029.
    - Technical: Reactive fast pyrolysis in a fluidized-bed reactor with catalyst regeneration and recycling.
    - Project management: No specific slides, but it is listed on Slide 17 with roles. The presenter also verbally elaborated on their roles.

  Progress and outcomes:
    - Details of biomass to be used, catalyst to be used.
    - The lab-scale fluidized-bed reactor used for the study with smaller-scale particles and product collection is well described.
    - Design work and 3D image for proposed fluidized system, to be completed by a subcontractor.
    - A summary of the RCFP catalyst testing with all phase yields was presented; however, the expected/desired outcomes (based on preliminary TEA estimates for yields) and comparison with it are not clear.
    - The biocrude upgrading results show an increase in O_2 content (0.86% to 6% from 10 hours to 140 hours TOS) and a corresponding decrease in H_2 content? This is indicative of rapid deactivation; during the presentation, the PI confirmed this. What are the mitigation plans? if the catalyst does not meet the criterion for short durations, what is the reason to move to scaled-up work?
      The process hazard analysis is by a consultant, Saltegra Consulting.
- Impact:
    - The project has limited time left to fabricate and demonstrate a very challenging fluidized-bed reactor with various recycle streams. This requires pressure balancing and observing the catalyst attrition and loss/makeup. There are difficulties in regenerating and feeding the catalyst, along with

product recovery and characterization. Given the remaining time, approximately 1 year, meeting the target goals is at high risk. The presenter mentioned that they have requested an extension for the project and will not use project time during the waiting period for receiving the fluidized-bed reactor unit. Also, the results shown for the hydrotreating catalyst are not encouraging for scale-up.

- The goal is to design, fabricate, and operate an HDO reactor that processes kilograms per hour. The process will use multiple condensers and an electrostatic precipitator to purify the biocrude. The process will require a catalyst regeneration step as the catalyst cokes and is oxidized during decoking, thus requiring a subsequent reduction. The process has been previously verified.
- A process hazard analysis was conducted due to the use of hydrogen.
- Hydrotreating was included to ensure proper oxygen removal, resulting in a more stable biocrude.
- The catalyst was tested for multiple regeneration cycles with no loss in activity.
- It seems that there is still quite a bit of work to be done. There was no risk assessment, though it seems that some problems have arisen, and some may be on the horizon.
- On the surface, it seems like a bad idea to have hydrogen pass through an electrostatic precipitator. In this case, the fuel and ignition source are present. Only an oxygen source is required for an explosion.
- This project has been subjected to extensive independent engineering review and has met the goals and recommendations. It is in the throes of finishing up, with the goal of producing a 100-L product, and the team seems on their way. I would like to have seen what they consider to be the figure-of-merit values to justify proceeding to the next TRL. Every step does not need to be at max performance but enough so that justification for further effort is warranted. This is a good team, and there is good interplay among them. They did a hazard and operability study at the engineering scale, which is very good. Their aqueous phase recycling is a plus. It is a worthy thing for BETO to have a project that provides the information and technology to allow for drop-in refinery products. This avoids a lot of the issues with fuel compatibility.
- This project appears to have been accounting for the carbon balance in a way that does not smoothly lend itself to subsequently performing an LCA of the system. The carbon reported for char and coke includes the carbon that is burned off from the coke. This carbon is not accounted for in the gas emissions, and the “gas” is pyrolysis gas; however, the division of carbon between the fraction that will remain in the char and the fraction that is burned off will make a difference in the calculations of potential carbon sequestration in the produced char (from the components that do not combust and that remain fixed in this material). Although the project team is well positioned for industry engagement, the project team might benefit from involving academics with LCA expertise or LCA professional consultants in these tasks to accurately determine the fate of carbon and the overall life cycle GHG emissions of the produced fuel. The project is in its last budget period, and the carbon footprint of the generated biofuels will affect its commercialization potential.
- The reviewer is concerned about the ability of the PI to deliver on the multiple BETO projects they have with competing priorities, especially as they noted challenges with hiring post pandemic. It is clear that they would not be able to make 100 gallons by the end of the project, and they are probably looking at an extension.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for taking the time to evaluate our project and providing constructive suggestions for improvement as the project continues into its final phase. As pointed out by the reviewers, we have quite a bit of scope remaining in the project and not much time to complete it. As a result, we anticipate requesting a 12-month no-cost time extension to complete the biocrude production and upgrading that is planned. The fabrication of the scaled-up unit continues, and we expect to take delivery of the completed system in November 2023. We expect that installation and commissioning will be completed in spring 2024, followed by 12 months of operation. The experimental results will be used to update existing process models that are the basis for the TEA. An LCA is also part of the final project deliverables. In the interim, we continue to work with our catalyst development partner, Topsoe, to finalize the procedure for producing a catalyst in a spray-dried format that has similar performance (45% carbon efficiency in the C4+ products with less than 15 wt % oxygen in the biocrude product) compared to the extrudates that were used to achieve the technical targets for the intermediate verification. Additional small batches will be produced by Topsoe and tested in RTI's two-fluidized-bed reactor system, the same reactor that has been used for all process development to date. Large batches for testing in the new unit will be produced once the catalyst formulation and synthesis have been finalized. We do not anticipate any delays in meeting that deliverable. The operation of the scaled-up unit will be invaluable in advancing the state of the RCFP technology. Two key objectives remain to be investigated during the final phase of this project: (1) optimizing process conditions to maximize biocrude yield and (2) producing enough RCFP biocrude to perform long-term hydrotreating to improve upgrading performance. To maximize biocrude, there are two design features in the scaled-up unit that need to be tested during the process optimization. First, the catalyst addition rate needs to be determined and balanced with the bed removal rate in an attempt to maintain steady-state RCFP catalyst performance. Catalyst samples can be collected to determine the extent of regeneration (carbon content on catalyst) because the catalyst regeneration is decoupled from the RCFP process. Second, the impact of recycling the hydrogen-rich tail gas on biocrude yield needs to be verified. Preliminary RCFP biocrude hydrotreating and coprocessing has been very promising. Deactivation of the hydrotreating catalyst is evident, but increasing pressure drop and reactor plugging has not been observed. This provides an opportunity to conduct long-term (greater than 150-hours TOS) hydrotreating experiments to understand catalyst deactivation mechanisms and establish process conditions to maximize TOS. Hydrotreating process conditions have historically not been changed to facilitate comparison with previous studies; however, results from select biocrude upgrading studies have indicated that hydrotreating catalyst activity can be recovered by increasing temperature. Therefore, increasing the initial hydrotreating temperature is one strategy for maintaining longer-term catalyst activity. There is also room for investigating different catalysts, catalyst dilution ratios, and catalyst dilution strategies.

BIOCRUDE PRODUCTION AND UPGRADING TO RENEWABLE DIESEL

Research Triangle Institute

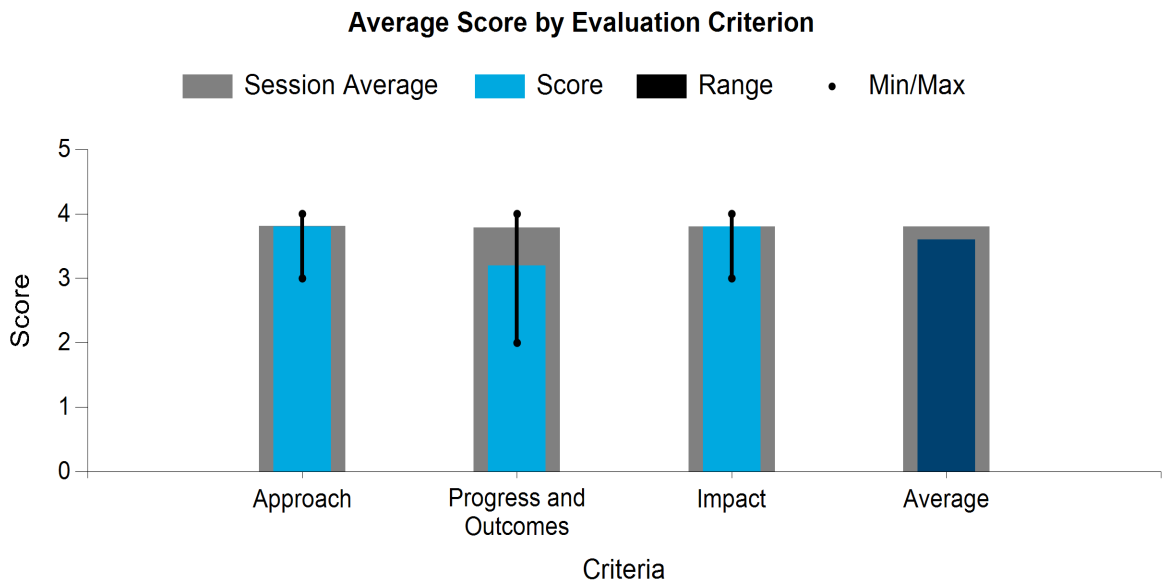
PROJECT DESCRIPTION

WBS:	3.5.1.301
Presenter(s):	Dave Dayton
Project Start Date:	10/01/2018
Planned Project End Date:	08/31/2023
Total Funding:	$3,192,405

A lot of activity in catalytic pyrolysis and hydroprocessing has occurred in the past 15–20 years with notable successes and failures; however, very little technical information is available in the open literature from continuous, integrated, pilot-scale studies. The next step along the technology commercialization pathway is to scale up the catalytic biomass pyrolysis process, integrate this technology with a hydroprocessing unit, and demonstrate the long-term operation and performance of the integrated process. RTI International is developing an advanced biofuels technology that integrates catalytic biomass pyrolysis and hydrotreating to produce hydrocarbon-based biofuels. Additional separation technology is being developed to recover valuable products from biocrude or fractionate biocrude prior to upgrading.

The goal of this project is to maximize the yield of biocrude from a catalytic biomass pyrolysis process and effectively and efficiently upgrade the biocrude intermediate into a renewable diesel blendstock. This goal is not unique; however, innovative approaches will be investigated to achieve the technical targets for an economically feasible, integrated, advanced biofuels process. The focus of the proposed project is to (1) optimize the physical and chemical characteristics of biomass feedstock, in a commercially viable manner, to maximize biocrude yields (independent of oxygen content) in catalytic biomass pyrolysis; and 2) improve biocrude upgrading efficiency by fractionating the liquid intermediate and independently hydroprocessing each fraction to maximize biofuel production.

The proposed project team builds on years of experience to seek innovative solutions that address technical challenges across the value chain—from feedstock preparation to biomass conversion, intermediate upgrading, and biofuel production. Idaho National Laboratory, in collaboration with Forest Concepts LLC, is evaluating physical property requirements for selected feedstocks to develop correlations that reduce the risk of feeding upsets in RTI's 1-TPD catalytic biomass pyrolysis unit. RTI and NREL collaborated on reactor modeling to optimize conversion process performance. RTI and Haldor Topsoe are developing a new strategy to upgrade biocrude that will minimize process severity while maximizing TOS. A systems approach will be taken to maximize the efficiency of biofuel production by fractionating biocrude, determining the most efficient way to process each fraction (hydrocracking or hydrotreating), or how best to recombine the fraction for ultimate biofuel production. Instead of trying to maximize deoxygenation during the catalytic biomass pyrolysis step, the goal is to optimize biocrude yields in the conversion step while managing downstream HDO by pretreating, fractionating, or coprocessing biocrude fractions to maximize biofuels carbon efficiency to improve the technical feasibility of renewable diesel production from cellulosic biomass. TEA, based on experimental results collected in the proposed project, will substantiate the economic viability of a fully integrated process design.



COMMENTS

- Approach: Technical—catalytic pyrolysis, with solvent extraction, aqueous phase recycling, and upgrading of various product intermediates via hydrotreating separately.
- There are two approaches for biocrude fractionation, solvent followed by water and vice versa, with the second approach showing less use of the solvent. Hydrotreating of various streams is analyzed separately.
- Progress and outcomes:
    - Four different sizes/biomass are tested to produce a total of close to 100 gallons of biocrude.
    - Biocrude, solvent extract and raffinate are well characterized, with up to 10%–15% unknowns.
    - The makeup solvent rate is not stated in the presentation. This could have a major impact on the overall cost. The reviewers request this information with run time data using actual feedstocks and loss rates.
    - Aqueous phase recycling is claimed to show major improvement in terms of reduction in the use of the water requirement, which is a significant achievement; however, for this stream level of impurities recycled, it has not been measured, verified, or addressed.
    - Three product intermediates are hydrotreated separately; it is a good approach to understand the impact on catalyst stability and identify the source. The results indicate that the hydrotreating catalyst is not stable for all three streams, and the lack of feed required to achieve steady state has been shown as the reason for the incomplete work.
    - The TEA case is well documented, with sensitivity analyses for two cases, where in one case aqueous organics are rejected with wastewater.
- Impact:

   - If successful (the project is in its last extended budget period), the project claims a reactor-ready feedstock and has well-defined approaches for product separations and impact on economics. If successful, the project can make a significant impact and aligns with various DOE programs.
   - What is not clear is the impact of intermediate quality on the hydrotreating catalyst. This has been the case for many years and a stumbling block for most fast pyrolysis technologies. What deactivation rates were observed, and how different are these from past data? The remaining time in the program and ability to generate enough quantities of intermediates required to do reasonable hydrotreating studies for various streams, as well as to come up with an overall commercial embodiment, and hence effective TEA to meet cost goals is quite limited. Overall, the project lacks the level of performance expected in last budget period.

- The project will produce upgraded biocrude from biomass using catalytic pyrolysis. Biomass of different sizes were investigated.
- The project compared the order of separations that use toluene or water as a solvent and found that the water separation should occur first. They have found significant catalyst deactivation issues that they are still trying to figure out.
- A TEA was carried out that found a fuel selling price of $3.33 and identified the most important factors that affect the price.
- The project has progressed, but the catalyst deactivation issues are an issue. The team has not yet produced the required amount of fuel, but they will have an extension to do so.
- This project has received considerable attention and analyses by the independent engineer. The comments from the previous review were direct, and some were not complimentary. The project team worked to address some of them, but they spent more time addressing the original goals of the project. Those goals were largely achieved, although some remain to be completed. The project progression is achieving TRL 6. The potential to go to higher TRLs is possible, and the sensitivity analyses were the right step in possibly going forward. Perhaps other industry partners will be needed to further this work. I am not sure if the project has defined the performance metrics it needs to complete the validation of the work.
- This project investigates and tests a pathway for biocrude production and upgrading to renewable diesel. A strength of this project is its analysis of the ability to recycle the aqueous coproduct so that water use and subsequent wastewater treatment needs can be reduced. The results of the hydrotreatment experiments also provide critical data to ultimately calculate the carbon footprint of the renewable diesel through this production process. With the data already collected by the project, an LCA could be performed in addition to the TEA that has been continuously developed during this project. It is part of the remaining tasks within the scope of the project, but the research would benefit from LCAs being performed at various stages to identify opportunities for improvement as the design develops. The project has received an extension.
- The yield is lower than expected. The characterization of the finished renewable diesel (cloud point/wax content/density, etc.) is required. The use of agricultural residue will result in a higher renewable identification number (RIN) value. Light cycle oils should be considered for use as a solvent. I am unsure if they will make 100 gallons by the end of the project. Likely a no-cost extension would be required.

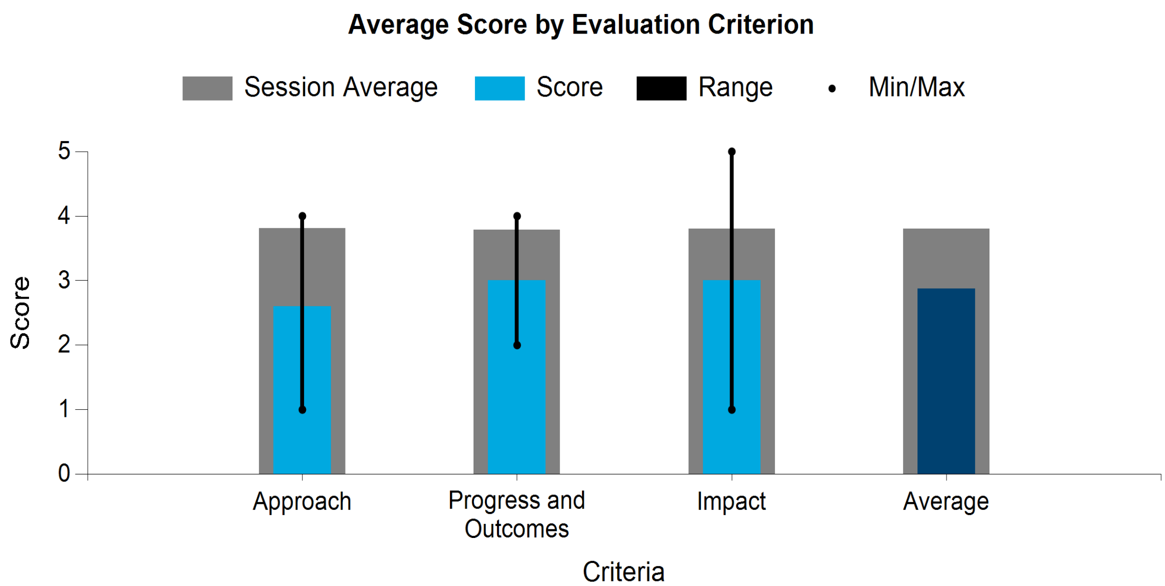
PI RESPONSE TO REVIEWER COMMENTS

- We would like to thank the reviewers for taking the time to evaluate our project and providing constructive suggestions for improvement as the project continues into its final phase. We would like to acknowledge the technical and contractual challenges encountered during this project. Lower-than-expected biocrude yields continue to be a dilemma that needs to be understood, and plugging hydrotreating reactors during biocrude upgrading is still quite common, though progress is being made to correlate the feed composition to hydrotreating performance. In addition, initial and intermediate verifications during the project took longer than planned, leading to significant delays in the technical work plan. Superimposed with the departure of key personnel and extensive pilot plant maintenance that has been required, we have requested a no-cost extension to complete the remaining scope of work. During the past 15 years, we have been conducting laboratory and pilot-scale R&D to advance the state of catalytic biomass pyrolysis technology to produce biofuels and bioproducts. The focus of these efforts has been to improve the CFP biocrude yield and the upgrading process at the pilot scale to demonstrate the techno-economic potential of an integrated biomass pyrolysis/hydrotreating pathway for renewable diesel production. This study builds on past projects that led to the design, fabrication, installation, and operation of pilot-scale unit operations for (1) CFP in a 1-TPD unit, (2) biocrude upgrading in a hydroprocessing reactor system, and (3) biocrude separation strategies to support bioproducts recovery and improved upgrading performance. The main objectives in this project address the key technical challenges associated with biomass conversion and separation and upgrading of intermediates. Preparing and feeding biomass has been a challenge for successfully scaling up and demonstrating thermochemical conversion technologies. One objective of this project is to evaluate the impact of feedstock preparation on cost and catalytic pyrolysis performance, particularly biocrude yields. Our partners at Forest Concepts are doing a detailed economic assessment of their technology for biomass preparation (drying and size reduction) as a function of particle size. We are then processing that feedstock in our 1-TPD catalytic biomass pyrolysis unit to evaluate the effect of particle size and feedstock type on biocrude yield and chemical composition. Recognizing that the absolute results may be reactor- or scale-specific, we expect the correlations to be relevant at a larger scale. In this final phase of the project, we will repeat the 1-mm and 2-mm Douglas fir CFP experiments for comparison to 1-mm and 2-mm alder CFP. Ten additional forest residual feedstocks will also be processed in the 1-TPD biomass unit. We will continue to explore optimized process conditions to maximize biocrude yields. Aqueous phase recycling not only reduces freshwater consumption (by 80%) in the process but also recycles organics back into the process, providing an opportunity to increase carbon efficiency. Continued sampling and analysis of the recycled aqueous stream will be used to follow the accumulation of specific biocrude components and help identify any impurities (alkali salts or nitrogen and sulfur-containing species) that may cause catalyst deactivation in downstream upgrading processes. The biocrude produced from the remaining biomass feedstock will subsequently be upgraded to renewable diesel. We have been exploring biocrude fractionation as a strategy to improve upgrading efficiency. Selected separation techniques are being used to segregate biocrude into fractions that are more easily upgraded and fractions that contain known components that cause fouling and plugging in the hydrotreating reactor. Fractionating the biocrude also puts less emphasis on HDO during CFP while putting a greater focus on increasing biocrude yield. In the final phase of this project, the second separations strategy (water washing followed by solvent extraction) will be demonstrated at the 7-gallon-batch laboratory scale to determine the relative separations efficiency, solvent use, and solvent recovery compared to the first strategy, where solvent extraction was followed by water washing. All hydrotreating products will be distilled to recover the renewable diesel fraction and characterized to determine if the fuel properties meet the ASTM D975 standard. The existing process model of the integrated catalytic biomass pyrolysis (CFP)/biocrude hydrotreating process will be updated with the experimental results collected during the final phase of this project. This model will form the basis of the final TEA for the integrated process to document the impact of the feedstock preparation on biocrude yield and quality as separations are used to achieve commercially relevant upgrading to biofuel. An LCA of the CFP/hydrotreating pathway will also be completed using the pilot-scale experimental results to evaluate the carbon intensity of the pathway for scenarios using the different feedstocks.

AGRICULTURAL AND WOODY BIOMASS TO DIESEL FUEL WITH FT INTERMEDIATE

West Biofuels LLC

WBS:	3.5.1.304
Presenter(s):	Matthew Summers
Project Start Date:	10/01/2018
Planned Project End Date:	12/31/2024
Total Funding:	$2,933,000



COMMENTS

- Approach: The project approach aligns with the metrics defined under Topic Area 2, DE-FOA-0001926.
  - Drop-in renewable diesel/jet fuel with >50% biogenic material, large-scale unit operations with commercial feedstock, mass/energy balance, TEA work, and minimum of 100 gallons final product. TEA/LCA with breakeven point; 1-dry TPD feedstock.
  - Gasification units, two Fischer-Tropsch units (slurry and fixed bed), and a combined Fischer-Tropsch wax, VGO upgrading at three different organizations.
  - Project management: Focus toward construction, commissioning, product transfer, and trials alignment.
- Progress and outcomes:
  - Gasification units commissioned and overhauled.
  - Fischer-Tropsch units commissioned but have not yet been tested.

- Fischer-Tropsch wax (product was obtained from other research groups/industry) and VGO upgrading/distillation. Product specification compared with ASTM requirements.
- 20%–40% coprocessed Fischer-Tropsch wax at the lab and pilot scale.
- The project is conducting similar work at two locations to better understand the type of gasifier, Fischer-Tropsch, and coprocessing results; however, it seems to be repeating a lot of work that has been conducted in this area (funded by DOE NETL/BETO) offices on past projects. The goals of the project in terms of the desired Fischer-Tropsch product distribution were not clear from this presentation. Is the goal to increase Fischer-Tropsch diesel cut or heavily rely on upgrading Fischer-Tropsch wax?

- Impact:
  - If successful (the project started in April 2021 and has completed two budget periods), the project will allow distributed intermediate product generation to be blended with existing refineries. The project is run at a scale that is representative for quality checks to meet the statistical requirements for blending/risk reduction. Fischer-Tropsch reactors are highly impacted by syngas quality; both chosen gasifiers show varying H_2/CO ratios and CO_2 concentration. Fischer-Tropsch data provided on Slide 7 show >50%–60 wt % wax (if that is the desired Fischer-Tropsch product distribution), and hence the project highly depends on wax recovery and upgrade. The work on the Fischer-Tropsch wax upgrade has not yet started. The project can highly benefit from past data and work in the choice of the Fischer-Tropsch reactor.

- The goal of this project is to produce diesel fuel using Fischer-Tropsch technology. The Fischer-Tropsch process is being carried out by West Biofuels using a fixed-bed catalyst as well as Best using a slurry bed reactor.

- The project has produced wax that can be used in a fluidized catalytic cracker resulting in acceptable fuel properties. A gasifier has been commissioned in Austria for Best, while West already has a gasifier on-site.

- There is no economic analysis that is important for this project. Fischer-Tropsch is a mature technology that has not had much, if any, sustained commercial success. The presentation did not include anything about the process that makes one believe that this one will be different. It certainly works, but it is not clear that it is cost-effective to do this.

- The project is on track to meet objectives. It is clear that this project addresses BETO’s strategies to produce drop-in fuels. There are some novel approaches with VGO and Fischer-Tropsch technology. These kinds of projects bolster the opportunities to look at the thermochemical processing of biomass for the production of oil refinery-type fuels. The project has a good risk analysis and mitigation strategies. The project needs to take a closer look at interface risks because that is always a hurdle to successful integration. This is a good team. Their long-term goal is to design and build their own operations, and they have a long way to go, but they are on track. They need to continue to assess local permitting and environmental issues to ensure they do not run into any snags that will delay their progress. Anticipate the worst, hope for the best.

- The project is investigating and developing a renewable diesel fuel production pathway through gasification, Fischer-Tropsch, coprocessing of the produced wax with VGO via FCC, and separation of produced diesel from other products, which could also be hydrotreated to generate diesel fuel. The project was originally funded in 2021, but it was affected by the pandemic; still, the initial verification has been completed, and industry involvement is well developed. The project team aims to quantify the biogenic versus fossil carbon flows through the system, which is necessary to identify the extent to which the produced diesel can be considered a renewable fuel due to the added fossil carbon inputs during FCC. This analysis would benefit from being extended into a full LCA to quantify the life cycle GHG emissions of the fuel, including emissions associated with its processing energy needs, VGO production, and hydrogen inputs, among other components. It is unknown whether this process generates a lower-carbon footprint diesel than conventional diesel without this analysis. This may also enable optimization toward lower GHG emissions as the project is analyzing the effects of different ratios of wax to VGO experimentally.

- The work is focused on replicating work done in Austria with feedstock from the United States and in the United States; however, no technical updates or modifications to the Austrian work appear to be planned. So, it is questionable if they are just replicating previous work done elsewhere and just reporting those results. The reviewer struggles to see the novelty of the approach or value of replicating work done elsewhere.

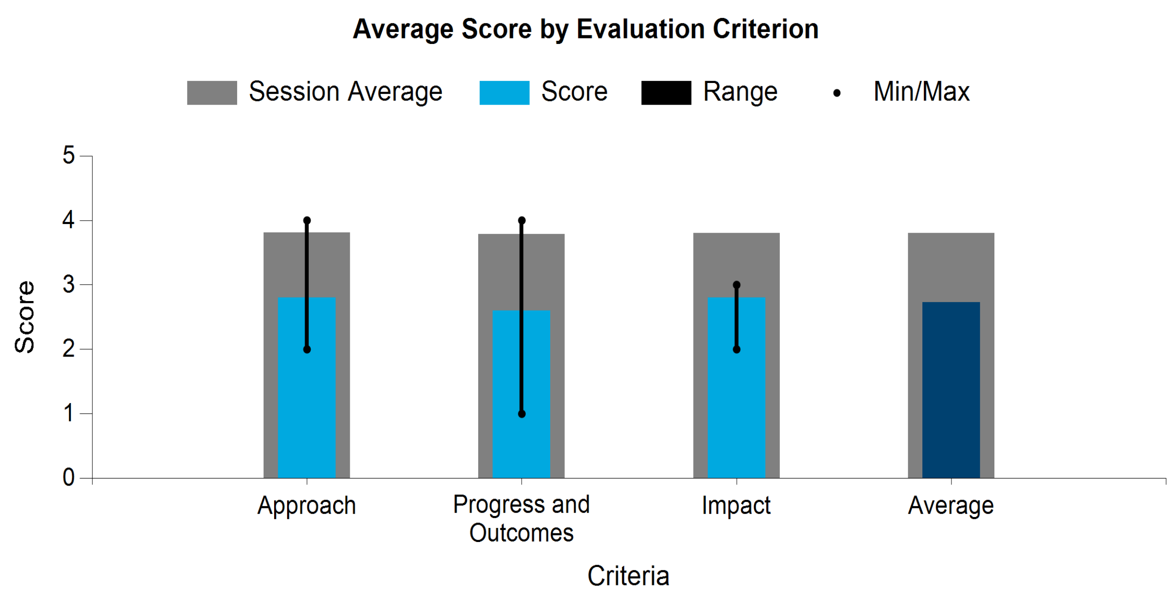
NOVEL METHOD FOR BIOMASS CONVERSION TO RENEWABLE JET FUEL BLEND

Technology Holding LLC

PROJECT DESCRIPTION

The overall objective of the proposed innovation is to demonstrate the techno-economic feasibility of an integrated process to produce drop-in jet fuel blend and isoprene as a coproduct from biomass hydrolysate such that private funding can be obtained after the initial governmental funded period. The technology will be matured from TRL 3 to TRL 4.

WBS:	3.5.1.401
Presenter(s):	Mukund Karanjikar
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2023
Total Funding:	$3,125,000



COMMENTS

- Approach: The project approach aligns with metrics defined under AOI-1 DE-FOA-0001926 in terms of gallons of product, selectivity toward cycloalkanes, improvement of required properties, and lower aromatic content. It is not clear if the level of GHG reduction has been met or included thus far in the project. The technical approach is to showcase a catalytic reaction to produce a cycloalkane/isoalkane mixture as a substitute for jet fuel without blending requirements. The project builds on past work for isoprene production via fermentation.

- Progress and outcomes: The verification stage and several other tasks have been successfully completed with up to 4 liters of dimethyl cyclooctanes (DMCO) production. The blends were tested with two HEFA and Jet A, showcasing meeting property requirements. The current focus is on pilot plant design. The team has made significant progress on all aspects. Some key questions that remain are TEA and justification for converting isoprene (a high-value/low-volume chemical) to SAF. Differences in the rate of productivity via fermentation (and hence scales) followed by Zeigler Natta-type chemistry.

- Impact: The project demonstrates (1) a shift toward cycloalkanes/isoalkane product with low or no aromatic content; (2) a unique approach using isoprene as an intermediate precursor; and (3) most importantly, showcasing that the property metrics requirement has been met at a greater detail.
- Questions: What is the rate of reaction for fermentation? What are the comparative sizes for fermentation versus catalysis? Was a model compound used for the catalysis reaction thus far and/or for pilot studies? What is the cost of the production of isoprene?
- The overall process consists of a fermentation to make isoprene, then isoprene is converted to cyclic alkanes using a catalyst. The fuel has been blended to make jet fuel, but it has the properties to be a stand-alone drop-in fuel. There was no discussion of the team (though it may just be Technology Holdings), and the discussion of risks are not specific enough, i.e., first-of-a-kind capital plant, to understand the technological advancement of the project.
- Most tasks have been accomplished with a pilot plant to be designed. The very different timescales for the fermentation and the catalytic process were not addressed. The catalytic process uses a homogeneous catalyst, but that was not described to know if it can be recovered. The production of impurities in the fermentation was not addressed. The idea that only the isoprene would leave the fermentation as a vapor does not seem reasonable.
- This is an interesting and novel route to cycloalkanes. Several important issues were not covered in the presentation, making it difficult to know what impact this process will have and the likelihood it will be possible as a fully integrated system.
- The project has achieved a measurable proof of concept. The results are noteworthy. There remains a long path ahead for fuel certification and the demonstration of an integrated system ready for piloting. The project should focus on how to put the pieces together with risk factors not on the global level but on the engineering-scale level. The potential of this approach is good for BETO's strategic goals; however, the presenter mostly spoke of future potential. The presentation would have been more meaningful if it had included some details of the process and how they were being conducted. I found this to be a major weakness of the presentation.
- This project focuses on assessing the feasibility of a processing pathway including fermentation that selects for isoprene and conversion of the isoprene to a jet fuel blend with DMCO. The project, which began in October 2018 and ended in March 2023, has met its goals of blend tests and partial fuel characterization, but not full characterization to assess the potential of the blend to meet ASTM standards, its fuel production goal of 10 gallons (although it has produced 4 liters of DMCO and started pilot plant design), LCA of the environmental impacts, or TEA. Without these data, it is unclear whether the project has commercialization potential despite the project team being in discussions with industry and the U.S. Department of Defense about the pathway.
- This project is addressing an unmet need in the space. The project is still not approved and needs to go through the ASTM approval process. The bigger challenge is the production of isoprene itself, with challenges in anaerobic fermentation. The project TRL is still partially unmet with FOA goals.

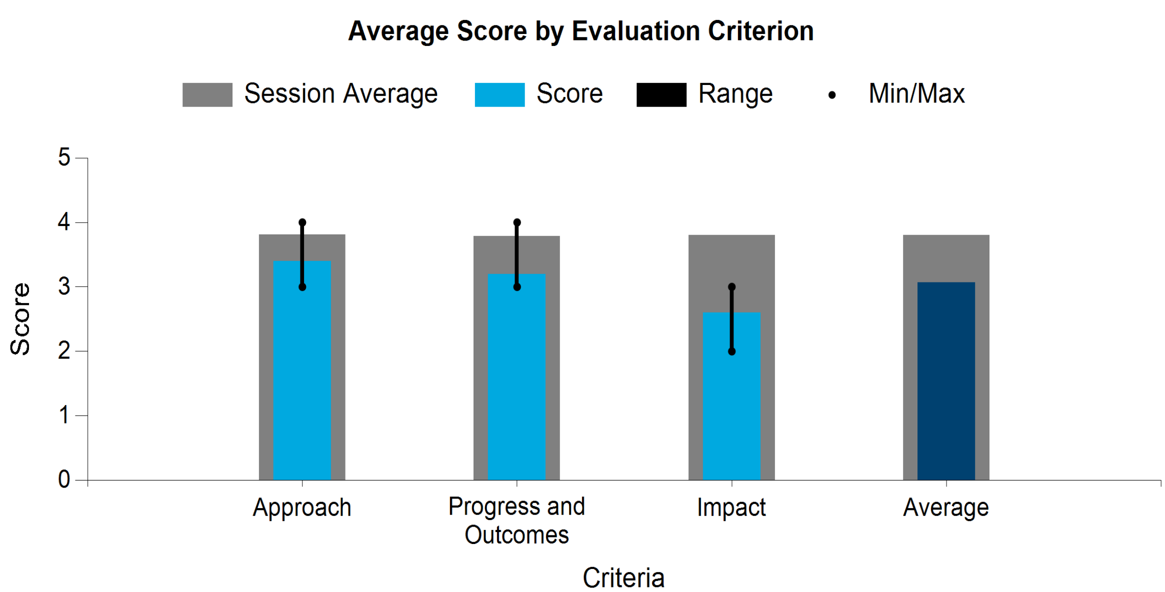
HYBRID HEFA-HDCJ PROCESS FOR THE PRODUCTION OF JET FUEL BLENDSTOCKS

Washington State University

PROJECT DESCRIPTION

WBS:	3.5.1.402
Presenter(s):	Manuel Garcia-Perez
Project Start Date:	10/01/2018
Planned Project End Date:	09/30/2023
Total Funding:	$3,472,904

The production of HEFA is the best current option for jet fuel production. HDO of bio-oils derived from pyrolysis and HTL of lignocellulosic materials produces jet fuel rich in aromatics, also known as hydrotreated depolymerized cellulosic jet (HDCJ). Relevance: Although HEFA is the most promising technology for jet fuel production, the construction of new units is limited by the availability of triglycerides. Pyrolysis and HTL bio-oils produced today are not accepted in any existing industrial facilities for further refining. Coprocessing triglycerides (yellow greases) with the phenolic-rich fraction of pyrolysis oils could help to increase feedstock availability for HEFA plants and create a path for bio-oil refining. Challenges: Our goal is to evaluate the technical and economic feasibility of using HEFA facilities to coprocess pyrolysis or HTL oils with yellow greases. Currently, our main challenge is to steadily operate the 400-mL continuous hydrotreatment reactor to produce larger quantities of jet fuel for tier beta and alpha tests. Accomplishments: We completed the oils collection, characterization, and emulsion stability studies. We have identified suitable conditions for coprocessing in a batch (250-mL) reactor and in a continuous 40-mL reactor. The fuel properties of the different cuts have been studied. The information collected is being used to conduct mass and energy balances and TEA and LCA of the hybrid HEFA-HDCJ technology. We are designing and evaluating a supply chain for the hybrid HEFA-HDCJ concept for the conditions of the state of Washington.



COMMENTS

- Approach: The project approach aligns with the metrics defined under AOI-1 DE-FOA-0001926 in terms of gallons of product, choice of feedstock, and scalability potential (merging with an existing process).

The technical approach is to increase the availability of feedstocks required for the HEFA process, which is currently limited by using yellow grease. The team has worked in tandem and showcased a large volume/amount of processing at each step. A major technical barrier was and still is coke formation and reactor clogging.

- Progress and outcomes: The verification stage and several other tasks at the laboratory scale—including product collection, product characterization, TEA, and LCA—have been successfully completed, with a long list of publications. The group has openly shared knowledge and made significant progress. TEA/LCA data are constantly updated. Only an area of concern is the limited product generation, and, as such, the project did not meet the FOA goal of a minimum 100 gallons of product and is less likely to achieve it in the remaining time. Higher hydrogen pressure with commercial catalysts that have a highly prescriptive catalyst presulfidation process might help reduce the coke and increase the life/TOS between regenerations. The main technical hurdle is the thermal coking of the pyrolysis oils prior to the catalyst bed or upper zones of the reactor bed.

- Impact: If the claims are realized, the project will demonstrate (1) an approach to reduce risk by combining hydrothermal and pyrolysis technology to advance the scalability of the HEFA process, (2) verification of the miscibility and product mix to generate feed for cohydrotreatment, and (3) reduction of experiments via TEA/LCA and lab results are well documented and help other technologists. Recommendation: The project can make a significant impact if more time/funds become available to do cohydrotreating work with industrial catalyst participation. Coke reduction for mixed-feed hydrotreating is at a more advanced stage than showcased here.

- The project cotreats bio-oils from liquefaction or pyrolysis with yellow greases. The management of the project with all task leads and progress in each task are presented very nicely. A major issue is coking of the catalyst, to be described next. It might be good to have a partner that can help with this issue.

- Coking in the scaled-up unit is a major issue that will require major reengineering of the process to avoid. The coking causes plugging of the system and shutdown, limiting the amount of continuous operation.

- Most tasks are not yet completed. The TEA and LCA are 90% complete, but they were not presented. Given the problems with plugging, the TEA or a modified TEA for a redesign could help determine whether to continue down this path.

- It seems that the plugging issues due to coking are severe issues that require much more time than is available to address. The results have been published in several papers, so much of the work is clearly important despite this major issue.

- This is a promising technology that has been evaluated in actuality at TRL 4–5. The encountered problems limited the team’s ability to meet the performance goals; however, these are not insurmountable, and the team is working to address them. They are using the right tools to assess the performance needs, but they probably need more time to scope all the potential risks. The team has made a good number of academic analyses that helped the project, and they made an honest assessment of the project’s progress; however, this process seems a long way from the finish line, and there is still a lot to prove that it has commercial potential. They have done a reasonably good job of assessing the feedstock sources. They may want to look to the Port of Umatilla, which was involved in gathering and collecting yellow-type greases for processing a few years back, to see if they have any avenues that would serve as suppliers for a process like this one.

- The project involves the development of a hybrid coprocessing pathway for pyrolysis oils and HTL oils with yellow greases to ultimately generate jet fuel. The project team has worked on supply chain analysis, LCA, and TEA in addition to performing bench-scale studies of cohydrotreatment of the oil and grease feedstocks. They have been able to test at small scales, but continuous coprocessing has faced issues at the lab and bench scales. Because the project is in its last year, the team shared that the original target of 100 gallons of jet fuel will not be reached. Additionally, there are biomass feedstock and yellow grease supply difficulties in the region (northwest United States), with a high likelihood of limiting commercialization potential. The lab-scale and bench-scale studies and modeling studies have provided some useful results that may assist in identifying future R&D directions; even the challenges experienced may inform new approaches that can overcome them in the future. As it stands however,, there is a relatively low likelihood of significant impact and commercialization potential, and new risk management strategies may need to be employed in any further study of this pathway.

- Challenges with coke formation and catalyst fouling continue to present barriers. The team has successfully demonstrated less than 1% coke formation.

PI RESPONSE TO REVIEWER COMMENTS

- The PIs thank the reviewers for the very constructive comments. Our main challenge today is to overcome the coke formation issues that are limiting our capacity to continuously operate our HDO unit. We were able to operate our 40-mL continuous unit for 255 hours in coprocessing (340 hours total run); however, when scaling to 400 mL, plugging happened at 26 hours of coprocessing (125 hours total run). Although we need more time to overcome these issues, we do not agree with Reviewer 2 regarding the low likelihood of a significant impact and commercialization potential. The encountered plugging issue is mainly due to the poor coke tolerance of trickle bed reactors and the fact that we cannot use very active precious metal hydrogenation catalysts due to the presence of sulfur in the feedstock. The coke levels achieved are low and tolerable by other reactors. In our opinion, the issue can be solved with the use a different type of reactor for the stabilization step (e.g., a slurry reactor) and by conducting a deeper stabilization of the oil before cohydrotreatment (perhaps using esterification strategies with alcohols, which are well described in the literature).

DROP-IN RENEWABLE JET FUEL FROM BROWN GREASE VIA THE BIOFUELS ISOCONVERSION PROCESS

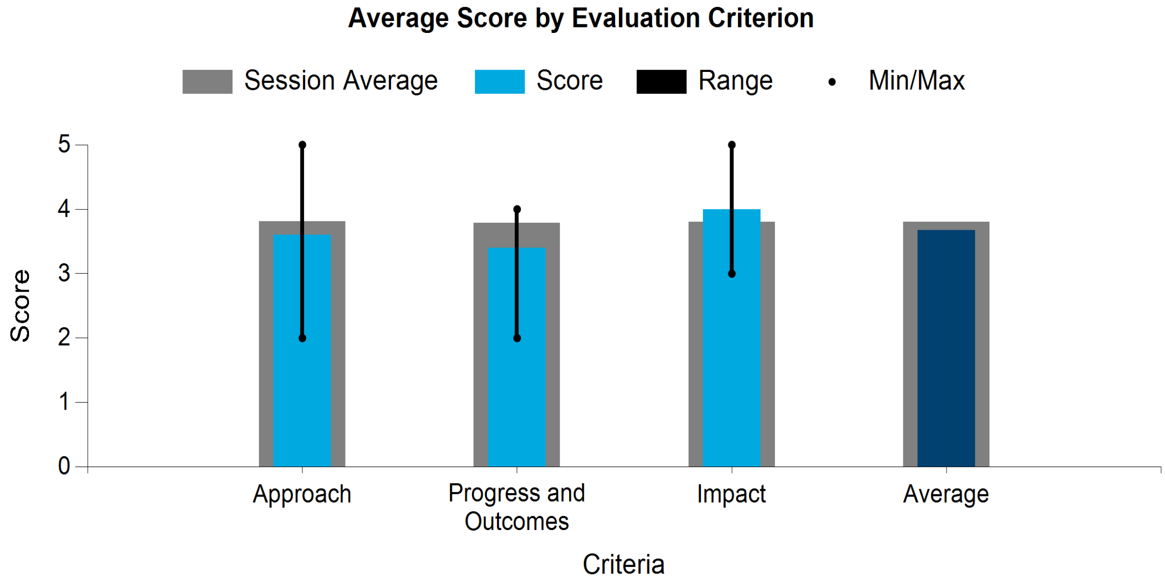
Applied Research Associates

PROJECT DESCRIPTION

WBS:	3.5.1.404
Presenter(s):	Jeff Rine
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2023
Total Funding:	$2,951,431

The Biofuels ISOCONVERSION process is a patented technology for converting lipids into naphtha, jet, and diesel fuels. The Biofuels ISOCONVERSION process consists of a hydrothermal cleanup (HCU) operation; a conversion operation, called catalytic hydrothermolysis; hydrotreating; and distillation into jet and diesel fuels. Catalytic hydrothermolysis jet (CHJ) from the Biofuels ISOCONVERSION process is an approved pathway under ASTM D7566 Annex 6 to produce commercial jet fuel. Brown grease is an acceptable feedstock for the Biofuels ISOCONVERSION process under Annex 6 and was the target feedstock for this DOE project. CHJ is a candidate for use as an unblended, 100% SAF because its chemical and physical properties are nearly identical to jet fuel derived from petroleum. Valuable coproducts from the Biofuels ISOCONVERSION process include diesel fuel that meets the ASTM D975 specification and naphtha that can be used as a gasoline or an E-85 blending component.

A goal of this DOE project is to demonstrate a “mature price goal” of less than $3/GGE. A key to meeting this goal is to demonstrate that the Biofuels ISOCONVERSION process can use highly contaminated, low-cost feedstocks, such as brown grease, to make jet fuel. Historically, brown grease costs approximately $0.10/lb ($0.75/gal), which is a small fraction of the cost of edible plant oils, such as soybean or canola oil. The Applied Research Associates (ARA) HCU process (U.S. Patent #10,071,322) removes metals, soaps, phospholipids, and other contaminants, producing a clean lipid feedstock for conversion into jet fuel via the Biofuels ISOCONVERSION process or other approved conversion processes. Pilot-scale testing during this project demonstrated that the HCU process reduces metals and phosphorus in highly contaminated brown grease to less than 5 ppm in a single step. Because HCU is a single-step, hydrothermal process that does not rely on conventional degumming and clay bleaching processes, solid wastes are eliminated, and the yield of clean oil is greater than 99%. Work performed during this project optimized HCU operating parameters to successfully reduce contaminants in brown grease. Brown grease cleanup and conversion was demonstrated in pilot systems with throughput capacities up to 3 barrels/day. Approximately 600 gallons of renewable crude from brown grease was produced for hydrotreating and distillation into 100 gallons of jet fuel meeting ASTM D7566 Annex 6. Initial pilot distillation of the hydrotreated product into CHJ demonstrated that all key specification requirements were met. Larger pilot distillation operations are underway, with an estimated completion date during FY 2023 Q2. Preliminary engineering is also underway for a commercial-scale facility capable of using brown grease as a feedstock to produce liquid fuels at less than $3/GGE. An estimated completion date for preliminary engineering is also FY 2023 Q2. The Biofuels ISOCONVERSION process is currently at TRL 7 for clean feedstocks. This project will increase the TRL for the HCU of brown grease from TRL 4 to TRL 7.



COMMENTS

- Approach: The project approach aligns with the metrics defined under AOI-1 DE-FOA-0001926 in terms of gallons of product, choice of feedstock, scalability, and hence cost. It is not clear if the level of GHG reduction has been met or is included thus far in the project.

- The technical approach is to showcase the removal of metals/impurities from brown grease and upgrade it to a blendstock for hydrotreating and distillation. The team has worked in tandem and has showcased a large volume/amount of processing at each step.

- Progress and outcomes: The verification stage and several other tasks have been successfully completed, with >400 gallons of intermediates. The hydrotreated crude and distillates were compared with jet fuel and diesel fuels, showcasing major agreement with desired properties. The current focus is on distillation and TEA. The team has made significant progress on all aspects; the ASTM 7566 Annex 6 criteria have been met. For the supercritical reaction step hazard and operability analysis, the team is working with a licensee. The project has one limitation of collecting the required amount of untreated brown grease. The team has made great technical progress. The water/gallon fuel used or recycled is to be confirmed. The project has been extended to Sept. 30, 2023.

- Impact: If the claims are realized, the project will demonstrate (1) a shift toward a new waste feedstock; (2) a unique approach using mixed feedstock with variability (a key risk of collection and homogenization); and (3) most importantly, showcasing that the property metrics requirement is met in greater detail for jet and diesel fuel. The next step to review the TEA results. The HCU and Biofuels ISOCONVERSION integrated process have already shown commercial traction. The low feedstock cost is advantageous. This project has clearly demonstrated the use of an underused feedstock to a fuel with great agreement with required properties. The work has been conducted at the pilot scale with good reproducibility. The project shows excellent process.

- The process uses HCU to clean brown grease, then catalytic thermolysis to make syncrude, which can be treated in a conventional hydrotreater and distillation column. The team comprises ARA, and they are using a tested method that they have developed. They have addressed a major risk involving the addition of lime to brown grease, which causes serious problems for their process. The Southwest Research Institute performed their hydrotreating and distillation.

- They have performed many milestones, with the TEA left. Their process is definitely possible using properly treated brown grease as a feedstock.
- Water is used in multiple steps in their process with little to no discussion of how much is lost in the different steps. The cost of generating supercritical water is expected to be quite large, yet there was no discussion of how much water was needed in the catalytic hydrothermolysis reactor. The cost of brown grease is going to change once it is used to create a fuel. This should be considered in the TEA report.
- The brown grease resource has needed a more thorough look to assess its potential. This project seems to be able to show that. The clean HCU product needs to meet the performance requirements, and it seems to have done that. The issue in all FOG systems is the efficient and cost-effective collection of the feedstock. Normally, people are glad to give it away, but if the value can be imputed to the product of processing, the suppliers may demand a cost for supplying the brown grease. It is not clear how they managed the waste streams.
- This project has very good potential to be demonstrated at a larger scale. There has always been potential in brown greases, and this project may be the right route to meeting that potential.
- The project is developing a Biofuels ISOCONVERSION (trademarked) process for drop-in renewable jet fuel production from brown grease, which is a low-cost wet waste feedstock generated from a variety of sources. With the high volumes of brown grease generated in the United States, there is potential for this process to convert a waste into a higher-value fuel product. Currently, however, collectors treat the brown grease with lime, which affects the conversion and "cleanup" processes by scaling the reactor. The project team is advised to test the solids generated in the reactor because previous studies of the HTL of calcium-rich feedstocks have generated hydroxyapatite (another higher-value product) along with a biocrude oil. Although these solids currently serve as an impediment to scale-up and commercialization in terms of their effects on the current reactors, they may provide additional economic benefits from the conversion process at the commercial scale if they are confirmed to be a high-value product like hydroxyapatite; however, the process still faces a challenge with the high volumes of oil-contaminated wastewater that would require treatment after separation. The wastewater has not been characterized, and the effects of changing the water-to-grease ratio have not been studied. The possible trade-offs in costs and environmental impacts from process to process along the life cycle of this fuel production pathway indicate the need for an LCA and TEA to better project the potential of this pathway. Despite this, industry partners are planning and constructing unit processes from the Biofuels ISOCONVERSION system. This 5-year project ended in March 2023, having met multiple goals but not the goal of producing 100 gallons of jet fuel through this process.
- The availability of brown grease is approximately 1.5 MM MT. Also, the supply chain is not segregated. The presence of calcium and other polymers will affect the reactor. D3 RIN credits for the diesel fraction should be explored.

HIGHER-ENERGY-CONTENT JET BLENDING COMPONENTS DERIVED FROM ETHANOL

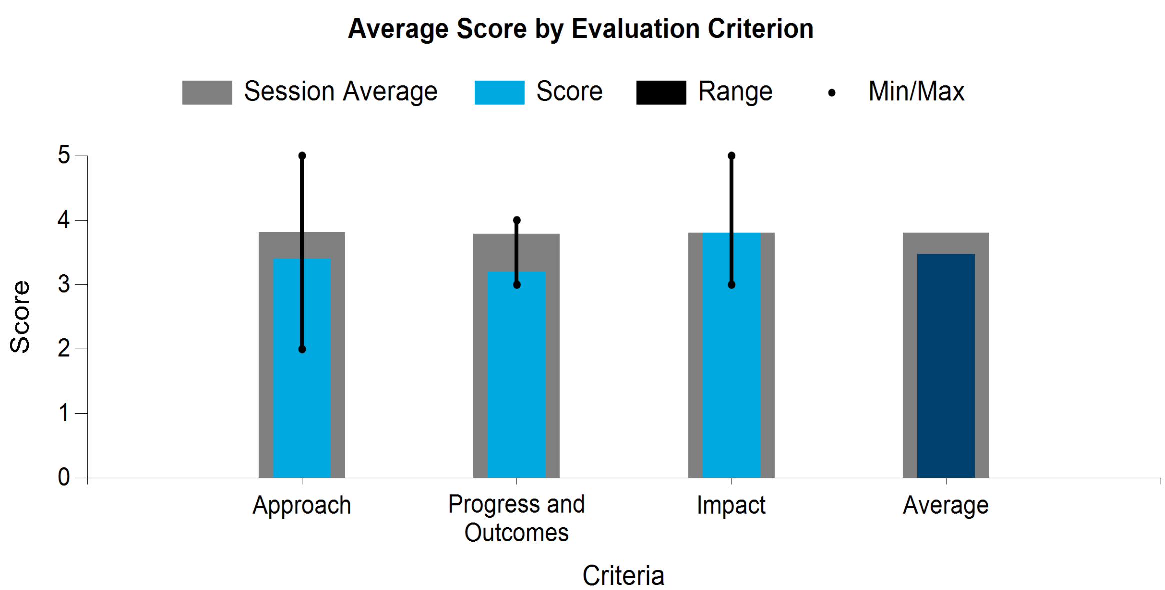
Purdue University

PROJECT DESCRIPTION

WBS:	3.5.1.408
Presenter(s):	Gozdem Kilaz
Project Start Date:	10/01/2019
Planned Project End Date:	07/31/2024
Total Funding:	$2,217,768

BETO's efforts in generating SAF have helped establish the production of isoparaffinic synthetic jet fuels with favorable properties, such as high energy density, excellent thermal stability, and favorable cold-flow performance. Combined with isoparaffins, cycloalkanes carry the potential of further fuel performance improvement with at least a 4% net increase in energy content. PNNL has already demonstrated a sustainable, nonpetroleum route to isoalkanes; however, the production of cycloalkanes from waste and biomass is challenged by hydrogen requirements, preferential selectivity to aromatic compounds, and low yields to jet-fuel-range components. Purdue University has partnered with PNNL and LanzaTech to create a strong team with the fuels, catalysis, process development, and scale-up expertise needed to successfully address these challenges.

Olefin intermediates will be produced from ethanol using existing technologies from the Chemical Catalysis for Bioenergy Consortium (ChemCatBio) and from PNNL/LanzaTech. In this project, we will leverage experience in converting a variety of olefins to jet- and diesel-range hydrocarbons to develop a new process with high selectivity to cycloalkanes. Processes such as hydroforming can convert alkanes and alkenes to cyclic alkanes (e.g., naphthalene from n-decane), and PNNL has demonstrated the production of cyclic alkanes from butene with 25% selectivity. The team will build on this established proof of concept in developing a process ready for scale-up using PNNL facilities to produce a minimum of 2 gallons of fuel blendstock. The project makes use of Purdue's extensive analytical capabilities to measure fuel properties that are indicative of the product's "drop-in" potential. Further experiments and analyses are currently executed to evaluate the end product's optimum blend proportions with conventional jet fuel.



COMMENTS

- Approach: The project approach aligns with the metrics defined under AOI-5 DE-FOA-0002029 in terms of gallons of product, selectivity toward cycloalkanes, improvement of required properties, lower aromatic content, scalability, and hence cost. It is not clear if the level of GHG reduction has been met or included thus far in the project. The approach is to showcase a catalytic reaction to produce >60 wt % cycloalkanes (using knowledge from isoalkane catalysis) as a substitute to jet blends to meet the high energy content and low swelling of O-ring materials requirements. The project builds on past work for feedstock generation for this reaction using industrial waste gases to olefins.

- Progress and outcomes: The verification stage has been successfully completed. The initial go/no-go was passed for the development of the analytical methods by April 30, 2022. Budget Period 2 work has focused on catalyst studies to improve cycloalkane yields and TOS. Results: 30 mol C% cycloalkanes, TOS 34 hours. The team has identified key cycloalkanes that maximize energy density (it is not clear how much of those are produced). The results on Slide 14 show a catalyst for alcohol dehydration to olefins (not the current focus of the study) and a literature citation for olefin to cycloalkane (up to 90% selectivity); it is not clear if this has been reproduced. The team has made significant progress on analytical methods in conjunction with identifying the impacts of what can potentially swell the seals, which is well documented with an understanding of the reasons behind it. The team has completed the key compound identification (cycloalkane trans- and cis-decalin) and the TEA/LCA model.

- Impact: If the claims are realized, the project will demonstrate (1) a shift toward cycloalkanes; (2) lower aromatic content and high energy density, and (3) improvement in lower swell properties. The project is geared toward meeting the required milestones and can advance the state of the art (SOA) by advancing new analytical methods and the impact of a new chemistry on O-ring swelling.

- The team comprises Purdue University, PNNL, and LanzaTech, giving a well-rounded team. Their goal is to convert alcohol to cycloalkanes to blend with jet fuel. They give specific goals for cycloalkane composition, with reasonable steps to take should they have problems meeting these goals.

- They completed the initial verification and have put a significant amount of effort into product identification. They have also identified target cycloalkanes that maximize energy density. They have also performed LCA and ring swelling analysis.

- The project has the potential to deliver high-cycloalkane-content jet fuel blending components. The identification of optimal cycloalkanes seems a bit too specific, and it is unreasonable to target those three cycloalkanes. It seems that the beginning and the end of the process have seen good progress, but the middle is lacking, and it is really needed to tie it all together.

- The project is designed to improve an existing process to produce a better SAF. Their approach is appropriate and addresses critical requirements for the LanzaTech process to be more relevant to producing jet fuel. Their approach is comprehensive, and they have a good risk management plan. They are a bit overambitious in planning for commercial-scale operation when they need to validate the findings at TRL 6 or TRL 7. They are not ready for TRL 8 because they are still in the system development stage. Overall, this is a well-managed project with an industry partner that has had success in commercializing technology.

- The project aims to develop and model a process for generating higher-energy-content jet blending components from ethanol to produce a jet fuel that has favorable fuel properties and that requires less hydrotreatment. The objectives include LCA and TEA of a 50-million-gallons/year commercial-scale process, catalyst development, analytical method development, process optimization through lab experiments, and the production of 2 gallons of cycloalkane fuel blendstock. The project has met its first two first milestones, but it has also adjusted its schedule to a no-cost time extension. The project team includes industry and aims to improve upon an existing PNNL/LanzaTech process. The potential for a significant impact is unclear; the data on selective catalytic formation of cycloalkanes and lab analysis methods emergent from the project could be useful to industry, but the approach appears to be a set of adjustments to a specific existing process used by one company. The preliminary LCA focuses more on the type of feedstock than on the conversion approach and comparing that to the impacts of other pathways; such results would be helpful in further optimizing the studied processing pathway.

- The project is limited by the pathway approval for SAF; however, it is important work toward addressing unmet questions in the development of SAF. The project is asking for a no-cost extension, and the reviewer wonders if the project team has adequate resources for the same.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the positive comments from the reviewers highlighting our innovative approach for producing cycloalkanes that maximizes energy density for jet blendstock; builds on past work for feedstock generation using industrial waste gases to make olefins; improves upon an existing PNNL/LanzaTech process; can advance the SOA for new analytical methods; demonstrates the impact of new chemistry on O-ring swelling; has strong teaming, with an industry partner with success in commercial technology; and shows a comprehensive approach, has good risk management, and is well managed.

- Regarding the question of whether GHG reductions have already been met, a >70% reduction in GHG has already been met by producing jet blendstock from renewably sourced ethanol. PNNL/LanzaTech already developed the ATJ processing for producing an isoparaffinic jet blendstock from ethanol. Here, we are working to improve this processing by shifting the product slate to cycloalkanes, which are more energy dense than isoparaffins. One reviewer mentioned that key cycloalkanes that maximize energy density were identified, but it was not clear how many of these have been produced experimentally. The target cycloalkanes were identified by researchers at Purdue separate from the conversion work being done at PNNL. The goal of the Purdue team was to identify the most promising molecules for maximizing energy density to (1) inform the PNNL experimental team and (2) provide this insight in a journal manuscript that is about to be submitted for publication. The Purdue team picked molecules to evaluate with guidance from PNNL on what products and mixtures might be possible to produce using the chemistry being developed. Details for how the degree of branching and other features affect energy density were discovered. This information will inform the research community as well as our own work moving forward.

- There was a question whether the results shown for olefin to cycloalkane selectively up to 90% had been reproduced by our team. We apologize for the confusion. No, this was from data reported from the literature. Thus far, we have had limited success in obtaining high cycloalkane selectivity with single-step processing; therefore, we showed the results from this paper as a proof of concept for producing high cycloalkane selectivity when using a two-step approach. Here, jet-range olefins are first produced followed by ring closure to produce a jet-range cycloalkane. We have recently pivoted our approach to this two-step processing, and we are working to reproduce results from this paper as part of this effort. We are also evaluating another two-step approach that also appears promising. We look forward to reporting on these results in the next review.

- There was a comment that we are ambitious in planning for commercial-scale operation. First, we point out that the TEA and LCA performed were assuming commercial-scale operation, as is typically done. Second, we made the point that, if successful, we could take advantage of the commercial platform already being built out by LanzaTech. Here, we use the same olefin intermediate for producing cycloalkanes as the current PNNL/LanzaTech process for producing isoparaffins as jet blendstock; thus, there would be the leverage of an ongoing commercial deployment activity already underway.

- There was a question whether this work could be useful to industry where our approach leverages a specific existing process. We point out that the olefin feedstock used here could be produced from a variety of sources, and thus we believe that this catalysis could be broadly impactful. The processes for producing aromatics from olefins are widely used in industry today. But commercial technology for producing cycloalkanes do not exist; thus, the new processing being develop here could lead the way for new cyclization chemistry.
- Finally, there was a comment that the project has asked for a no-cost extension (actually two), and the reviewer wonders if the project team has the resources to do so. The team is, indeed, running out of resources, but, fortunately, the team believes it will soon have the data required to meet the very challenging go/no-go criteria to move into the final budget period.

CELLULOSIC-DERIVED ADVANTAGE JET FUEL

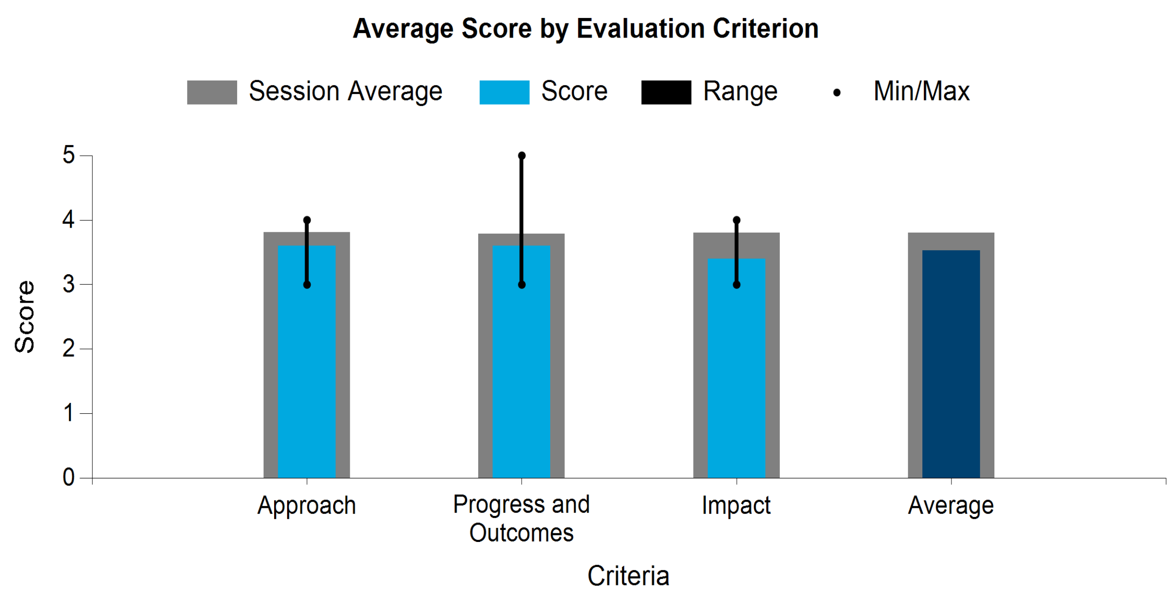
The Regents of the University of Colorado

PROJECT DESCRIPTION

WBS:	3.5.1.410
Presenter(s):	J. Will Medlin
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2024
Total Funding:	$2,705,048

This project will produce a jet fuel from cellulosic-derived sugars using a novel catalytic processing technology. The produced liquid fuel will have high content of cyclo-paraffins and dicyclo-paraffins, compounds that have high energy density, thermal stability, and a low freeze point, all of which are desirable properties for jet fuel. The process of generating jet fuel from cellulosic feedstocks provides a route for generating a large volume of product (7–14 billion gallons) from corn stover at a competitive price. This project will provide the necessary evidence for improved yields and operability to allow this technology to move toward commercialization.

The project is led by the University of Colorado Boulder in partnership with NREL, Shell, and Virent. This project combines the deacetylation and mechanical refining (DMR) deconstruction technology developed by NREL with a novel catalytic conversion technology discovered by Virent. NREL is working with Virent to design and commission a catalytic process unit to produce 2 gallons of on-specification jet fuel. Shell, one of the leading providers of jet fuel to the aviation industry, will provide analytical support by conducting analysis for ASTM approval as well as conducting blending studies of the generated jet fuel. The University of Colorado Boulder will lead the project and conduct fundamental studies of the required condensation chemistry to guide improvements of the catalytic process.



COMMENTS

- The project approach aligns with the metrics defined under AOI-5 DE-FOA-0002029 in terms of gallons of product, product stability/compatibility, and MFSP. It is not clear if the level of GHG reduction and aromatic content (8%) metrics have been included thus far in the project. The approach is to reduce ash content using NREL's DMR technology and improve the condensation catalyst stability and the process optimization. Key innovations are high-yield/low-ash-content sugars and an improved condensation catalyst, minimizing competing reactions. The verification stage has been successfully completed. Budget Period 2 work has been completed for one quarter on the condensation catalyst as a bench-scale test using model compounds. A schematic for the reaction paths and setup is shown, but no data are provided for the conversion/selectivity or the stability of the catalyst (the presenter verbally mentioned 3–4 weeks). Similarly, the benefits of the DMR technology are listed, and a product profile with an ash profile and sugar yield is required to determine the impact of its benefit on the process and if sugar meets the specifications required for downstream catalysis. Overall, the four-step proposed process has three hydrogenation steps, and as such quite high hydrogen demand, and this needs to be reported and accounted for in the TEA.

- The project has a good mix of university, national lab, and industry participation. That the national lab contributor is the founder of one of the industry partners seems to be a major strength. A technical problem that deals with the relative rates of the different potential reactions is being handled well by looking at the model compounds and model reactions. This kinetic information should be helpful in predicting the potential range of products. The metrics for the catalyst stability were not clear. Typically, catalysts deactivate over time, so giving a performance benchmark for a particular amount of time would be a better description.

- Despite how recently the project started, it seems that the lab experiments are up and running. It is of interest to the project that smaller molecules react faster and should be considered for the kinetics. A process flow diagram of the overall system was presented, which is encouraging. A phase separator between the first and second reactor showed that everything went to the second reactor.

- It seems that Virent is working on variations of this. Without a TEA or LCA, it is truly difficult to assess the overall impact. It does seem that a more stable condensation catalyst was the main goal of the work. More information on how this would be scaled up from the lab reactor would be helpful because this is going to be an important piece. Though Virent has done this in the past, more information could be shared.

- This project is on track and has met the first critical decision requirements to continue. The project is at TRL 6 of evaluation and seems to have the pieces necessary to complete this level. The project team should focus less on improving each step and more on how integrating the unit operations work together. Interface issues may be a risk they need to address. Whole-system issues are more important to look at than the efficiency of each unit operation. DMR is still a process; the team is working on delivering adequate quantities of clean sugars, so that area will need to be eventually addressed. Virent has been working on this technology for a long time, and I expected a bit more advancement than what has been shown.

- This project involves the development of a novel pathway to produce jet fuel involving catalytic hydrogenation, HDO, and condensation. The start of the 3-year project was January 2022, and the team has spent less than 2% of their budget; they passed the initial verification in 2022 and are on track toward their June 2024 go/no-go decision point. In this first phase of the project, they have involved industry in the unit process design (one PIs is the founder of the company) and made progress on the bench-scale testing of possible catalysts for the steps toward producing jet fuel. The project has the potential to improve yields from the conversion of sugars to jet fuel, and it is considering the risks involved with catalyst stability. There is the potential for the coproduction of other fuels besides jet fuel, providing greater commercialization potential; however, there are sustainability considerations that should be investigated as the project develops, particularly because of the separate steps involving catalysts and the reliance on hydrogen throughout conversion and upgrading: (1) the hydrogen demand per gallon of jet fuel, (2) the treatment of waste streams such as the 1 gallon of wastewater produced per gallon of jet fuel, (3) the materials and energy involved in catalyst production and regeneration (also affected by catalyst lifetime, which is already within the team's scope of study), and (4) the proportions of jet fuel versus other fuels that would result from the pathway (would this process ultimately be best commercialized toward a different end product that may be generated in greater quantities?). Some of these aspects might be quantified as the team assesses the economics of the pathway in the future as planned, but some might weigh more heavily toward the carbon footprint of the jet fuel than its costs. If the carbon footprint of this biomass-derived jet fuel is higher than that of conventional jet fuel due to high energy, hydrogen, wastewater treatment, and the carbon footprint of the catalyst production, this could substantially affect the scale-up success of the NREL DMR with Virent processing pathway.

- The level of blending that can be accomplished and the yield per ton of biomass are unclear, though I am not penalizing the project for that because it was not part of the original FOA. The key concerns are around using the DMR process and the cleanup required around DMR to meet the feedstock specifications for making SAF using the Virent process. The ion-exclusion technology is not sufficient to meet the feedstock specifications they desire. Also, finally, the SAF pathway meets all the specifications but is not necessarily tied to the stover feedstock.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The project approach aligns with the metrics defined under AOI-5 DE-FOA-0002029 in terms of gallons of product, product stability/compatibility, and MFSP. It is not clear if the level of GHG reduction and aromatic content (8%) metrics have been included thus far in the project. The approach is to reduce ash content using NREL's DMR technology and improve the condensation catalyst stability and the process optimization. Key innovations are high-yield/low-ash-content sugars and an improved condensation catalyst, minimizing competing reactions. The verification stage has been successfully completed. Budget Period 2 work has been completed for one quarter on the condensation catalyst as a bench-scale test using model compounds. A schematic for the reaction paths and setup is shown, but no data are provided for the conversion/selectivity or the stability of the catalyst (the presenter verbally mentioned 3–4 weeks). Similarly, the benefits of the DMR technology are listed, and a product profile with an ash profile and sugar yield is required to determine the impact of its benefit on the process and if sugar meets the specifications required for downstream catalysis. Overall, the four-step proposed process has three hydrogenation steps, and as such quite high hydrogen demand, and this needs to be reported and accounted for in the TEA.

- Response: We appreciate the comments. The TOS profiles are being collected as part of the ongoing work to enable quantitative comparisons of catalyst stability across different materials and operating conditions. The suggested analysis of the DMR technology, as well as the impact of hydrogen demand for the total process, will be included in the TEA. Validation data provided to the validation team from previous work at Virent is included here, which shows that the hydrogen consumption for the overall process was 0.16 kg of hydrogen per kilogram of final hydrocarbon products (includes gases and liquid organic products): "Table C.2.4. Hydrogen input rates and consumption data. Benchmark. Intermediate Final H_2 Input Rate (mol H_2/mol C) 2.12 1.24 0.96 H_2 Consumption (kg/kg liquid fuel product) 0.3 0.17 0.16."

- Comments: The project has a good mix of university, national lab, and industry participation. That the national lab contributor is the founder of one of the industry partners seems to be a major strength. A technical problem that deals with the relative rates of the different potential reactions is being handled well by looking at the model compounds and model reactions. This kinetic information should be helpful in predicting the potential range of products. The metrics for the catalyst stability were not clear. Typically, catalysts deactivate over time, so giving a performance benchmark for a particular amount of time would be a better description. Despite how recently the project started, it seems that the lab experiments are up and running. It is of interest to the project that smaller molecules react faster and should be considered for the kinetics. A process flow diagram of the overall system was presented, which is encouraging. A phase separator between the first and second reactor showed that everything went to the second reactor. It seems that Virent is working on variations of this. Without a TEA or LCA, it is truly difficult to assess the overall impact. It does seem that a more stable condensation catalyst was the main goal of the work. More information on how this would be scaled up from the lab reactor would be helpful because this is going to be an important piece. Though Virent has done this in the past, more information could be shared.

- Response: Thanks for the helpful suggestions. We agree about the importance of a TEA for elucidating the overall impact, and we acknowledge that scale-up issues may be significant. These will both be addressed during the coming months of the grant.

- Comments: This project is on track and has met the first critical decision requirements to continue. The project is at TRL 6 of evaluation and seems to have the pieces necessary to complete this level. The project team should focus less on improving each step and more on how integrating the unit operations work together. Interface issues may be a risk they need to address. Whole-system issues are more important to look at than the efficiency of each unit operation. DMR is still a process; the team is working on delivering adequate quantities of clean sugars, so that area will need to be eventually addressed. Virent has been working on this technology for a long time, and I expected a bit more advancement than what has been shown.

- Response: We appreciate this comment. The reason for the major focus on the condensation step is related to a point made in this comment. Virent (and others) have developed relatively advanced technology for many key steps in the reaction process, particularly related to hydrogenation and HDO. Condensation, on the other hand, is much less developed, and technology improvements are needed to advance the overall process. Nevertheless, we acknowledge that the integration of all process units is critical for the success of the project, and that will be the major focus of our upcoming work (and is the key step for our go/no-go decision). This work must also include the analysis of the DMR process that is suggested in this comment.

- Comments: This project involves the development of a novel pathway to produce jet fuel involving catalytic hydrogenation, HDO, and condensation. The start of the 3-year project was January 2022, and the team has spent less than 2% of their budget; they passed the initial verification in 2022 and are on track toward their June 2024 go/no-go decision point. In this first phase of the project, they have involved industry in the unit process design (one PIs is the founder of the company) and made progress on the bench-scale testing of possible catalysts for the steps toward producing jet fuel. The project has the potential to improve yields from the conversion of sugars to jet fuel, and it is considering the risks involved with catalyst stability. There is the potential for the coproduction of other fuels besides jet fuel, providing greater commercialization potential; however, there are sustainability considerations that should be investigated as the project develops, particularly because of the separate steps involving catalysts and the reliance on hydrogen throughout conversion and upgrading: (1) the hydrogen demand per gallon of jet fuel, (2) the treatment of waste streams such as the 1 gallon of wastewater produced per gallon of jet fuel, (3) the materials and energy involved in catalyst production and regeneration (also affected by catalyst lifetime, which is already within the team's scope of study), and (4) the proportions of jet fuel versus other fuels that would result from the pathway (would this process ultimately be best commercialized toward a different end product that may be generated in greater quantities?). Some of these aspects might be quantified as the team assesses the economics of the pathway in the future as planned, but some might weigh more heavily toward the carbon footprint of the jet fuel than its costs. If the carbon footprint of this biomass-derived jet fuel is higher than that of conventional jet fuel due to high energy, hydrogen, wastewater treatment, and the carbon footprint of the catalyst production, this could substantially affect the scale-up success of the NREL DMR with Virent processing pathway.

- Response: As noted, the hydrogen demand for this process is potentially a significant limitation, and this aspect will be investigated via TEA as the project proceeds. This comment raises an excellent point about the appropriate analysis of waste streams, such as the water produced from the HDO and condensation reactions, which will be significant due to the high oxygen content of the original biomass; we will attempt to incorporate such analysis in our future work. As the comment mentions, the energy and materials inputs for the catalysts are a key motivation for this project; the primary negative impact of having a catalyst with low stability is the inputs required to regenerate the catalyst (and corresponding efficiency losses). We also acknowledge the point about the process potentially generating product fractions that may best fit outside the jet fuel (blend) range, although it is worth mentioning that the process has been specifically designed to produce high yields of cycloparaffins in the appropriate molecular weight range for jet fuel. Finally, we agree that, ultimately, it will be important to demonstrate the carbon footprint of jet fuel generated from this process.
- Comments: The level of blending that can be accomplished and the yield per ton of biomass are unclear, though I am not penalizing the project for that because it was not part of the original FOA. The key concerns are around using the DMR process and the cleanup required around DMR to meet the feedstock specifications for making SAF using the Virent process. The ion-exclusion technology is not sufficient to meet the feedstock specifications they desire. Also, finally, the SAF pathway meets all the specifications but is not necessarily tied to the stover feedstock.
- Response: Thanks for the comments. The level of blending that can be obtained will be a focus of studies after the generation of jet fuel by the integrated process. Yield information was not directly presented in the presentation, but our goal is to produce 70 gallons of jet fuel per ton of corn stover. Ion exclusion by itself will not meet the final feedstock specification because a finishing ion exchange step will be required to remove the small amount of contaminates that remain after ion exclusion. The advantage of ion-exclusion technology is that it eliminates the necessity of using ion exchange to remove all the contaminates, which would be more expensive.

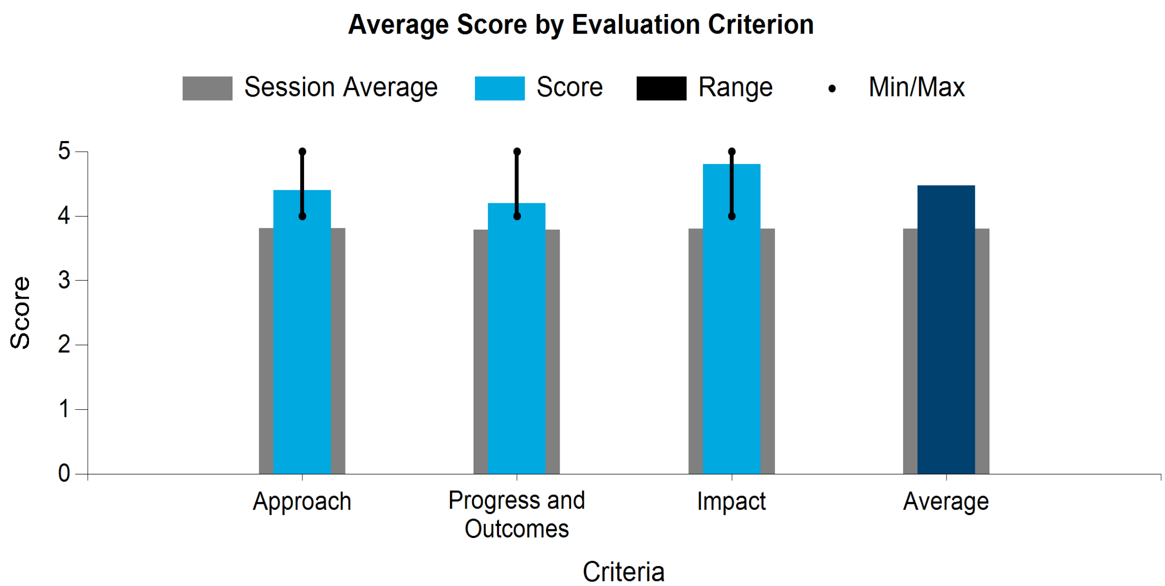
PRODUCTION OF RENEWABLE CYCLOALKANES FROM ETHANOL FOR BLENDING WITH JET FUEL TO ENHANCE ENERGY DENSITY AND MATERIAL COMPATIBILITY AND REDUCE PARTICULATE EMISSIONS

Vertimass LLC

PROJECT DESCRIPTION

WBS:	3.5.1.412
Presenter(s):	John Hannon
Project Start Date:	10/01/2019
Planned Project End Date:	03/30/2024
Total Funding:	$1,793,423

Previous DOE BETO funding advanced technology from lab to pilot for production of high-octane gasoline and aromatics. Overall liquid yields were increased from 36% to 82%, catalyst was moved from lab powder to low-cost commercial extrudates, and the process was scaled up 300 times. Current project goals are to (1) scale up from pilot to demonstration with Technip Energies to obtain engineering data for commercialization; (2) shift carbon number range from 4–12 to 75% as 7–17 (jet fuel); (3) reduce aromatics from approximately 50% by weight to less than 20% weight while increasing cycloalkanes to a max of 30% by weight; (4) increase energy density; and (5) minimize emissions.



COMMENTS

- Approach: The project approach aligns with the metrics defined under AOI-5 DE-FOA-0002029 in terms of gallons of product, selectivity toward jet fuel range, scalability, and hence cost. It is not clear whether product stability/compatibility, level of GHG reduction, and aromatic content (8%) as opposed to less than 20% metrics have been met or included thus far in the project. The approach is to showcase a single-step reaction for an ATJ fuel mix product using a commercially available catalyst and to qualify product against identified jet fuel blend analogues. A key innovation is a single-step reactor using a commercial catalyst from a strong, active team with substantial work on this reaction over years. Another substantial improvement is no use of H_2.

- Progress and outcomes: The verification stage has been successfully completed. The initial go/no-go was passed March 2022. Budget Period 2 work has focused on shifting the product range toward C7; lab results show up to 82.5% product in this range, although with very high aromatic content, 83.5%, of the product.
- The project involves several companies with varied capabilities that make for a comprehensive team with expertise in catalysis and scale-up. The main goal is to shift the composition of their alcohol-to-cycloalkane process to higher and more cycloalkanes with less aromatics. Their process can use any alcohol, but results for ethanol were presented.
- Challenges were presented, but they seemed to be at a high level, i.e., qualifying a suitable product. This does not address the technical challenge they are trying to overcome.
- It is interesting that they can use such a diluted form of ethanol. The discussion of the reactor's operating conditions, however, did not tie into this issue. Changing the reactor conditions is going to have a major impact on costs if the primary feedstock is at 50% concentration.
- They have passed the initial verification. They have performed experiments where they have increased the amount of cycloalkanes (and aromatics) through adjusting the operating conditions and catalysts. Without specifics besides adiabatic versus isothermal, it is difficult to understand how tunable the reactor is. All reactors are tunable with the number of potential changes that can be made to their operation.
- Without TEA and LCA, it is difficult to determine the impact and potential for this project. They have clearly shown that they can produce a better component to blend with jet fuels. It would be interesting to see the effect of other alcohols, especially methanol and butanol, on product composition.
- The progress has been good and is on track. I am concerned about interface issues between unit operations. The team seems to have obtained the results they wanted and has met goals, but they did not discuss any interface issues, which typically are what sidetracks fully integrated systems. They need to focus on one or two product streams over extended periods of time before considering commercial operation. They have kind of met the TRL 7 requirements with the Technip work, but they have not completed the system development to go to TRL 8 or TRL 9. This is a well-managed and good team with good potential to go to the next level of development and be successful.
- This project focuses on the development of a primarily ethanol-to-jet-fuel process, consolidated alcohol deoxygenation and oligomerization, which also has the potential to generate a multitude of coproducts, such as propane, butane, plastics, and other fuels beyond jet fuel. The one-step conversion approach has the potential for commercialization and for a lower-life cycle impact. The technical approach involves a team with extensive experience in scale-up, commercial catalysts, optimization of key parameters, lab development, and modeling of fuel properties and techno-economics, and they have established additional key partnerships during the span of the project. A reactor has been designed, constructed, and is currently operational; the project has reached its intended demonstration scale. The catalyst lifetime has been substantially extended, but reducing the high-aromatics content is still in progress. The project has spent only $123,401 of a total budget of $1,434,738 since starting in March 2022. As the demonstration scale is tested, the life cycle energy inputs and carbon footprint should be compared against those of conventional jet fuel production and pathways of SAF production because it is currently unknown whether this particular pathway of single-step conversion will truly be an improvement beyond the reduction in unit processes.
- The work on Hannon et al. that forms the basis of this project is seminal. It is delivering a significant increase in hydrocarbon yield and the use of the ATJ pathway. Concerns are with high levels of aromatics and cycloalkanes. Blending would be limited because of that.

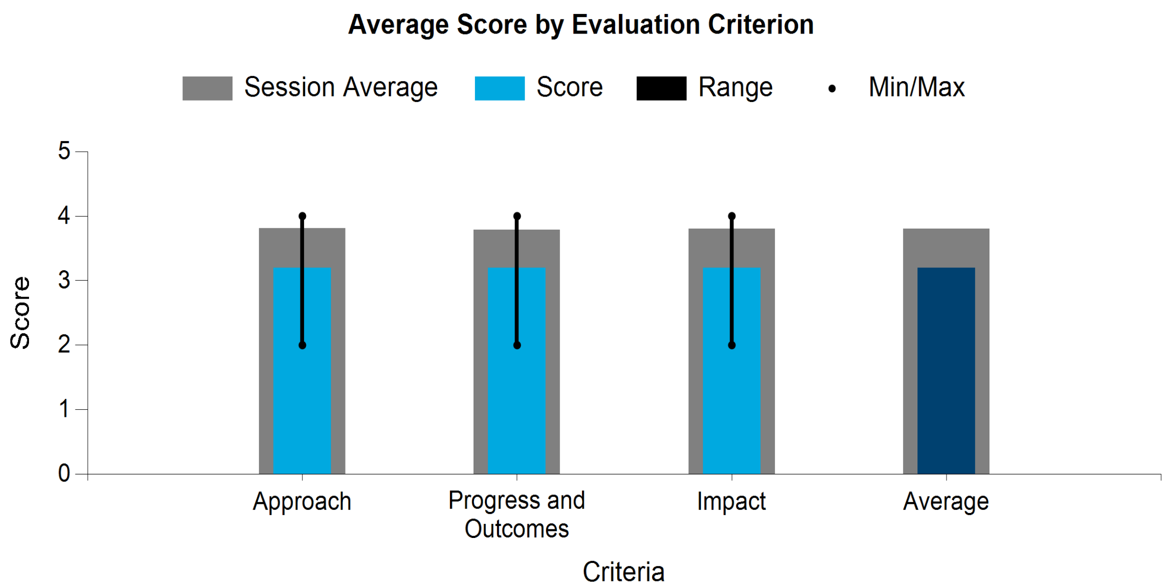
PI RESPONSE TO REVIEWER COMMENTS

- We thank you for organizing a great peer review, and we appreciate all the reviewers' observations and comments.
- Response to Comment 1: Thank you for the review and comments. The Vertimass technology converts ethanol into a variety of jet-fuel-range aromatics and cycloparaffins with smaller amounts of paraffins and isoparaffins. We intend to blend this SAF with other technologies that only produce paraffins and isoparaffins to make a more complete fuel. This is the main reason we partnered with World Energy—to complement their HEFA-derived SAF that contains no aromatics or cycloparaffins and to increase their potential volumes because we can use widely available ethanol feedstocks. We also believe that this technology will substantially advance the SOA to convert alcohols into hydrocarbons in one low-cost step.
- Response to Comment 2: Thank you for the review and comments. The combination of using different catalysts and operating conditions has allowed us to vary the product slate, and we are still determining the best combination for our SAF blendstocks. We believe this new tunable and cost-effective process has the potential to dramatically change the SAF landscape.
- Response to Comment 3: Thank you for the review and comments. Our scale-up partner, Technip Energies, is currently working on a fully integrated plant design that addresses the interfaces with an ethanol plant. Technip Energies has had commercial success with plant integration, and we will have this engineering design completed in FY 2023 Q3.
- Response to Comment 4: Thank you for the review and comments. Our scale-up partner, Technip Energies, is currently working on a fully integrated plant design that will quantify all the process inputs/outputs so that we can more accurately determine the LCA. We are also working with Life Cycle Associates and ANL to quantify the LCA.
- Response to Comment 5: Thank you for the review and comments. The Vertimass technology produces elevated levels of aromatics, but this SAF blendstock complements other SAF technologies that have zero aromatic content to make a more complete jet fuel. Thank you again, and please feel free to reach out to us with any more follow-up questions at jhannon@vertimass.com.

MULTISTREAM INTEGRATED BIOREFINERY ENABLED BY WASTE PROCESSING

Texas A&M Agrilife Research

WBS:	3.5.1.501
Presenter(s):	Susie Dai
Project Start Date:	06/01/2018
Planned Project End Date:	11/30/2023
Total Funding:	$2,795,267



COMMENTS

- Approach: The project approach aligns with the metrics defined under Topic Area 2, DE-FOA-0001689.
    - Technical lignin utilization for carbon fibers; lignin-to-asphalt binder modifier.
    - Project management: The outcomes suggest that the program is well managed via monthly teleconferences between the partner organizations and the DOE program manager.
    - The two process streams downselection is based on the TEA and performance.
- Progress and outcomes:
    - The team has made significant progress on identifying and meeting the required properties for two major applications compared to the benchmark. It is not clear if the benchmark numbers reflect the minimum carbon fiber specifications. T300, a basic carbon fiber by Toray, has a tensile strength of 3,530 Mpa, MOE 230 GPa, strain 1.5% with density and filament diameter requirements; however, for automobile applications, lower specifications are acceptable. No measurements on strain rates have been presented; this is a minimum requirement.

- The results are not sufficient to evaluate progress on asphalt binders.
- The addition of back-end fermentation helps remove small lignin molecules, which is required to improve carbon fiber properties to meet 1.4-GPa tensile strength.

- Impact:
  - The project team has clearly demonstrated scientific advancement and the utilization of waste streams for very-high-valued product streams. Even if small volumes are used, it will have a major impact on the biofuels industry. Thirty-one publications and three patents on this topic have also added a lot of value for the scientific and industry community. It is a bit unclear how the benchmark values were selected; a few references on this could be helpful. The team is well organized, has access to past data on lignin characterization, and has shown enthusiasm and vigor in achieving goals that align well with BETO's goals. The program lacks clarity on commercially acceptable specifications; more industry engagement is recommended.
- This project focuses on producing asphalt binders and carbon fibers from lignin. A significant analysis of the products was presented, as well as economic feasibility, along with some sensitivity analysis.
- The asphalt that can be generated has seen major improvements and has met the team's benchmarks.
- The carbon fibers have seen improvements in properties, though they have not reached their modulus or tensile strength goals.
- A TEA has been completed that found the team can achieve $1.88 for a selling price and $2.56/GGE.
- It is greatly appreciated that a sensitivity analysis was completed, but it seems that the minimum ethanol selling price is extremely sensitive to the price of the carbon fiber. A small decrease from the $20/kg assumed for carbon fiber greatly reduces or eliminates the economic feasibility.
- It may benefit the team to have more input consultants who have lignin, asphalt, and/or carbon fiber manufacturing experience.
- This project is useful to examine the potential coproduct streams from a biorefinery. It is a good exercise and poses some potential. It is more of an academic exercise than one based on reality because it takes much more than just good numbers to see any of the processes implemented in an operating biorefinery. The team listened to previous reviews and limited the coproducts, which was good and showed the potential for them to work. In the asphalt area, they might have wanted to compare what competition exists, such as lignosulfonates from pulp mills. As previously noted, they should continue to work with potential end users but recognize that they are still far from implementing these in real situations.
- This project is investigating pathways for a multistream integrated biorefinery that yields an array of products from biomass-derived lignin—including carbon fiber, asphalt binder, bioplastics, and lipids—for fuel upgrading. It incorporates LCA and TEA to evaluate possible pathways and improve process design. The diagram provided on the summary of estimated carbon dioxide emissions is difficult to interpret, although the other process diagrams are helpful for following the various options studied. The project has met its milestones for Budget Period 2, and currently it has less than 1 year remaining. The project has produced 31 publications. The presentation focused on the potential significance of the work once scaled up more than the work undertaken thus far. Consequently, it is unclear at what scales the experiments were conducted and how this can truly scale up for commercialization. Similarly, the models appear to be developed for small flows through a biorefinery. An investigation into the extent to

which the results at the laboratory scale may be representative of outcomes at the commercial scale is recommended.

- The project is quite wide in scope and would benefit from narrowing the focus areas. Resourcing appears very limited, and the project should be more specific and directed.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' enthusiastic support of the project, including "significant progress," "well managed," "significant analysis of the products," "listened to previous reviews," "good exercise and poses some potential." With all these supportive comments, this response primarily focuses on the concerns of the project.

- For Reviewer 1, the comments are in four categories. (1) The choice of the specs and relevance to industry: "It is not clear if the benchmark numbers reflect the minimum carbon fiber specifications. T300, a basic carbon fiber by Toray, has a tensile strength of 3530 Mpa, MOE 230 GPa, strain 1.5% with density and filament diameter requirements; however, for automobile applications, lower specifications are acceptable." "It is a bit unclear how the benchmark values were selected; a few references on this can be helpful." And "The program lacks clarity on commercially acceptable specifications." We appreciate the reviewer's comment. First, we substantially considered the industrial relevance during the proposal development and project implementation. With carbon fiber as an example, the project focuses on automobile industry applications because they are the most relevant to energy efficiency and carbon emissions reduction in the transportation sectors. That said, T300 from Toray is a lower grade for the aviation industry application. Instead, we benchmarked our carbon fiber performance against DOE's automobile industry carbon fiber specifications (tensile strength of 1.72 GPa and a modulus of 172 GPa). The project aims to reach tensile strength at 2 GPa (higher than 1.72 GPa) and modulus at 100 GPa (lower than 172 GPa) [1]. Our target considered the carbon-fiber-reinforced polymer development. For the asphalt binder modifier, we also considered commercial applications. In particular, we focused on improving high-temperature performance without compromising low-temperature performance [2]. The resultant asphalt binder will improve 1 to 2 PG, which accounts for a $100 to $200 increase in market value; therefore, the lignin could be sold at $1,000 to $2,000 for the value added to the asphalt binder in a 10% mixture. The focus on high-temperature performance aims to address the climate change-related infrastructure challenges. The benchmark value was justified by previous publications from the group [2]–[4]; therefore, all benchmarks and milestones are justified, and the milestones are directly relevant to commercial potential and industrial applications. (2) "No measurements on strain rates have been presented." The strain rates were calculated in all samples. Here are some examples from Table 1: "Table 1. Strain rate for the before and after fermentation lignin (AESA: after fermentation; AESM: before fermentation and modified; AESAM: after fermentation and modified) Strain rate (1/s) Dev AES 0.000421366 5.72E-05 AESA 0.000338317 1.97E-05 AESM 0.000340513 1.32E-05 AESAM 0.000342423 3.24E-05 3." (3) "The results are not sufficient to evaluate progress on asphalt binders." The asphalt binder techniques have met the milestones from the last peer review; therefore, we are not repeating the data from the last peer review. (4) "More industry engagement is recommended." We agree with the reviewer's comment and are taking action to engage more end users, even though the lignocellulosic biorefinery had some setbacks. In fact, we have engaged different commercial partners, including those involved in SAF efforts.

- For Reviewer 2, the major concern is, "It may benefit the team to have more input consultants who have lignin, asphalt, and/or carbon fiber manufacturing experience." We agree with the comments. In fact, the team has most of the expertise on lignin and asphalt binder. We also consulted with experts on carbon fiber manufacturing and developed two additional strategies to improve carbon fiber properties.

- For Reviewer 3, the primary comment is as follows: "In the asphalt area, they might have wanted to compare what competition exists, such as lignosulfonates from pulp mills. As previously noted, they should continue to work with potential end users but recognize that they are still far from implementing these in real situations." We actually carried out the comparison of Kraft lignin in previous studies [2]. In fact, previous studies from the team have shown that lignosulfonates will not serve the purpose because it decreases the low-temperature performance while improving the high-temperature ones. The lignin from the paper and pulping industries needs special treatment before using it as a quality asphalt binder modifier. On the contrary, the biorefinery lignin from this project, with the proper pretreatment technologies developed in this project, addressed the challenge to derive lignin with improved high-temperature performance without compromising low-temperature performance. As mentioned, we are engaging commercial partners.

- For Reviewer 4, the primary comment is, "Consequently, it is unclear at what scales the experiments were conducted and how this can truly scale up for commercialization. Similarly, the models appear to be developed for small flows through a biorefinery. An investigation into the extent to which the results at the laboratory scale may be representative of outcomes at the commercial scale is recommended." The reviewer also has difficulties interpreting the carbon emissions data. In our quarterly reports, we thoroughly discussed carbon emissions and LCA. In fact, we will publish the data soon. We totally agree with the reviewer on the scale. We are working with NREL to scale the technology to half-dry TPD. (References: [1] doi.org/10.1002/app.39273, [2] doi.org/10.1021/acssuschemeng.6b03064, [3] doi.org/10.1039/C6GC03555H, [4] doi.org/10.1039/C7TA01187C.)

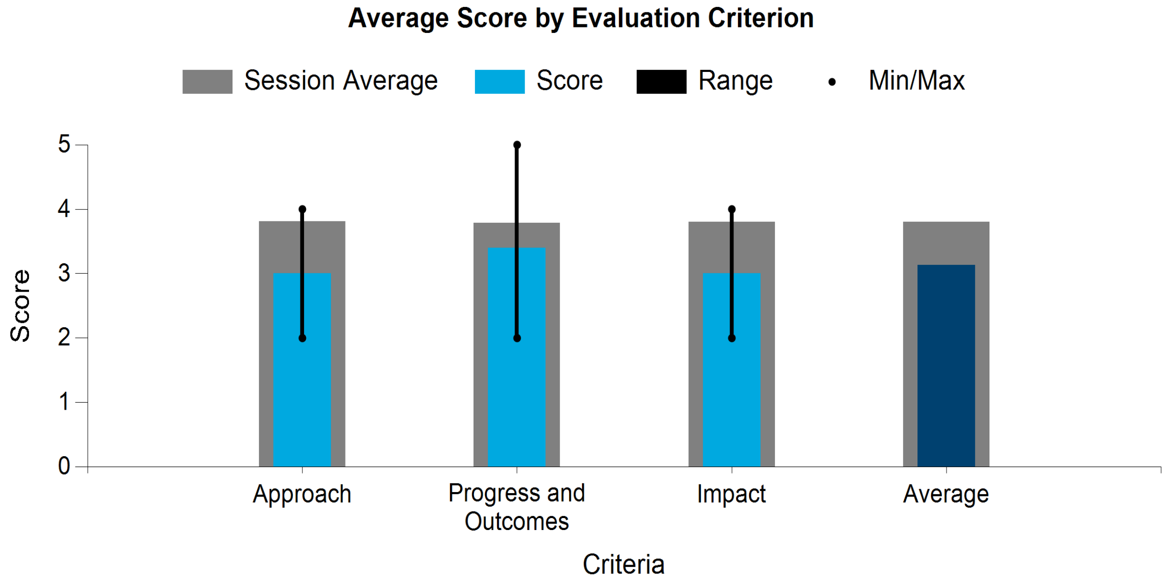
NEAR-CRITICAL FLUIDS TREATMENT FOR LIQUEFACTION AND EXTRACTION OF BIOFUELS

University of Maryland

PROJECT DESCRIPTION

WBS:	3.5.1.601
Presenter(s):	Ashwani Gupta; Cassie Moore
Project Start Date:	10/01/2021
Planned Project End Date:	04/30/2026
Total Funding:	$3,876,702

We propose to develop the liquefaction of biomass and biowaste feedstocks in the presence of near-critical fluids, such as supercritical CO_2 (sCO_2), and subcritical water to form oil products and subsequently extract hydrotreating-suitable biocrude to produce liquid biofuels and valuable chemicals. The proposed process will build on the emerging HTL process for biocrude products by using the synergistic solvent properties of sCO_2 and subcritical water to improve the quality of biocrude and provide robust operation and fuel extraction. The low viscosity and high density of these near-critical fluids will improve the process operation while the tunability in the solvent properties with temperature and pressure will provide efficient product extraction to remove the water, metal, and O content of biocrude. This improved biocrude composition will provide improved aging stability, carbon content, heating value, and compatibility to industrially established hydrotreating processes to obtain transportation fuels. In addition, near-critical fluids mitigate the energy-intensive moisture control requirements in feedstocks and thus also allow for the conversion of diverse moisture grades of biomass into liquid fuels. This improvement in biocrude quality, yield, efficient dewatering, and product extraction will provide reduced GHG emissions to beyond 70% reduction compared to petroleum-based alternatives. The integration of dewatering, liquefaction, and sCO_2-extraction can be achieved for efficient operation and potentially reduced capital costs. For this research, process components—mainly feedstock dewatering, near-critical liquefaction, and sCO_2-biocrude extraction—will be developed for continuous mode and investigated to build predictive models of their operation. These reactor studies will be carried out at an FOA-relevant scale to gain design knowledge of the operational requirements and process output. Different real feedstock samples will be examined, each from different classes, including lignocellulosic, algal, and wet biomass, and sorted municipal solid wastes. The influence of operational parameters (such as temperature, pressure, solvent/feedstock ratio, feedstock loading, residence time, and solvent requirement) on process output (such as energy input, GHG impact, water and CO_2 recyclability, product quality, and yield) and byproducts will be obtained using these process tests. Biocrude and sCO_2-extracted crude components' quality will be judged in terms of parameters such as O/C, H/C, composition, viscosity, aging stability, water content, density, and heating value. The goal will be to obtain biocrude with capabilities to be incorporated into hydrotreating plants of petroleum crude that yield transportation fuels. This will be demonstrated based on ASTM standard characterization of the extracted biocrude and its similarity with petroleum crude. Predictive process models will be developed based on these investigations, which will be further incorporated into the LCA and TEA of incorporating these components into an integrated process from feedstock-to-product deployment. These analyses will be used to determine the economic, GHG, and fuel cost impact of the process, along with the optimal conditions needed for maximizing these benefits.



COMMENTS

- The project approach aligns with the metrics defined under the FY 2021 pre-pilot: \$2.75/GGE and 70% reduction.
  - Technical: sCO_2 dewatering, liquefaction under sCO_2 and sCO_2 recovery.
  - Project management: Dr. Gupta's and Dr. Sandborn's groups are working on experimental and modeling, respectively.
  - DEI: There is active participation from Historically Black Colleges and Universities McNair Scholars, interns, graduate researcher, and training.
- Progress and outcomes:
  - Batch reactions are conducted, with char and biocrude fractions quantified for verification purposes.
  - The sCO_2 process claims low metal content, water, and oxygenates in biocrude. The team compares it with biocrude feed. It would be nice to see if this can be compared with other types of biocrude, as shown in additional slides.
  - The team claims higher stability of bio-oils with respect to viscosity, acidity, and oxygen number.
  - It is unclear if the process can be scaled to meet the pressure feed requirements for the sCO_2 process at this stage. TEA/LCA work has not been started, and it is recommended to start preliminary work to estimate/understand the impact of key unit operations using sCO_2 as a fluid.
- Impact: If successful (the project started in October 2021 and has completed two budget periods; the project has passed the initial verification and completed 1 year of work post verification), it will enable the utilization of sCO_2 as a fluid/reactant medium to dewater and liquefy biomass to biocrude with low impurities and a reduction in the complexity of separations. It is, however, not clear how biomass will be fed at such high pressures and temperatures in a continuous reactor. This is a pre-pilot program with

expectations to produce enough product for characterization. The current facilities are limited to small batch reactors.

- This project looks to convert biomass to biocrude using sCO_2 for dewatering, liquefaction, and extraction. The scaled-up plant will also include LCA and TEA. The project is being led by two faculty members with many students and postdocs. They have recruited undergraduate students from the University of Texas at El Paso, a Hispanic-serving institution.

- The small-scale system that has been built though this program is quite new. The verification is complete. Students have been recruited to work on this project.

- The presentation outlined technological advantages to using sCO_2, but the main drawback has always been economics. The proposal does not yet have data on the economic feasibility, though given that it is widely known that the cost is prohibitive, some calculations could have been included. Estimates of the amount of sCO_2 needed per mass of biocrude would also be helpful to get some rough estimate. The team would also benefit from having someone with supercritical experience at the industrial scale, though that person may be difficult to find.

- The proposal does have a good DEI plan, especially with outreach and training. Recruiting from a Hispanic-serving institution is also a good step, as are the research talks at the Hispanic-serving institution.

- This project must prove concepts at a batch-scale level. The success will be in the value of the graphite product, and comparing two types of pyrolysis oils is germane and appropriate. The impacts will be less on the biofuels market because it will be on the U.S. economy. The team appropriately points out that the supply chain needs to be more internal to the United States versus foreign countries, and that is easily obtainable via the biomass resources that exist in the United States. It is a project that looks at biomass use in a different way but that could have a good impact. Good diversity efforts.

- The project team is developing a near-critical integrated liquefaction and extraction pathway to convert biomass and wastes to deployable biofuels. They have graduate and undergraduate students assigned to key tasks, including design, process modeling, lab experiments, and analysis of costs and life cycle GHG emissions. DEI efforts include implicit bias training, participant climate surveys, and recruitment and mentoring of students from historically marginalized groups in engineering. The project leadership team has previously supported summer research students in publishing their research. Following the "pipeline" outcomes from the project would be an interesting addition to these initiatives—for example, tracking the percentage of summer-term research students who pursue other research opportunities or return to this project or who apply to and enter a graduate program and comparing that against expected rates. The presentation mixed cost-specific parameters into its discussion of a stochastic LCA model under development, and key parameters related to the life cycle GHG emissions were missing from the list. It is unclear whether the project is fully tracking the flows of carbon throughout the pathway and end products (for example, the amount of carbon that might be sequestered in the generated chars). The project team may benefit from the services of an LCA practitioner or researcher to ensure that their accounting of life cycle GHG emissions (for which the team has a >70% reduction target) is thorough. The project is currently completing Task 1.0, the initial verification, and has been active since October 2021.

- The challenge is the scalability of sCO_2 processing. CapEx barriers and materials-of-construction issues with equipment remain to be addressed. The team also needs to further reduce the oxygen content of the biofuels for scalability. The project is more at TRL 2 or TRL 3.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The project approach aligns with the metrics defined under the FY 2021 pre-pilot: \$2.75/GGE and 70% reduction. Technical: sCO_2 dewatering, liquefaction under sCO_2 and sCO_2 recovery. Project management: Dr. Gupta's and Dr. Sandborn's groups are working on experimental and modeling, respectively. DEI: There is active participation from Historically Black Colleges and Universities McNair Scholars, interns, graduate researcher, and training. Progress and outcomes: Batch reactions are conducted, with char and biocrude fractions quantified for verification purposes. The sCO_2 process claims low metal content, water, and oxygenates in biocrude. The team compares it with biocrude feed. It would be nice to see if this can be compared with other types of biocrude, as shown in additional slides. The team claims higher stability of bio-oils with respect to viscosity, acidity, and oxygen number. It is unclear if the process can be scaled to meet the pressure feed requirements for the sCO_2 process at this stage. TEA/LCA work has not been started, and it is recommended to start preliminary work to estimate/understand the impact of key unit operations using sCO_2 as a fluid. Impact: If successful (the project started in October 2021 and has completed two budget periods; the project has passed the initial verification and completed 1 year of work post verification), it will enable the utilization of sCO_2 as a fluid/reactant medium to dewater and liquefy biomass to biocrude with low impurities and a reduction in the complexity of separations. It is, however, not clear how biomass will be fed at such high pressures and temperatures in a continuous reactor. This is a pre-pilot program with expectations to produce enough product for characterization. The current facilities are limited to small batch reactors.

- Response: We thank the reviewer for the valuable comments. The project has just finished Budget Period 1 with passing the initial verification. The sCO_2 extraction of biocrude significantly improves the viscosity, acid number, and oxygen along with reducing the metal and water content compared to the biocrude feed. Currently, this is the extent of the literature available, and it is limited to only one type of biocrude. We will perform these studies and will provide comparisons as the project progresses. The scalability of high-pressure feeding is a technical risk associated with the process, and we intend to address this with efforts to resolve the loading and unloading times in the batch process so that it can be operated in a continuous fashion. We have started some preliminary TEA/LCA work already; we are currently looking into the impact of CO_2 and biomass feedstock availability. The NILE process will be a batch process but with capabilities to be operated in a continuous fashion. We intend to start our design into biomass loading at high pressure and temperature early in the project, with the goal to load and unload the biomass batches with low downtime and avoiding cooling or depressurization. Although the current facilities are small batch reactors, we intend to identify the operational conditions at this scale, along with potential solutions to scalability challenges, and then move to larger-scale reactor studies to minimize costs and project risk.

- Comments: This project looks to convert biomass to biocrude using sCO_2 for dewatering, liquefaction, and extraction. The scaled-up plant will also include LCA and TEA. The project is being led by two faculty members with many students and postdocs. They have recruited undergraduate students from the University of Texas at El Paso, a Hispanic-serving institution. The small-scale system that has been built though this program is quite new. The verification is complete. Students have been recruited to work on this project. The presentation outlined technological advantages to using sCO_2, but the main drawback has always been economics. The proposal does not yet have data on the economic feasibility, though given that it is widely known that the cost is prohibitive, some calculations could have been included. Estimates of the amount of sCO_2 needed per mass of biocrude would also be helpful to get some rough estimate. The team would also benefit from having someone with supercritical experience at the industrial scale, though that person may be difficult to find. The proposal does have a good DEI plan, especially with outreach and training. Recruiting from a Hispanic-serving institution is also a good step, as are the research talks at the Hispanic-serving institution.

- Response: We thank the reviewer for the valuable feedback. For the economics, we have started working on developing the TEA of the process in terms of CO_2 and biomass availability, biomass collection, biomass piles and transportation logistics, plant location, byproducts, and oil demand (and selling price contract), as some parameters. The proposed process will need at least a one-to-one ratio of sCO_2 with respect to the feed, but that is during the process, and it will not be consumed and will just act as a solvent. In the NILE process, we intend to recycle the CO_2 after usage to avoid any CO_2 loss, and one subtask is associated with CO_2 recycling via purification and pressurizing for reuse in the process. We are currently looking for partners with industrial supercritical experience for insights into potential issues at scale.
- Comments: This project must prove concepts at a batch-scale level. The success will be in the value of the graphite product, and comparing two types of pyrolysis oils is germane and appropriate. The impacts will be less on the biofuels market because it will be on the U.S. economy. The team appropriately points out that the supply chain needs to be more internal to the United States versus foreign countries, and that is easily obtainable via the biomass resources that exist in the United States. It is a project that looks at biomass use in a different way but that could have a good impact. Good diversity efforts.
- Response: We thank the reviewer for the valuable comments. The project's initial tasks are set to prove the performance improvements at the batch scale.
- Comments: The project team is developing a near-critical integrated liquefaction and extraction pathway to convert biomass and wastes to deployable biofuels. They have graduate and undergraduate students assigned to key tasks, including design, process modeling, lab experiments, and analysis of costs and life cycle GHG emissions. DEI efforts include implicit bias training, participant climate surveys, and recruitment and mentoring of students from historically marginalized groups in engineering. The project leadership team has previously supported summer research students in publishing their research. Following the "pipeline" outcomes from the project would be an interesting addition to these initiatives—for example, tracking the percentage of summer-term research students who pursue other research opportunities or return to this project or who apply to and enter a graduate program and comparing that against expected rates. The presentation mixed cost-specific parameters into its discussion of a stochastic LCA model under development, and key parameters related to the life cycle GHG emissions were missing from the list. It is unclear whether the project is fully tracking the flows of carbon throughout the pathway and end products (for example, the amount of carbon that might be sequestered in the generated chars). The project team may benefit from the services of an LCA practitioner or researcher to ensure that their accounting of life cycle GHG emissions (for which the team has a >70% reduction target) is thorough. The project is currently completing Task 1.0, the initial verification, and has been active since October 2021.
- Response: We thank the reviewer for the valuable feedback. As per the suggestion, we will include pipeline outcomes from the project to track the students, their learnings, and their path forward in research and graduate studies. Life cycle GHG emissions that originate from the feedstock logistics process (collecting, transporting, and piling feedstock), the conversion of feedstock to biocrude, and the logistics associated with moving the resulting biocrude to refineries (and other byproducts to their final destination) will be determined by the LCA from the system dynamics model (TEA) outputs. The system dynamics model for TEA will also provide the amount of biochar as an output. The carbon sequestered in the generated biochar will be determined by the LCA from the amount (and resulting final properties) of the biochar. The LCA will be performed by an undergraduate student team that will be overseen by a graduate student and an advisor from the environmental policy department.

- Comments: The challenge is the scalability of sCO_2 processing. CapEx barriers and materials-of-construction issues with equipment remain to be addressed. The team also needs to further reduce the oxygen content of the biofuels for scalability. The project is more at TRL 2 or TRL 3.
- Response: We plan to address the scalability challenges at the laboratory scale with efforts starting early in the project. We plan to modify the reaction conditions to minimize the CapEx barriers for scalable design and construction, and, additionally, these challenges will be considered in the TEA/LCA to guide the project for scalability (the TEA will include both CapEx and OpEx). Literature on hydrotreating the CO_2 extracted biofuel was found to reduce oxygen to 1.6% as the starting point. During the project, we plan to improve the conditions to further minimize the oxygen content and improve the overall compatibility of the biofuels produced. The components of the project are TRL 3, while the overall process may be at TRL 2 or TRL 3, and that is the starting point for this program.

ADVANCED LOW-EMISSION RESIDENTIAL FLUID-BED BIOMASS COMBUSTOR

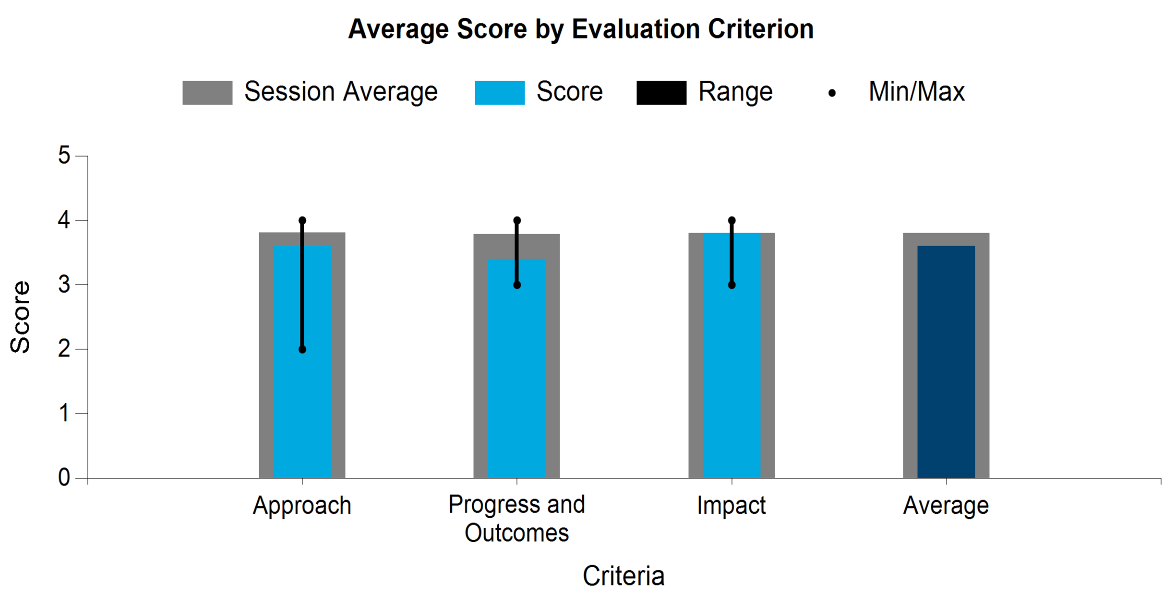
NtreTech LLC

PROJECT DESCRIPTION

WBS:	3.5.2.604
Presenter(s):	Bartev Sakadjian
Project Start Date:	10/01/2020
Planned Project End Date:	04/30/2024
Total Funding:	$3,038,823

NtreTech LLC, Babcock and Wilcox, and Ohio State University recognize the limitations of current residential wood-fired heater designs and their fixed-bed (stoker)-type operation. To achieve a step-change reduction in emissions, heater designs need to adopt more advanced combustion technologies. The novel application of fluidized-bed technology to residential wood-fired central heaters will help meet current and future regulations. Although fluidized-bed technology is currently commercially offered for large-scale utility applications, there are significant challenges to overcome to adopt the technology in residential applications. The project work will help bridge technological gaps by prototyping a transformative approach to firing wood in residential heating applications.

Fluidized-bed operation improves air/fuel mixing and increases heat transfer, which results in more complete combustion of the fuel. Due to the fluidization properties of the bed, the combustion temperature can be more uniformly controlled, which reduces the formation of NO_X. Higher combustion rates also result in lower CO and volatile organic compound (VOC) emissions. Moisture content, air velocity/staging, and bed temperature can be adjusted to control the combustion process and the emissions. The potential to use different types of bed materials, including catalytic bed additives, can further enhance combustion characteristics and decrease emissions. Due to the improved combustion process in a fluidized bed, the uncontrolled NO_X, CO, and VOC emissions are typically 10%–25% less for a given biomass fuel than for a stoker. The use of fluidized-bed technology in residential wood-fired central heaters enables a step change in emissions reductions. The use of modern sensors and low-cost microprocessors would provide the needed automation to overcome the operational complexities of a fluidized-bed wood-fired heater.



COMMENTS

- Approach: The project approach aligns with the metrics defined under (FY 2020) Topic Area 5, DE-FOA-0002203.
    - Domestic-manufactured, low-emissions, high-efficiency, residential wood heaters.
    - Quantitative goals: room wood heater—2.0 or 2.5 g/hour (cord wood alternative) particulate matter emissions limit; hydronic wood heater—0.1 lb/MMBTU particulate matter emissions limit, or 0.15 lb/MMBTU particulate matter emissions limit for forced air; amounting to a 25% emissions reduction and 5%–15% efficiency improvements.
    - Technical fluidized-bed stove/heater.
    - Project management: Babcock and Wilcox and Ohio State University as partners; NtreTech is the lead and has a process engineering specialist.
    - Issues scaling down, simplification for use, frequent load variations.
    - DEI student engagement and training, ample industry participation and guidance. Mainly skilled labor development.
- Progress and outcomes:
    - The project has completed 1 year of work.
    - The team is in the verification stage.
    - The initial stages of design, operations, and operating procedures have been conducted in the labs.
    - Downscaling from 150 MWth to 0.09 MWth was done in the past at this scale.
    - This technology is focused on chips' fluidized nature compared to other wood burners.
    - Fluidized-bed walls are heat-recuperated for hot water.
    - A steady-state fuel flow test was conducted at Ohio State University.
    - The team is reviewing cold-flow testing and modeling the pressure balance impact on a fluidized bed.
    - Process model to check for mass and energy balance and emissions/combustion efficiency load range from 25% to 100%.
- Impact: The project team has made reasonable progress on a new design for a stove. Modeling of a simplified system and the setup of equipment to verify the simplified model has been carried out. The design is bit complex for residential use and draws upon past experience on a large-scale, fluidized-bed system. Scaling down such systems is usually not easy, especially for variable-load requirements.
- The project relies on the vast experience of the company in designing larger-scale, fluidized-bed systems to design a small-scale system for residential wood heating. This heater would focus on the use of pellets or chips.
- Some fluidization work has been completed.

- The process seems too complicated for residential use, which is not monitored and transitory; however, the process shows improvement in other emissions that will likely be regulated down the road.
- This is a good assessment of key challenges. This shows a good team effort that is yielding the desired results. Using fluidized-bed technology does not seem to be a challenge because the operation is actually better at smaller scales. This team should be able to assess whether that approach is feasible from a cost and performance perspective. The desire is to produce a system that can operate unattended for extended periods of time, which will be their challenge, and they know this is an issue. It may be best suited for a central heating system than single-home use due to the potential maintenance requirements for sensors, etc. This is an area that needs to be looked at by BETO, and this team will be able to do it. Having Babcock and Wilcox as a partner is a major plus.
- This project focuses on the combustion of wood chips and wood pellets using residential-scale bubbling fluidized-bed technology. The project team has performed lab tests and design and will be fabricating a prototype and performing parametric testing. The completed progress tasks align with the project schedule. The approach includes a specific commercialization plan to be initiated in the last budget phase of the project, during which the team will be advised by an industry review committee. The project team also includes industry partners. One risk of the project is the possible complexity of a fluidized-bed heater for individual households, which may intimidate potential consumers despite automation and other simplifying features. A possible approach to mitigate this risk is to consider a different target population that is at a community scale, such as apartment buildings, college campuses and dormitories, or small-district heating networks.
- There is limited potential for the home market. The project is directed toward a more industrial user base.

PI RESPONSE TO REVIEWER COMMENTS

- The project team thanks the reviewers for providing not only the comments but also the insightful questions and discussions during the presentation. As the reviewers noted, the team brings extensive experience and background to the project and has made good progress on the development efforts. As our team progresses with our design and development efforts, we will consider the reviewers' comments in our risk analysis task as well as the design efforts and ultimately our commercialization endeavors. As noted, the complexity of the system may lead to some reluctance on the side of consumers to adopt the technology. We are mindful of the potential for the technology to impact the end user, and it is our intent to account for that and design the user interface such that it provides streamlined, simple, and easy-to-use features. Perception regarding the complex nature of fluidized-bed technology has been experienced in the past within the industrial market. The technology has since shown that it can provide ease of operation and require less operator interface than competing technologies when coupled with modern advanced controls. The project team is therefore tasked with the challenge of incorporating modern advancements in automation and controls into a residential package to help realize the advantages of the system within our target market. The operation of the unit through the various transient loads will be carried out during the Phase 3 testing and optimization tasks, which will demonstrate the system's ability to meet the desired level of operational flexibility. Transient operation is a key focus area of the project. As noted in the comments, though the development focuses on residential applications, the advances made in realizing the final design of the prototype can find applications in other markets.

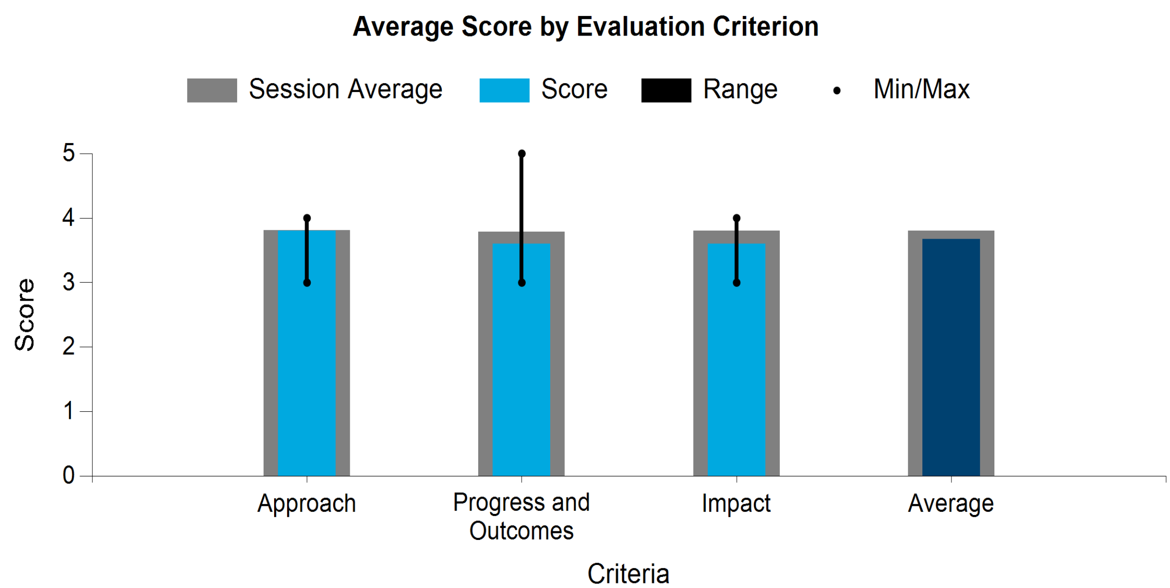
SIMULATION-DRIVEN DESIGN OPTIMIZATION AND AUTOMATION FOR CORDWOOD-FUELED ROOM HEATERS

Ohio State University

PROJECT DESCRIPTION

WBS:	3.5.2.605
Presenter(s):	Shawn Midlam-Mohler
Project Start Date:	10/01/2020
Planned Project End Date:	12/31/2025
Total Funding:	$3,143,161

The goal of this project is to position the domestic wood-fueled room heater industry to meet current and future DOE and EPA goals for efficiency and emissions by modernizing the products and product-development processes. Automation and simulation have revolutionized products and design processes in many other industry sectors, whereas these technologies have largely bypassed the domestic wood-fueled heater industry. This project will develop two wood-fired room heater prototypes to demonstrate the efficacy of these technologies to improve wood heater performance. The project team will also work to transfer this knowledge directly and broadly into the domestic woodstove industry to support their adoption of these technologies. The work unifies expertise from several organizations to form the required multidisciplinary team. The Ohio State University team brings the requisite experience in model-based design, automation for combustion/emissions control, and professional development. The University at Buffalo brings deep expertise in modeling combustion and gaseous emissions in wood combustion as well as experimental facilities for testing wood-burning appliances. ORNL provides expertise in particulate matter (PM) modeling. New Buck Corporation is a domestic stove manufacturer with more than 30 years of experience and provides prototyping capability. NAFEMS America is the primary national organization for companies conducting modeling and simulation and is well positioned to support the transfer of technology from this proposed project into the domestic woodstove industry. All partners have a track record of expertise in their respective areas.



COMMENTS

- Approach: The project approach aligns with the metrics defined under (FY 2020) Topic Area 5, DE-FOA-0002203.
  - Domestic-manufactured, low-emissions, high-efficiency, residential wood heaters.
  - Quantitative goals: room wood heater—2.0 or 2.5 g/hour (cord wood alternative) PM emissions limit; hydronic wood heater—0.1 lb/MMBTU PM emissions limit, or 0.15 lb/MMBTU PM emissions limit for forced air; amounting to a 25% emissions reduction and 5%–15% efficiency improvements.
  - Technical: Modeling and simulation-aided design of woodstoves, guided by aerospace industry practices.
  - An 8% efficiency improvement and PM emissions reduction of 65% for catalytic and 7% and 70% for non-catalytic stoves.
  - Project management: NAFEMS does education and adoption of simulation technologies and can help advance the technology.
  - NAFEM, the University of Buffalo, Ohio State University lead, ORNL, New Buck Corporation.
  - Issues: wood combustion; adoption risks for advanced models/costs of products.
- Progress and outcomes:
  - The project has completed 1 year of work.
  - The team has passed the verification stage.
  - December 2023 is the next go/no-go first prototype testing.
  - The Ohio State University CFD models and accuracy milestone has been passed.
  - Baselines stoves are meshed for CFD.
  - Two setups for testing: one at the University of Buffalo and one at Ohio State University.
  - Non-catalytic and catalytic systems are being tested for shakeout.
- The goal of this project is to work closely with the industry partner to improve their stoves based on CFD models. The project supports a number of students from two universities.
- Modeling of a particular stove has been used to see the effects mostly of modifying different aspects of secondary air. The goal is that qualitative improvements can be determined from the model and then implemented in these stoves.
- On one hand, the study is limited to one brand of stoves; however, modeling can reduce the number of costly experiments needed to optimize the wood heater. If successful, this could be a path for other heater manufacturers to improve their systems.
- I appreciated their risk analysis approach to addressing the work plan. This has the potential for implementation because it seeks to modify existing designs, not create new ones. It would have been helpful if some type of figure of merit or benchmark were provided to understand how the results were

positive, as stated in Slide 12. I am not sure the project will be able to reach TRL 7 but, surely, they can achieve TRL 6. The team should probably assess the cost of risk reduction in terms of contingency planning—scope, dollars, or time. Their estimates of efficiency may only be a modest reflection of what they can achieve. Good agreement with CFD.

- This project will develop models and automation technology to support simulations of woodstoves to be used in optimizing the design of domestic woodstoves toward low PM emissions and higher efficiencies. This has the potential for industry-wide adoption and technology improvements. The project's technical targets are to demonstrate a catalytic stove and a non-catalytic stove meeting efficiency improvement and PM emissions reduction goals by the end of the project. In this first contracted year of the project, 19% of the budget has been expended, and the work performed has primarily been simulation studies, but experimental facilities have also been established during that time, and the project team has involved multiple graduate and undergraduate students and two postdoctoral researchers at two universities. The graduate students and postdoctoral researchers are building expertise in CFD, design, and automation that will enable comprehensive modeling of the full physics of wood combustion during the project. The milestones thus far have been met as scheduled. The project team has incorporated technology transfer to the woodstove industry and mitigation of added costs into their approach and their risk management plan, increasing the chances of success in commercialization in the future.
- The efficiency improvement goals are too modest. No emissions reduction results were reported.

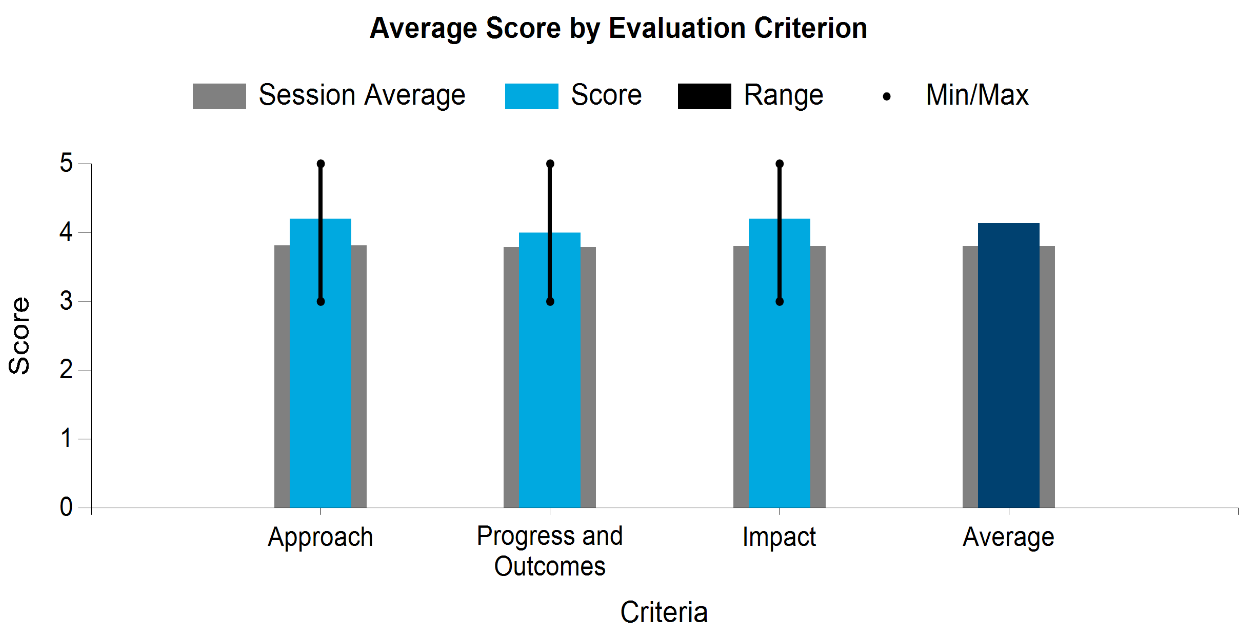
SCALING UP BIOCRUDE-DERIVED ANODE MATERIAL (BDAM)

North Carolina State University

PROJECT DESCRIPTION

WBS:	3.7.3.005
Presenter(s):	Sunkyu Park
Project Start Date:	10/01/2020
Planned Project End Date:	12/31/2025
Total Funding:	$5,492,007

The primary objective of this project is to scale up the key process ("delayed coker") for converting biocrude pyrolysis oil into high-quality graphite that is economically and environmentally preferred as anode materials in lithium-ion batteries. Lab-scale work at North Carolina State University and NREL has shown that a fraction of biocrude oils from the fast pyrolysis of woody biomass can be converted into graphite, which perform as well as commercial lithium-ion battery anode materials. The remaining biocrude is preferred for biofuels production. This project will reduce commercialization risks by scaling the initial critical carbonization process, delayed coker, which is common in most petroleum refineries. Experimental data collected in this project will be used to design, build, and operate a pilot-scale delayed coker. The reactor will be demonstrated for 500 hours with fast pyrolysis biocrude. The performance of graphite and hard carbon in lithium-ion batteries will be coupled with TEA and LCA to identify and improve the specific process steps that have the greatest impact on costs and sustainability, respectively. Once proven at scale, the new carbon materials have the potential to reduce the cost of biofuels and enhance the supply of high-quality carbon products.



COMMENTS

- Approach: The team is focusing on the production of graphite for battery electrodes with the utilization of known delayed coking processes as a key step for upgrading fast pyrolysis oils. The team comprises various university-led groups, industry, and national labs.

- Progress and outcomes: The project recently passed the initial verification and has completed only one-quarter of the work for Budget Period 1. The team has made significant progress on producing lab quantities of graphitic carbon, property comparison with commercial samples, and coupon performance tests. One proposed method is to use a catalyst for accelerated coking; this optimization was conducted. Impurity tracking and the impact of process parameters are well documented. The approach toward scale-up and work distribution is well planned.

- Impact: The team proposes a low-severity method to produce a high-demand critical material for lithium-ion batteries. Given the quality of varying types of biocrudes and intended volumes that may result if pyrolysis or HTL technologies are successful, the project is well positioned to convert biocrudes to graphite, a high-value product, by diverting some feedstock, hence improving the overall economics of the process. Overall, the team has shown great progress and is well aligned with the goals of enabling low-cost biofuels by creating additional revenue streams for bioproduct sales.

- The project aims to use pyrolysis oil to produce graphite. The team consists of multiple universities, NREL, and companies. The presenter also mentioned including a consultant who has previously worked in the graphite industry. The project will scale up a process developed by the PI.

- They have passed the initial verification and made the biocrude they will need. They are beginning to make graphite and have had batches tested. They have not yet achieved the necessary purity. They have identified issues with foaming that they need to address as they continue the project.

- There is going to be a major need for graphite to produce batteries moving forward. At the moment, there is little capacity to do so in the United States. It is not clear if that is on purpose or not. It seems that ramping up production could happen in the United States, but it has not yet happened. There are issues with reaching the necessary purity that they still need to solve. The idea that their impurities are different than those in other sources of graphite should be taken seriously because those impurities, even in parts-per-million quantities, may have a major effect on the product.

- The projected product has real value and is a high-impact material. They met the initial verification milestone. They have a new project member with experience in making graphite. The team seems adequate, and they are on track to meet their December 2023 go/no-go decision point. Their scope is good, and they should be able to provide DOE with information suitable for showing the value of the process.

- This project investigates scale-up pathways for biocrude pyrolysis oil to be converted into high-quality graphite, which is a substantial component of lithium-ion batteries. This pathway has the potential to bypass natural graphite mining and avoid its environmental impacts. The project team includes an LCA expert to accurately quantify the life cycle environmental impacts of the studied pathways as well as a TEA counterpart. They have a management plan to integrate analyses across institutions (which include academia, industry, and a national lab), and they have brought everyone together in person to coordinate within the first few months. The project started 6 to 9 months ago, and the team has multiple tasks already in progress and has completed the initial verification and production of more than 20 kg of biocrude oil by the company on the project team. Experiments on the production of biographite and analyses of its properties are underway. The project team's approach is appropriate to provide actionable data on the production of biographite and to minimize its life cycle costs and GHG emissions. This project has the potential to guide a nascent industry in the production of graphite from biomass feedstocks and to identify viable pathways for commercialization.

- The project is novel and works to address a novel need: graphite; however, the desired purity levels are still not achieved, even with acid washing. An alternate approach might need to be considered. No data on graphite quality, yield, density, etc., were provided. It would be helpful to compare it to coke-based graphite.

PI RESPONSE TO REVIEWER COMMENTS

- The project team thanks the review panel for their encouraging and thoughtful comments as well as their recognition of the novelty, work progress, management, and potential impact. Based on the reviewers' comments, we will further investigate the method to improve the graphite purity. This will include a multiple-stage acid reflux/water washing, thermal treatment (above 1,500°C), or a combination of acid washing and thermal treatment. In addition to the total inorganic impurities, we will carefully monitor individual inorganic elements because some are more sensitive than others in terms of battery performance.

SWIRL STOVE: SWIRLING COMBUSTION FOR EFFICIENT WOOD BURNING

MF Fire Inc.

PROJECT DESCRIPTION

WBS:	5.5.1.101
Presenter(s):	Paul LaPorte
Project Start Date:	10/01/2019
Planned Project End Date:	06/30/2023
Total Funding:	$1,249,747

MF Fire Inc. proposes to create and validate a novel, commercially viable technology for use in woodstove design for mixing combustion air with gasification products to achieve a more complete burn, thereby reducing emissions and increasing efficiency. This novel innovation involves the swirling of inlet air, as described in MF Fire's patent application, US 2018 / 0051886 A1. The project would leverage MF Fire's existing EPA Step 2 certified woodstove, Nova, as a baseline design with corresponding baseline data for emissions, efficiency, and CO.

A critical method to yield an optimal wood burn with low emissions and high efficiency is to homogenously mix air and gasified wood fuel in a specific ratio throughout a burn chamber. Our technology is based on proven combustion science associated with a swirl phenomenon whereby high-speed spinning air movement in a singular direction forms a vortex that centrally concentrates combustion in a burn chamber, away from walls or other impediments, leading to a near burn of available fuel, including PM. This approach has been successfully demonstrated in other fuel types (gas, diesel, oil, etc.) but never with cordwood. This innovation will lead to a substantially cleaner method for burning cordwood in a woodstove and enable industry-wide design adoption on future woodstove products.

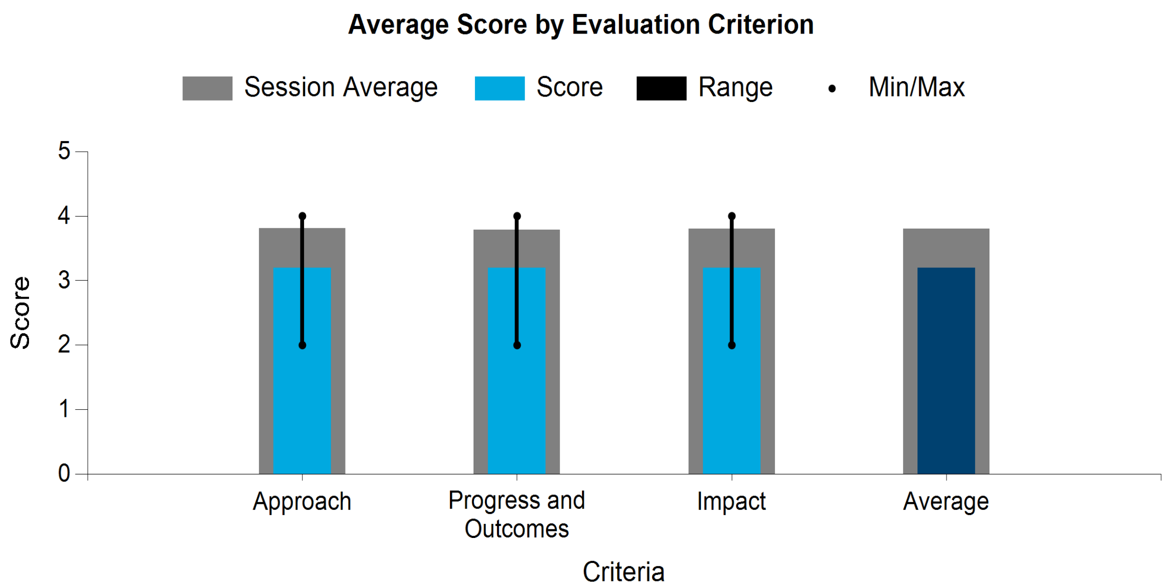
The proposed technology targets reducing particulate emissions production to less than 0.5 g/h, a 75% reduction over MF Fire's current firebox design (1.9 g/h). Initial testing of a prototype design yields significant improvements in carbon monoxide (92% reduction) and PM (PM 2.5) (75% reduction) in an open burn environment compared to testing with secondary combustion pollutant mitigation alone. These performance enhancements are comparable to the results obtained by the inclusion of a catalyst—but without the significant additional cost of the catalyst (saving consumers $300–$500). Alternatively, a catalyst can be used in combination with swirl technology for additional emissions reduction.

Historically, burn chamber geometries and airflow designs do not afford an opportunity for homogenous mixing due to dead spots, inefficient gas transport, and localized eddies, resulting in incomplete combustion and pockets of residual PM. This leads to unnecessarily high PM emissions and suboptimal efficiency. Key challenges for implementing the proposed technology involve sustaining airflow with a sufficient swirl number and an appropriate air-to-fuel ratio despite nonhomogeneous fuel characteristics.

The proposed technology will overcome imperfect, nonhomogeneous air-fuel mixtures by introducing a novel airflow system, as shown in images associated with the pending patent US 2018 / 0051886 A1. This airflow system thoroughly mixes air with fuel while concentrating combustion in a central vortex, created by the laminar, circular air movement. To optimize air-to-fuel ratio, passive (bimetallic strip) or active (air fan, electronic regulators, etc.) air control strategies will be tested and implemented.

This project has the potential to eliminate combustion inefficiencies introduced by suboptimal air movement and incomplete air-fuel mixing. The estimated impact to emissions is to reduce baseline emissions between 50%–75%, depending on the original stove burn chamber geometry and other pollution mitigation measures. It is possible, with the inclusion of a catalyst and the introduction of swirl combustion, that 0 particulate emissions could be achieved.

Efficiency gains will also be realized. A more complete burn cycle yields higher combustion efficiency because more heat potential is realized from the fuel. A lower pressure drop allows for greater heat recovery in natural draft woodstoves, improving thermal efficiency and delivered heat. In preliminary testing, net efficiency gains of 15% were achieved.



COMMENTS

- The project approach aligns with the metrics defined under (FY 2019) Topic Area 3, DE-FOA-0002029.
    - Quantitative goals: Minimum 25% reduction and 5%–15% efficiency improvement for residential wood heaters relative to the current baseline residential wood heater design. The team managed the wood heater challenge.
    - Technical: 75% reduction and overall 85% efficiency; swirling combustion.
    - The team tried conducting swirling combustion with cordwood with measuring the emissions rate to be less than the baseline 4.5 g/hour.
    - No clear DEI goals or work.
- Progress and outcomes:
    - The project claims but has not met milestones.
    - Swirl patterns were modeled in CFD to improve heat transfer.
    - Secondary air introduction approaches were used to increase swirl in the flow path.
    - Chosen swirl vane, secondary air. R1 model.
    - R2 model designs for aesthetics, removal of dead space.
    - Emissions testing is incomplete.

- Impact: The project team has prototyped a new type of stove combustor but has not met the emissions reduction and efficiency requirements. The approach is quite new and adopted from the gas flow industry, wherein flow characteristics can be controlled in a more defined manner. The project is close to the end, and it seems to have fewer chances to showcase or meet all objectives; however, if the team can continue on its own or if there is continued funding, the project may help define the requirements for a new design. The proposed design also does not meet the criterion to support the FOA goal to make the low-cost wood burners required to serve economically weak sections of society.

- The proposed wood heater uses a swirling combustion approach to decrease emissions and increase efficiency by improving mixing of the fuel and air. The project uses CFD modeling to inform the design of the heaters and experiments to carry out.

- CFD modeling has been used to help inform the system design. Though a limited number of experiments can be carried out due to the expense, the CFD modeling did help in the design. A furnace has been built with a viewing chamber to see the flame. It seems that there is still interfacing of the metallic and glass components of the heater. Unfortunately, emissions and efficiency numbers were not presented.

- The presenter mentioned that the visual appeal is currently the main selling point. The selling price will be well out of range for those who rely on wood heat for economic reasons, which is unfortunate though needed for market introduction. As a comment, the ability to retrofit this into fireplaces may be another way to increase adoption.

- The presenter made an excellent comment about the heater burning too hot, which may lead to fewer emissions at the cost of going through cordwood too quickly.

- The project has made modest progress from the last review period. It seems to be a bit slow in achieving the goals. There is concern over the ability to address risks. I am concerned about materials-of-construction issues that may arise with implementing the swirl technology. I believe the swirl technology can be successful in achieving reduced emissions. The cost may eliminate their market opportunity.

- This project is developing a partially clear chimney for a high-end woodstove that allows users to see a fire tornado while using the stove, which would have both aesthetic value and the potential to reduce PM emissions. The project team has met the milestones and completed the tasks up to completing the prototype development, including CFD modeling and testing the first prototype. The fire tornado or swirling combustion has not yet been sustained for long periods of time, and the geometry of the prototype has changed from the first to the second version for the design to appeal to the target market of higher-income consumers, which led to design and implementation challenges with the curved glass fitting the metal chimney. There is potential for commercialization, but the target market may be small, especially because this is best suited for vacation homes in remote and/or cold climate locations; however, the project team is in an industry that has reached the same target market with previous products. The efficiency of the prototype has not yet been determined and compared to existing stoves.

- The stove is focused on a very premium market and does not reduce PM emissions compared to other models on the market. There is limited adoption potential, and the increase in efficiency is not demonstrated.

AUTOMATED WOOD STOVE UFEC23

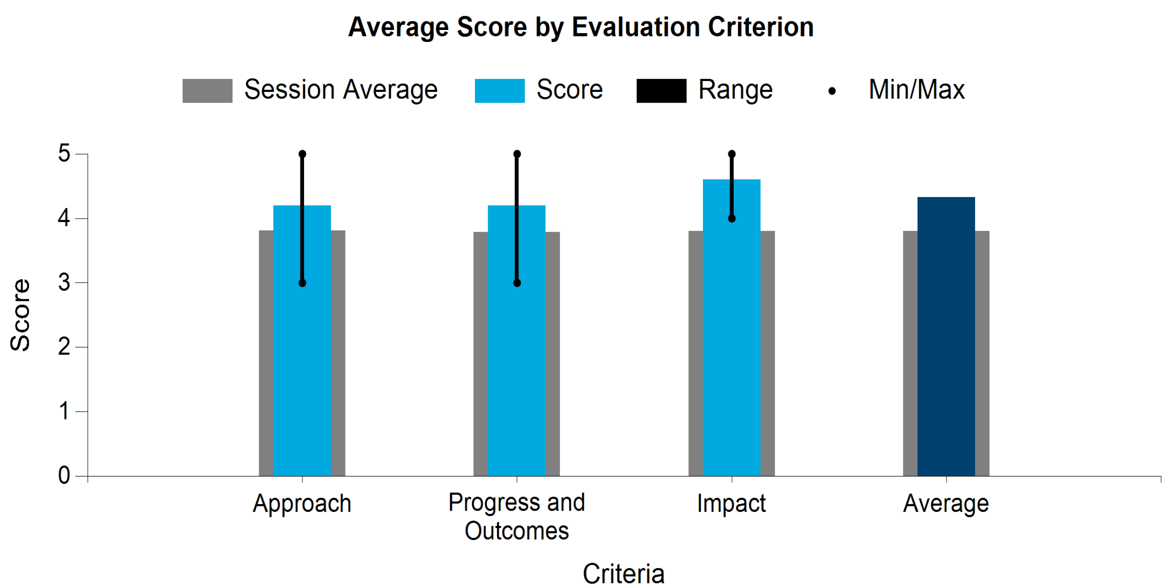
ISB Marketing

PROJECT DESCRIPTION

WBS:	5.5.1.102
Presenter(s):	Guillaume Thibodeau-Fortin; Louis-Pierre Cote
Project Start Date:	10/01/2019
Planned Project End Date:	04/30/2024
Total Funding:	$1,274,714

Our goal is to make a stove that will compensate for any "bad action" from the consumer due to their misunderstanding of the combustion process or lack of knowledge about combustion parameters in general. The critical success factors are:

- Design an automated stove that has a maximum particulate emissions rate of 1.2 g/h and an overall efficiency greater than 75% (higher heating value).
- Design an artificial intelligence algorithm that will limit emissions to no more than 2.0 g/h, regardless of the loading method used by a reasonable consumer.
- Design a stove that is easy to operate, reliable, safe, cost-effective to manufacture, and aesthetically pleasing.



COMMENTS

- The project approach aligns with the metrics defined under (FY 2019) Topic Area 3, DE-FOA-0002029.
    - Quantitative goals: Minimum 25% reduction, which aligns with BETO's FOA requirement of 50% based on a revised EPA target midway through the program
    - Technical: Flame view area, radiative heating. Smoke emissions in real time. Baseline verification and Empire Comfort System (ECS) testing

- Project management: ISB Marketing is the PI; Stove Builder International (SBI) and ECS seem to be a small, cohesive team, heavily involved in the project
- Issues: Emissions reduction, commercial acceptance, and costs
- DEI: Environmental, social, and governance policies are well implemented at the level of the company scale.

- Progress and outcomes:
  - Customer survey to understand requirements—high-efficiency thermostat integrated with remote control, and good flow in areas where heater is not installed.
  - ECS baseline testing.
  - Air intakes and electronics sensor controls; air intakes primary—primary above glass and secondary air to burn gases.
  - CFD model for steady and transient station to measure and verify flue temperature, CO_2 percentage, wood gas flow rate. Key performance indicators—increase in residence time for gas flow/PM?
  - Combustion: 80% higher heating value on low fire with non-catalytic combustion.
  - Smoke sensor optical sensor, backscattered light using ambient light.
  - Demonstrated 58% emissions reduction and 12% efficiency increase.
  - Beta prototype for EPA and safety certification.
  - Negotiating with EPA for new types of tests.
- Impact: The project team has clearly demonstrated scientific advancement and a beta prototype with the required emissions reduction and efficiency improvements. Improvements include the redesign of the airflow intake, a new test method using a smoke sensor, and improving residence time for hot air and PM in the equipment. Some of the items produced using research can be stand-alone achievements, such as the smoke sensor. The company has an open and fast approach—it is listening to customers, working with regulatory bodies, contracting with the right people, and has a commercialization path.
- The goal of this project is to automate wood heaters. The project seeks a furnace that can essentially emulate a fireplace that can monitor efficiency and smoke events in real time as well as incorporate machine learning to predict and prevent smoke events. The presentation included DEI efforts, though they were not required in the FOA.
- The company has produced CFD models of the combustion process in a simulated furnace. They have met their goals for emissions and efficiency. They have also developed a smoke sensor that can be used to monitor emissions. They are at the point where they have a prototype that they would like to start commercializing. The machine learning portion was not a success and was dropped from the project.
- The fact that they are about ready to sell a real unit is great. It would be interesting to know if these units could be retrofit into an existing fireplace.
- The project obtained sufficient results from new designs to produce improved results for this technology. The team made a good analysis of challenges and then went forward to address them. The final effort

will be telling as to the value of these advancements to the SOA. This is a good team that is involved throughout the process.

- The project team is in the beta prototype step of developing an automated wood stove using machine learning to prevent smoke events and increase efficiency. The approach aims to compensate for improper woodstove user behavior. The prototype tests have demonstrated emissions reductions and efficiency increases. The project team is on track to have 25 automated stoves installed in homes in the coming winter. To meet the needs of the target population, the team is analyzing how to reduce the stove's cost while the beta prototype is being developed. There is an opportunity for sharing their air emissions testing data, combustion CFD simulation graphics, and comparisons of automated controls to standard user control on a website shared on flyers by local stores in communities that might be the most affected by the PM emissions of household stoves, thus reaching more of the target population and increasing commercialization success. The team's approach, progress, and outcomes appear promising.
- The project is more focused on the expensive end of the consumer base; however, eventually automation and technology improvements would be beneficial to the industry. I recommend ongoing support for the industry as a whole to develop lower-cost technology solutions.

PI RESPONSE TO REVIEWER COMMENTS

- Thank you all for your comments. To provide a short update, we are continuing to improve the combustion algorithm using the signal of the smoke sensor. A complete prototype was built and is much closer to the end-user product. We had great news from the EPA: We will be able to install our product in 25 homes in the United States and Canada and have them burn for a full season before doing the emissions certification testing. This will allow us to update the combustion software following real-life experience. The conditions still need to be written and accepted by all involved parties. This news delays the discussion on the test method to use. We will wait to see how the industry adapts to the cordwood testing restrictions. SBI will attempt a certification testing using a new method on another wood heater; their experience will guide our choice for the test method. Currently, we are doing multiple different looks to present to our distributors in a few weeks. After, we will build a program to find 25 participants. The goal of the project is to test multiple technologies in the field to find what is reliable enough to go for mass production. Our wish is to be able to provide myriad wood-burning products that will introduce new technologies to the market while being affordable (small to large stoves and small to large inbuilt fireplaces).

FIRE MAPS – SECURE PERFORMANCE MONITORING AND USER ALERTS SYSTEM (FOR WOOD-BURNING STOVES)

MF Fire Inc.

PROJECT DESCRIPTION

WBS:	5.5.1.103
Presenter(s):	Paul LaPorte
Project Start Date:	10/01/2019
Planned Project End Date:	03/31/2023
Total Funding:	$1,245,144

All woodstoves are dramatically more polluting in real-world use than in a test lab. This is due in part to users who do not have sufficient knowledge or data to guide them in proper woodstove operation. MF Fire proposes to create a unique, commercially viable technology for woodstoves, called Fire MAPS (Monitoring, Alerts, and Performance System), for delivering secure, real-time performance monitoring and user guidance to improve user control and stove burn management in any existing woodstove, thereby reducing emissions and increasing efficiency. This technology establishes a first-ever comprehensive burn database that securely captures detailed burn information that enables regulators and clean air advocates to understand real-world stove use and make informed policy decisions. The use of inadequate burning conditions in woodstoves can cause an emissions increase as high as sixfold over controlled, ideal burns.

This technology would comprise (1) sensors, (2) a controller, (3) a user application or display unit, and (4) a burn database. Sensors include multiple thermocouples, a door, and bypass monitoring. The controller is an Internet of Things device, including a central processing unit and wireless connectivity. The user alert system delivers information via an application to a user device. The database powers the guidance and alerts the engine. The Fire MAPS system could be used in both new and existing woodstoves, enabling large-scale adoption for vast emissions reductions and efficiency gains. This innovation leverages unique insights gained from users of MF Fire's Catalyst (EPA Step 2 certified) woodstove, which is equipped with data-collecting sensors and a basic user alert system triggered by sensor data.

Sensor data provide critical information triggering real-time user guidance on what action to take to achieve the best results regarding low emissions and high efficiency during real-world use. Monitoring and guidance would cover a broad set of conditions and events, such as:

- Combustion phases: cold start, steady state, overfire, long/slow burns, and burnout.
- State transitions: ignition, warm reload, catalyst engagement, overfire, and door open.

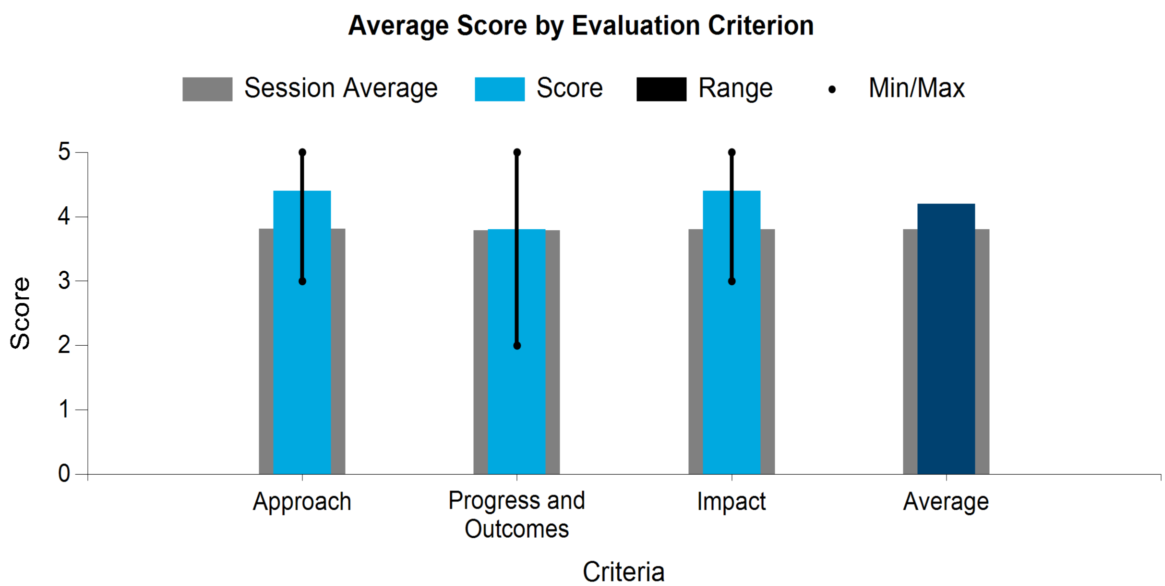
Guidance would be proactively sent to a user's device, including cell phone, tablet, or other display. This project would leverage Nova (EPA Step 2 certified) for baseline data.

Burn information would be securely and anonymously stored in a burn database to provide a comprehensive view of burn habits and real-world use, from which machine learning would help continuously improve guidance and alerts, resulting in further emissions and efficiency gains. This unique database, referred to as the Fire MAPS Database, could be used by various agencies to aid in air quality management decisions and to provide supporting evidence that various DOE and EPA programs have a positive impact.

User-specific contributions to woodstove emissions have been reported as high as a 600% increase over certified stove baseline emissions. This technology could address and suggest improvements to all these deficiencies. MF Fire estimates that the proposed technology will significantly improve user behavior and eliminate greater than 60% of user-contributed emissions, or approximately 300% of a stove's certified emissions level.

The proposed technology overcomes users' knowledge limitations and woodstove operation errors by automatically monitoring the stove's key performance indicators and providing real-time guidance that allows users to implement best practices and learn proper operation.

This project has the potential to eliminate excess emissions and improve low efficiency due to poor stove management, insufficient knowhow, and burn information. The estimated impact is a 60% real-world emissions reduction measured from in-home burning. Fire MAPS could be installed on up to 500 stoves for a pilot as part of the project to populate the burn database and expanded through commercial sales after the project to encompass thousands more.



COMMENTS

- Approach: The project approach aligns with the metrics defined under (FY 021) Topic Area 4, DE-FOA-0002936.
    - Quantitative goals: room wood heater—2.0 or 2.5 g/hour (cord wood alternative) PM emissions limit; hydronic wood heater—0.1 lb/MMBTU PM emissions limit, or 0.15 lb/MMBTU PM emissions limit for forced air; amounting to a 25% emissions reduction and 5%–15% efficiency improvements.
    - Technical software/hardware platform to reduce user-contributed emissions for nonoptimal use. It has been noticed that user-contributed emissions can be as high as 600%.
    - Hypothesis: Monitor performance in real time; helps eliminate 50%–80% of user-contributed emissions if used correctly based on guidance.
    - Mimics user conditions in the lab to create data matrix and measure impacts.
    - Uses this data to create software/hardware solution.

- Guidance system to act on basis.
- Project management was not discussed much.
- Issues: These were well discussed, and there is a need for a software/hardware system; see above.

- Progress and outcomes:
  - Fifty home trials have been completed.
  - The project has been able to collect more data than planned—30 days versus 2 years.
  - Long-term use in many cases is not 30 days, but it is the best data available.
  - The goals achieved over the large data set are not known; however, point-of-reference results show reduced emissions and increased efficiency.
  - The system includes a door sensor, thermocouple, and a stack thermocouple coupled with the controller, cloud, and application.
  - Baseline user profiles were created to compare with post-controller installed profiles. Anecdotal evidence shows a 38% reduction in emissions for a small set of data.
- Impact:
  - The project team has created a hardware system coupled with cloud and real-time guidance for customers to take action to reduce emissions and increase efficiency. The tool is model agnostic and can be used for all types of furnaces. It addresses a major concern that user-contributed emissions are much higher than the furnace rating. This allows for user training and helps reduce emissions. It can have a major impact. See above for the data analyzed thus far—38% reductions have been demonstrated, which is very significant given that wood burners have 600% emissions due to improper use. This scheme allowed for 38% reductions, which is equivalent to 600*0.4 = 240%, more than twice the base emissions rating.
- The goal of this project is to develop software that informs heater users on how to better manage their wood heater system based on their behavior collected over some time period. The software system is potentially educational as a short-term device or more performance related as a longer-term device. The device can be self-installed for personal use.
- The software/hardware platform has been developed. Their database collects information on individual users, so in that sense it can educate users about their own heater system.
- The communication relies on electricity and wired home access, which could be a problem for some disadvantaged populations or those who have the furnace in a secluded seasonal home. Communication that relies solely on cell phone access would be an improvement. The ability for the user to input their own data, such as log size, and to include atmospheric information, such as temperature/humidity, is good to have. If it does not have it, something that shows how much more efficient the heater system is using their software would be meaningful to users. A more robust system that uses more sensors may be desirable to some end users as well.
- Technologically, this project has produced a product that can help operators of wood-burning stoves achieve better operation, leading to reduced emissions and improved efficiency. Their initial results are encouraging and could lead to wider incorporation into operating units. They do need a larger sample

size because the limited testing size may not be sufficient. The education risk is high, as evidenced by other attempts to introduce technology to the public that falter after extended use. The team needs to ask themselves how much contingency is needed in their plans to achieve the predictability of having a reliable and useable product. The cost to the user is not too exorbitant, allowing for broader market adoption.

- This project addresses a critical concern in the use of woodstoves: suboptimal user behavior. The project team made a test matrix of user behaviors and then tested it in a lab and measured the impacts of those behaviors on emissions from woodstoves. This informed the creation of a free technology-agnostic application with notifications linked to a $299–$399 sensor installed by users, which is a similar setup to smart thermostats (though those are automated, and automation is not permitted in retrofitting existing woodstoves), and thus has high potential for commercialization and woodstove user adoption. The emissions from woodstoves resulting from user actions are timing-dependent and require real-time feedback to inform a user on what to do to decrease emissions, so the use of an application to direct user behavior is an impactful approach. The project team conducted more than 50 in-home trials with woodstove owners and monitored them over time to collect data on how the application (Fire MAPS) affected user behavior and unnecessary emissions. Eighty percent of test users were still using the device after the 30-day trial period, and some continued to use it two seasons later. The project team is discussing collaborations with local air quality boards who are interested in this new approach to decreasing PM emissions and has also developed a customer support and research tool with an interface that displays emissions data over time. This project has high potential for significant impact to PM emissions from woodstoves and high commercialization potential.
- Improvements in automation are not necessarily resulting in any higher PM reduction or energy efficiency. The data presented are anecdotal (five users only).

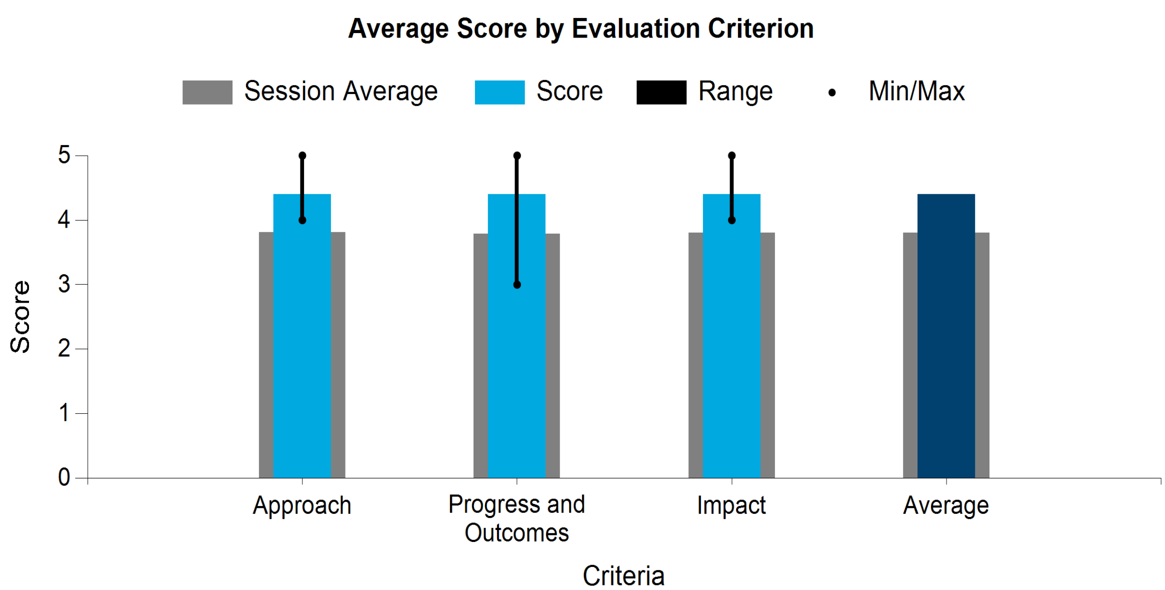
ADVANCING WOOD HEATER EVALUATION METHODOLOGY FOR ACCELERATING INNOVATION—LBNL, BNL

Brookhaven National Laboratory

PROJECT DESCRIPTION

WBS:	5.5.1.105
Presenter(s):	Rebecca Trojanowski
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2022
Total Funding:	$1,995,692

Brookhaven National Laboratory and Lawrence Berkeley National Laboratory aim to accelerate wood heater innovation and commercialization by developing rapid, cost-effective performance test methodologies for biomass-fired heaters. These simplified methods aim to reduce R&D cycle times, allowing manufacturers to efficiently evaluate performance metrics before costly certification. This project aligns with BETO's mission to support the development of low-emission, high-efficiency wood heaters, enabling broader access to clean and affordable heating solutions. Challenges lie in accurately measuring emissions, and considering concentrations, types, and burn phases, all while managing the associated costs. Our literature review explored current certification and measurement methods with recommendations for simplified methods, informing our technical approach. Specifically, our approach developed instrumentation suites suitable for both laboratory and field use. Cost considerations were paramount, but accuracy and range were also prioritized to effectively measure a spectrum of emissions, from cold start emissions to steady-state emissions. Furthermore, three virtual workshops were hosted as part of the 5th Wood Heater Design Challenge to discuss advances in wood heater design and technology, instrumentation advancements, and adoption of new technologies.



COMMENTS

- The project approach aligns with the metrics defined under (FY 2019) Topic Area 3, DE-FOA-0002029.
- Quantitative goals: Minimum 25% reduction. This aligns with the 50%–80% (in the FOA) because a standard was revised, reducing emissions to half, midway through the program, so, overall, 25% is equivalent to 50% emissions reductions relative to their current baseline residential wood heater design.

And 5%–15% efficiency improvement for residential wood heaters relative to their current baseline residential wood heater design. The team managed the wood heater challenge.

- Technical scope: Low-cost measurement method simplifying the method to test—ASTM E2779; utilize inputs from industry on standards and test method requirements.
- Project management: The Alliance for Green Heat is a collaborator, the rest of the team is from LBNL.
- Issues: Wood heating is a relatively higher emissions sector compared to comparable high-temperature industries in other sectors. It is used because of a lack of income and/or no connection with gas or the electric grid.
- Progress and outcomes:
    - The team has made significant progress on identifying and meeting the test methods. Challenges include emissions—carbon rich, flue gas flow, measured gas phase CO_2/CO; stack loss measurements for efficiency. ASTM E2779 was used to verify the stoves at different labs using the same fuel feedstock.
    - Flow measurement through dilution tunnel for flue gas; VOC, PM, and gas phase measured, also velocity.
    - Community engagement: three workshops—100 participants; industry feedback; innovations in the European Union were well incorporated.
    - Three winning teams were identified.
- Impact: The project team has clearly demonstrated scientific advancement and simplification to guide the industry on the measurement of emissions and help them standardize with some limitations. The goal of this project seems to provide a platform for testing and unification and serves as a resource for the industry to go back and look at their innovations and help them get tested. The EPA considers all the work that goes to the national labs. The winning teams get an opportunity to come test at the labs.
- This project has multiple national lab partners acting as a resource for wood heater manufacturers by developing protocols, analysis, and measurement tools that can be used to verify performance measures. They act as an interface to take inputs from manufacturers and to support them.
- The labs have set up validation facilities, developed simpler protocols, developed a user interface for analysis, and held workshops to engage and connect stakeholders.
- It is important for manufacturers to obtain this help and guidance to reduce the R&D barrier. A major issue with wood heating is the tendency for lower-income communities to rely on wood heating, and thus expensive solutions will not always be the best even though the profit margins may be higher. The role that the lab participants are playing is critical and a good fit. An industry consortium is not likely due to the fact that many companies are smaller and not able to participate in a consortium-type exercise.
- National labs provide an independent analysis for addressing the problems of emissions. They have provided an early assessment of possible improvements but also, even more importantly, the development of analytical methods that can be used. The issue will be how viable are these measurement methods going to be, and that is what they are evaluating. This effort is needed to begin to address the issues of achieving efficient wood-burning stoves. The effort is designed to be used as a monitoring tool, not a certification. There is good attendance at workshops. The involvement of the stakeholders and communities is commendable.

- The Wood Heater Design Challenge has a demonstrated impact as a previous winner has secured their own project funding and further developed their technology. The project team has also completed reviews of test methods and recommended and developed simplified woodstove emissions measurement methods. The wood heater industry has been vocal about challenges involved with certification test methods, so these outcomes from the project are aligned with industry needs. The project team has convened community engagement workshops and competitions beyond the Wood Heater Design Challenge, which catalyze exploratory R&D in this field. The project has less than 1 year remaining, and it has been achieving its milestones as scheduled. Its unique programs have brought greater attention to the needs of the wood heater industry and have supported the commercialization of promising technologies.
- The work is merited and is needed in the industry to standardize wood heater designs and provide ratings to the consumers. This is a very effective project and addresses several sustainable justice goals. It is highly recommended.

DEVELOPMENT OF FORCED-AIR COMBUSTION SYSTEMS WITH AUTOMATED CONTROLS TO REDUCE EMISSIONS FROM CORDWOOD ROOM HEATERS IN EVERYDAY USE

Oregon State University

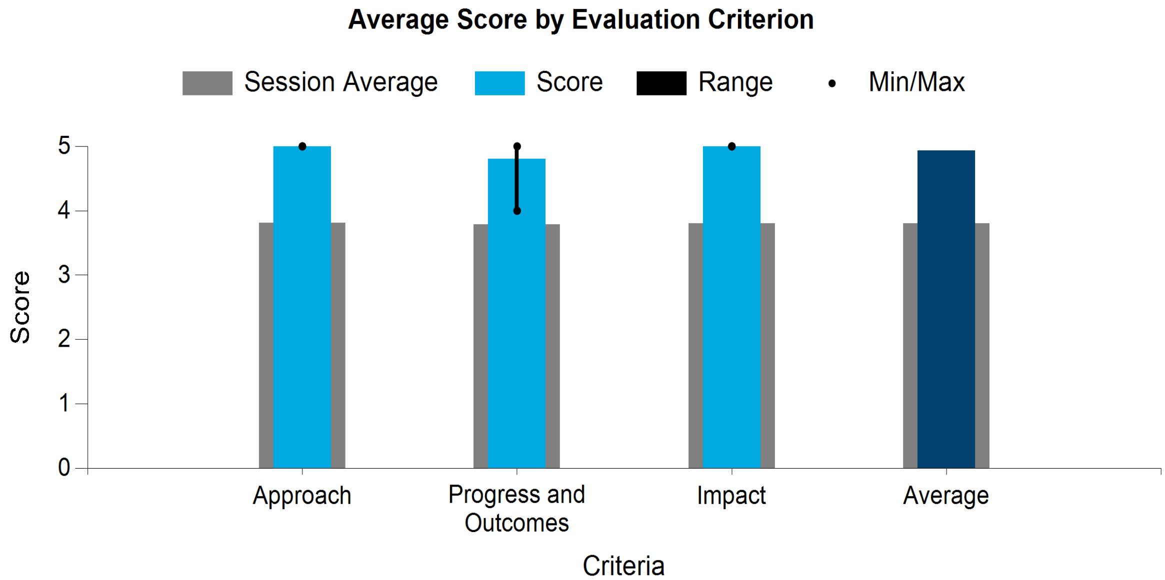
PROJECT DESCRIPTION

WBS:	5.5.1.106
Presenter(s):	Nordica MacCarty
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$3,127,067

This project aims to undertake the development needed to reduce PM emissions throughout the real-world burn cycle of cordwood room heaters by incorporating turbulent jets of forced air into the firebox. To achieve this, we will develop two retrofits that bring common legacy wood-heating stoves up to 2020 EPA emissions and efficiency requirements under the real-world operating conditions identified by extensive user research. The major tasks to achieve these outcomes include fundamental combustion experiments with small- and full-scale prototypes to inform lightweight models that will be used to develop prototypes that will be operationalized with closed-loop sensors and control algorithms. Plans are also in place for market transformation with regulatory oversight and with knowledge sharing among partner manufacturers and the industry at large.

The impacts of this work include the development of a technology and design rules that reduce PM 2.5 during both ideal and nonideal (e.g., wet wood, overfeed) operating conditions. Addressing issues with the latter is particularly important because these conditions contribute the most to PM 2.5 emissions yet have often been neglected during R&D. In addition, initially focusing on retrofit technology is key to enabling rapid and affordable implementation in underserved and tribal communities that suffer disproportionate health effects from wood smoke exposure.

Our team includes faculty and students from mechanical engineering and anthropology at two OSU campuses, Aprovecho Research Center, Blaze King Industries; three tribal communities in the Pacific Northwest; as well as industry, regulatory, and tribal advisory groups.



COMMENTS

- Approach: The project approach aligns with the metrics defined under (FY 2021) Topic Area 4, DE-FOA-0002936.
  - Quantitative goals: room wood heater—2.0 or 2.5 g/hour (cord wood alternative) PM emissions limit; hydronic wood heater—0.1 lb/MMBTU PM emissions limit, or 0.15 lb/MMBTU PM emissions limit for forced air; amounting to a 25% emissions reduction and 5%–15% efficiency improvements
  - Technical forced-air combustion; detailed combustion diagnostics chemical reactor network modeling to 2020 EPA guidelines
  - Project management guidance from industry; regulatory and tribal advisory; OSU, Aprovecho Research Center, Combustion Consulting Services, Blaze King Industries, Nez Perce Tribe; communication map seems complex but is per budget period in terms of type of communication needed
  - Design retrofit for the two most common types of used stoves
  - New project, in the seventh month, has not yet reached any go/no-go
  - The DEI project has active team members from underserved communities. The PI has a legacy of working with nonprofit organizations.
- Progress and outcomes:
  - The team is developing a combustion model using sophisticated laboratory equipment. They are ahead of schedule in the setup of the system that is required to make these measurements. The team is creating a chemical reactor network model. They are performing a baseline, prototyping, and user tests. They are focusing on market transformation and open-source design. Note that these tasks are for a period of 46 months; the project is in the seventh month.

  - Verification test baseline: 9.36 g/hour; forced-air system: 1.63 g/hour, 82.5% reduction meets criterion; baseline versus tested: 79% versus 81%.
  - The team has made great progress; it includes an advisory board from industry, regulatory, and tribal advisor.

- Impact: The project team has made significant progress in 7 months. In terms of the emissions reductions and efficiency improvement over the chosen baseline of the most commonly used stoves using forced convection, the project is promising. Overall, the team has maintained high momentum on all Tasks 1–5, and although this is not required, this will help a lot with the project's success and in forecasting challenges. The proposal is open source, directly targets low-income populations and their choice of stoves; they are performing community testing at an early stage. The team has made good use of sophisticated lab equipment to correlate data versus field-testing. This is an excellent team, and they have made great progress.
- The team consists of university, industry, tribal, and regulatory stakeholders who seek to bring legacy stoves into compliance through retrofitting using forced-air jets. The results will remain open access in that design rules will be published. The approach consists of a well-thought-out DEI plan.
- The team has started all tasks and has started measuring furnace efficiencies. The plan is to go with manual control first, then implement automatic process control.
- This project truly addresses the social justice issues associated with wood heating. Improvements in wood heating, if appropriately focused on, as this project does, can improve the health and welfare of communities that rely on wood heating.
- The team did a good job of identifying risks and an approach to mitigation. The potential to retrofit is real. There is some concern over the materials of construction for the forced-air system. They need extended testing to see if the whole approach holds up. They may want to look at retrofitting options for other stove configurations. They have an excellent risk analysis. They have made systematic progress. They have a particularly aggressive approach to involve underserved communities and hence to reach potential stakeholders and users.
- This project aims to develop design rules and a retrofit kit for existing woodstoves, with automated controls and forced-air fans, that fit the needs of underserved populations relying on cordwood heaters. The lead project team at OSU has a variety of partners on the project, involving tribes, research centers, and industry. There is a structure to their integration and collaboration, and it appears that there has been communication and progress on all fronts within these first 7 months of the project. The project team is well designed to perform impactful and reliable research; it includes an anthropologist who is conducting the user needs assessment survey, and the lead has a 25-year record in cookstoves for underserved populations. In these first 7 months, the team has passed their first go/no-go decision point, conducted more than 50 interviews with various stakeholders, obtained lab and field equipment after consultation with advisors, and began collecting data through field and user tests—while spending only $17,021 of the budget. The project has a thoughtfully developed DEI plan as well as a dissemination plan that shows high potential for implementation success of the woodstove retrofits. The cost of the retrofits are also considered; although the parts are currently roughly $400 per stove, the project team aims to develop a training program for tribal members to be installers in their communities. Overall, the project has stellar potential for impact, has made excellent progress with useful outcomes, and has a genuinely well-developed and effective approach.
- The team shows strong work with a good DEI plan and community engagement. Even by the seventh month, they have achieved the majority of the project's goals. The reviewer has no concerns regarding

higher heating value. I am wondering what happens when the power/forced air is not available. Preheating of incoming secondary air should be explored. The reduction in carbon emissions does not include the energy for the fan. It is important to highlight the social justice impact and participation of the PI. The project PI clearly demonstrated an excellent passion and ownership of the goals. I strongly recommend additional support and funding on the same. Clearly, this is one of the exceptional presentations at the 2023 Project Peer Review.

PI RESPONSE TO REVIEWER COMMENTS

- Our team sincerely thanks the reviewers for the detailed feedback, kind words, and encouragement about our approach. We appreciate the notes to consider the impact of power outages, secondary air preheating, forced-air construction/durability, and carbon accounting of electricity usage, and we will look into each of these during the project. We look forward to continued progress in these areas and sharing results as they are available.

CLEAN COMBUSTION TECHNOLOGY WITH EFFICIENT AND AUTONOMOUS WOOD HEATER OPERATION OVER THE FULL CYCLE

The University of Alabama

PROJECT DESCRIPTION

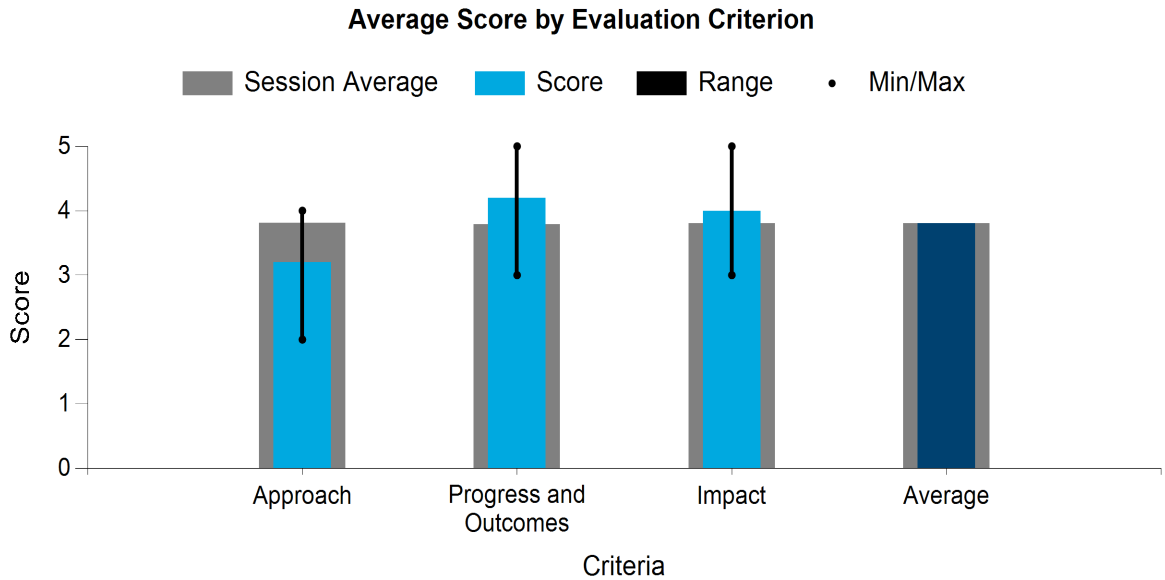
WBS:	5.5.1.107
Presenter(s):	Ajay Agrawal
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$2,080,683

The objective of this project is to develop a modern non-catalytic wood heater for residential applications using wood chips, cordwood, and wood pellets. Experimental and computational techniques will be used to advance the wood heater technology in four areas: (1) novel and innovative designs of combustion chamber geometry, airflow distribution, mixing of combustion air with gasification products, etc., to reduce emissions; (2) thermoelectric generators (TEGs) to produce electricity and manage battery power distribution to operate the wood heater independent of the grid; (3) effective heat extraction methods to increase the average efficiency; and (4) automation to optimize the operation for all phases of the wood-burning cycle, including startup, steady state, overfeeding, overnight burn, and burnout. All electrical and mechanical systems will be integrated to produce the wood heater prototype for testing. The project will use a baseline wood heater that meets the 2020 EPA regulations and is sold by our industry collaborator.

Clean combustion will be achieved by segmenting the combustor into distinct primary and secondary zones, and combustion air will be supplied by forced convection as opposed to natural convection in current systems. The combustor design will demonstrate a reduction in PM emissions by 25%–50% compared to the 2020 EPA emissions limits. Stand-alone power will be generated by solid-state TEGs integrated into the wood heater to ensure that a surplus of energy will be available to replenish the energy stored in a battery during the burn cycle. The electrical and thermal subsystems will be developed independently, and then the combined system will be integrated with the wood heater. Heat removal by radiation and natural convection will be supplemented on demand by convection heat transfer using strategically located variable-speed fan(s). The final system will demonstrate an increase in efficiency of 5%–15% compared to the baseline design. The wood heater will be automated through the evaluation of robust sensors, controller hardware/software development, and a smart control algorithm to convert sensor outputs into control signals to vary the speeds of combustion and convection airflow fans in real time. A prototype will be built and undergo extensive dilution tunnel (following EPA Method 5G) testing to optimize and quantify performance over the complete wood-burning cycle. The total cost of the wood heater installation is expected to remain within 10% of the total cost of the baseline system. The final prototype will be integrated with smart apps and will be ready for field-testing.

The wood heater developed in this project will operate at high efficiency and produce low emissions during all stages of the wood-burning cycle. The heat release rate in the wood heater will adjust to the heating load demand of the residence to always attain high efficiency. It will be a direct vent system, the first of a kind in the industry; replacing the flue pipe with a vent pipe will increase efficiency and save costs both for installation and maintenance. Results of the study will be widely disseminated to help the wood heater industry and the technical community at large.

Major participants of the project are the University of Alabama, Unforgettable Fire LLC (a small U.S. business with existing wood heater products in the market), and Virginia Tech.



COMMENTS

- Approach: The project approach aligns with the metrics defined under (FY 2021) Topic Area 4, DE-FOA-0002936.
    - Quantitative goals: room wood heater—2.0 or 2.5 g/hour (cord wood alternative) PM emissions limit; hydronic wood heater—0.1 lb/MMBTU PM emissions limit, or 0.15 lb/MMBTU PM emissions limit for forced air; amounting to a 25% emissions reduction and 5%–15% efficiency improvements Technical: Two-stage combustion gasification followed by combustion.
    - Fan-assisted heat extraction.
    - TEG to produce and manage power.
    - Automation for phase burning.
    - Project management: Virgina Tech CFD analysis.
    - DEI not mentioned.
    - Issues: Natural conversion control; catalytic high performance cost.
- Progress and outcomes:
    - The project is in the early stages and has just completed verification.
    - The team is using a component-level testing approach.
    - The baseline heater chosen is high efficiency, 1.3 g/hour and 79% efficient. This is a high-level baseline to improve beyond the market requirements.
    - The team installed a new katydid heater.
    - The team installed a soot measurement system.

  - Modeling prep work was conducted by partner Virginia Tech at the early stages.
  - The team created a 2D model, 3D concept, and fabricated a prototype.
  - The TEG design and prototype work was shared and tested to verify the vendor specification.
- Impact:
  - The project team has made significant progress in the very early phases of the project.
  - This is an expensive design but an exceptional project at a university that definitely advances the SOA and allows industry to pick and choose features that are commercially relevant. The team has high baseline and high performance goals, which is great, but they may be implemented in a smaller market. Nevertheless, the university project is on the right line. Something that might help the project and was highlighted by other reviewers as well is a focus on ash management and its impact on downstream TEG. Consider or estimate the use of wood as a fuel required for partial oxidation to overcome endotherm for gasification and its impact on overall efficiency. The DEI lacks details and is mostly built on Alabama University's existing practices. It is bit overlooked at the early stages of the project, and it can be improved.
- The project includes two universities and one company collaborating on a two-stage combustion process. The proposed heater includes forced air, two-zone combustion, TEG, and automation. The DEI plan is not very well detailed beyond working with university offices.
- Verification has been completed, and a prototype for their idea has been built. Work has been done on TEG and CFD modeling.
- The proposed furnace contains many key elements that will be valuable to better understand individually as well as in a complete system. The design is unique and complex on a technical level, relying on forced air, but it seems reasonably simple for a potential user.
- This is a good approach to looking at the combustion dynamics to craft a wood-fired system that is not normally employed in wood-burning operations. The team has made progress toward a prototype that will need validation, but they have a good plan for getting there. Some aspects of the downdraft combustion effort could improve overall efficiencies, such as heat transfer to the environment, and also augment heating the combustion chambers. The team has a good grasp of combustion issues and should be able to provide answers on the feasibility of this approach if they can get it all done. There is concern about the level of work to be done and the ability to complete it. There is little light on DEI efforts, i.e., they have offloaded that to others and perhaps need to take a larger role in that.
- The project, which started in December 2022, has completed initial verification, built a prototype of a dilution channel, and built a prototype wood heater to test individual improvements toward the goal of developing a two-stage combustion, automated wood heater with fan-assisted heat extraction and TEGs. The thermoelectric module has been designed, and preliminary laboratory tests have been conducted. Although the project is only within its first few months, it has been developing at an expeditious pace. The wood heater improvements are expected to reduce emissions and improve thermal efficiency relative to the baseline design of the industry partner. Ultimately, the results could be extended to new designs of other wood heaters, thus producing a useful impact throughout this industry. One weakness in the project's approach is their DEI plan. It appears to rely on existing efforts at the lead institution and nearby minority-serving institutions, which may cause an unjust burden to those who are working to improve DEI outcomes and who are expected to support the project without budget items allocated to their efforts. Beyond the intended engagement and recruitment of students from historically marginalized

communities in science and engineering, there is a missed opportunity to test unique ways to engage stakeholders who use wood heaters to meet their needs in the design of the autonomous wood heater or to identify ways to reduce costs in the final design so that the wood heater has commercial success if its target population is rural, low-income households.

- The DEI plan is quite weak and needs to be further developed. The integration of different unit operations is lacking, and the overall prototype design still needs to be optimized.

SYSTEMS DEVELOPMENT AND INTEGRATION: SCALE-UP

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Systems Development and Integration – Scale-Up Portfolio (SDI-SUP) Technology Area is one of 12 technology areas reviewed during the 2023 Bioenergy Technologies Office (BETO) Project Peer Review, which took place April 3–7, 2023, in Denver, Colorado. A total of 28 presentations were reviewed in the SDI-SUP session by five external experts from industry and academia. For information about the structure, strategy, and implementation of the technology area and its relation to BETO's overall mission, please refer to the corresponding Program and Technology Area Overview presentation slide decks (www.energy.gov/eere/bioenergy/systems-development-integration-scale-portfolio).

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $93.7 million, which represents approximately 17% of the BETO portfolio reviewed during the 2023 Project Peer Review. During the Project Peer Review meeting, the presenter for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their approach, impact, and progress and outcomes. This section of the report contains the Review Panel Summary Report, the Technology Area Programmatic Response, and the full results of the Project Peer Review, including scoring information for each project, comments from each reviewer, and the response provided by the project team.

BETO designated Robert Natelson as the SDI-SUP Technology Area review lead, with contractor support from Remy Biron of Boston Government Services. In this capacity, Robert Natelson was responsible for all aspects of review planning and implementation.

SYSTEMS DEVELOPMENT AND INTEGRATION – SCALE-UP PORTFOLIO REVIEW PANEL

Name	Affiliation
Ray Miller*	Verdecute Consulting
Joaquín Alarcón	Catalyxx Inc.
Susan van Dyk	University of British Columbia; SVD Consulting
Mary Dinh	Avangrid Renewables
Siva Sivasubramanian	Independent consultant

* Lead Reviewer

SYSTEMS DEVELOPMENT AND INTEGRATION – SCALE-UP PORTFOLIO REVIEW PANEL SUMMARY REPORT

Prepared by the Systems Development and Integration – Scale-Up Portfolio Review Panel

INTRODUCTION

The SDI subprogram was reviewed by a team of industry subject matter experts at the request of BETO management. The projects reviewed covered a wide range of areas, including:

- Project risk management
- Biomass pretreatment equipment improvements
- Adding value from lignin market development
- National laboratory process development and demonstration facilities
- Algae deployment
- Bio-based alcohols to advanced fuels
- Biomass processing to advanced fuels
- Biogas processing to advanced fuels.

STRATEGY

The BETO 2023 plans and strategies across the portfolio are strongly consistent with the current national goals for climate-impacting carbon emissions. The primary concern of this review panel centers on the robustness of the technologies being developed, which need to be both effective and economic to ensure implementation. This concern points to the need for a critical assessment of the funding and probability of success for each program so that a go/no-go decision can be promptly made before the demand for resources starts to dramatically ramp up.

The SDI portfolio has a clear set of goals and targets. It has significantly benefitted from industry and stakeholder input during the past few years, and now it is focused on greenhouse gas (GHG) emissions reduction projects that will greatly impact the development and scale-up of technologies to produce sustainable aviation, rail, heavy-duty transport, and maritime fuels versus light-duty vehicle transportation fuels, especially gasoline. That seems to be an appropriate shift due to the increasing emphasis on more widely available and effective electrification technology for cars and light-duty trucks; however, it should not be at the total exclusion of gasoline replacement and use reduction opportunities to improve average passenger car fleet mileage through other means, such as light-weighting, that use more mature technologies and do not require the extensive infrastructure investments that large-scale electric vehicle employment will require. Fuel additives and engine improvements would also fall into that category because the return on investment would be quicker.

Another important gap that is being addressed in the future is the decarbonization of chemicals and materials. There are many challenges in attempting to convert traditional plastic and chemical products into renewably sourced materials, especially matching the cost and quality of existing products; however, some newer bio-based materials are under development or are recently launched that combine renewable content with advanced performance. Examples include Sorona (polytrimethylene terephthalate) as a partially renewable replacement for nylon 6 and polylactic acid as a renewable replacement of disposable packaging and implements from polystyrene. There are other valuable bioproducts/chemicals in development, and if at all possible, they should be supported during their early stages.

Funding for these new, first-of-a-kind technologies has always been a challenge, so the selective use of both funding opportunity announcement (FOA) and annual operating procedure funding mechanisms is necessary to support and leverage developments in that area. In addition, feedback from industry and subject matter experts should continue to be a critical assessment tool to ensure that progress is made and that projects that are not performing are curtailed.

There is clear evidence that most, although not all, the projects currently funded in this technology area are making good progress toward the established goals, although meeting them on the desired timeline will be quite challenging. More focus on the projects that are nearer to implementation may be needed, even at the expense of some of the more innovative but less probable for success projects. Active management of the programs is necessary to ensure that short-term deliverables are obtained considering the looming crisis of global warming.

There should be increasing focus on selecting and scaling up new technology to address major gaps in sustainable fuel production as well as bioproducts, and implementation is necessary to meet climate change goals. Leveraging public and private investment in developing and proving out these technologies is an effective way to fund them. Pilot and precommercial demonstration units are critical to proving that these technologies are robust and to meeting the goals of these projects. These projects must be encouraged to use the resources of the national labs to capitalize on the already developed infrastructure and experienced resource pool. Using outside expertise to evaluate progress is an essential tool to objectively critique programs. The SDI portfolio is a good start.

STRATEGY IMPLEMENTATION AND PROGRESS

Detailed comments on each project are included in the body of this report. Selected comments on each major area are summarized in the following overview. The portfolio of projects is quite comprehensive, and good progress is being made in most areas.

Project Risk Management

The SDI's project success rate can likely be improved by implementing a uniform framework that focuses on risk identification and mitigation as well as maintenance of a risk register for BETO's scale-up projects. The framework should consider various types of risks—such as technical, implementation, unforeseen events, and the identification and allocation of resources—along with cost (on-budget) and timeline (on-schedule) risks. Standards used by the chemical, engineering, and aeronautical industries could be incorporated into the calculation methodology. Based on the risk score, only projects with acceptable risk levels should be selected for implementation. SDI has supported "Risk Management Program for BETO Scale-Up Projects" to develop a uniform process for risk management. After the completion of this project at the Pacific Northwest National Laboratory (PNNL), the developed tool should be made available to all FOA submitters, and funding should include a contingency budget (e.g., 15% of the requested budget) for any unforeseen risks. As identified risks are mitigated, the contingency budget could be accordingly reduced. Additionally, tasks should be included in this project for technology transfer efforts, especially to the SDI team. BETO would greatly benefit from the implementation of this risk management framework to ensure the successful scaling up of projects.

Biomass Pretreatment Equipment Improvements

Modeling the disc refiner is very useful and informative, provided that the operation of the disc refiner can be tested at conditions that would be used in a biorefinery, such as with actual feedstocks and solids concentration. This will identify whether the improvements in sugar yield and energy consumption will still be achievable at relevant conditions. Also, it would be useful to observe disc deterioration and performance over lengthy periods of time.

Similarly, a very systematic approach to selecting and improving the materials of construction of the Szego Mill rollers to improve wear and corrosion resistance is proving useful. An additional benefit of this work might be noise reduction for this unit operation. This kind of analysis would be useful for any other pretreatment unit operations that are subject to mechanical wear or corrosion damage. It might also be useful to consider other materials of construction, such as advanced ceramic composites, which are both tough and unaffected by corrosion; however, several questions still remain about this unit operation, for example, whether the conditions of high speed and tight clearances are causing cavitation, which might impact wear and noise. A different configuration might allow for higher residence time, thus allowing for slower and less damaging speeds.

Added Value from Lignin Market Development

Adding value above fuel value to the lignin can significantly increase the investment return for biomass-fed processes; however, separation of solid lignin from the cellulosic components presents a significant operational challenge. The deacetylation and mechanical refining (DMR) process is showing promising results in laboratory and pilot-scale studies. The separation of sugars and solids before fermentation may be necessary to optimize the fermentation process efficiency because lignin can hinder the fermentation process by binding to microorganisms and thus inhibiting their growth. Additionally, sugars in the solid fraction will not be readily available for fermentation, resulting in lower product yields. Although there is a potential loss of sugar during the washing of solid lignin, efficient separation processes can minimize this loss. The concentration step following the washing can increase the sugar concentration of the feed to a fermenter, resulting in higher product yields. Clean lignin isolation opens possibilities to convert cyclohexanes from phenolic compounds in the lignin fraction of corn stover after DMR, providing an important blending component for sustainable aviation fuel (SAF) in place of aromatics. In another project, a pilot-scale hydrothermal process produced high-value biocarbon and carbon nanofibers. These are all promising options for adding value to lignin after extracting the sugars from biomass.

National Laboratory Process Development and Demonstration Facilities

The national laboratories reported on efforts to expand their equipment and expertise in biomass sorting, processing, and conversion processes. Consistent feedstock handling and feeding remain significant challenges in biomass projects, and leveraging the expertise of engineering firms and equipment vendors in collaborative engagement projects will improve feedstock preprocessing, particularly in the area of densification, to ensure a consistent and stable feed for end users. PNNL's hydrothermal process development unit (PDU) provides a valuable facility for testing, scaling, and commercializing hydrothermal projects and valorizing wet waste feedstocks. PNNL has learned from tar sands for solids separation and wastewater treatment plants to eliminate heat exchangers and their associated fouling problems. Similarly, the National Renewable Energy Laboratory's (NREL's) Thermal and Catalytic Process Development Unit (TCPDU) is a valuable resource that enables research and development (R&D) for developing, de-risking, and scaling thermochemical conversion processes, which are capital-intensive steps. Continued investment to maintain the TCPDU as a state-of-the-art (SOA) facility is a key component of developing large-scale biofuels and the biochemicals industry. Idaho National Laboratory's (INL's) Biomass Feedstock National User Facility (BFNUF) provides a valuable facility for feedstock testing, handling, scaling, and de-risking the commercialization of biochemical conversion. Continued investment to upgrade all these facilities with SOA technologies is a well-spent investment to continue innovations and the commercialization of biochemical conversion processes.

Algae Deployment

The use of algae as a means to capture carbon dioxide (CO_2) and generate feedstock for biofuels and bioproducts has gained significant interest due to an improved algal growth rate, higher lipid content, and ability to grow in a variety of environments. New technology to dry and extract lipids and meal from algae are also helping to grow this approach; however, there are still concerns with respect to water use, water recycle after separation, and land use that remain to be answered. Also, the cost of producing biofuels from algal biorefineries is currently prohibitively expensive, which limits the impact as well as the widespread adoption of this technology. These challenges will need to be addressed to ensure that the industry is sustainable and does not negatively impact other sectors, such as agriculture.

Bio-Based Alcohols to Advanced Fuels

Meeting the goals of the advanced fuels, such as SAF, or other sustainable advanced fuels, such as low-sulfur diesel, will require the development of low-cost cellulosic ethanol. One option being explored is using energy-dedicated feedstocks, such as miscanthus, grown on marginal soils. Another option being worked on involves upgrading the alcohol to 2,3-butanediol (BDO) and then converting it to SAF. The lack of success of previous commercialization of cellulosic ethanol has spurred the development of the DMR process, which has been demonstrated with clean feedstock of consistent quality, but this is an ideal situation. It is well documented that feedstock harvesting, storage, handling, high contaminants, and inconsistent quality caused some of the most important challenges and impediments to the commercialization of cellulosic ethanol.

Biomass Processing to Advanced Fuels

Various projects are exploring thermal processing to break down biomass into fractions that can be upgraded to advanced fuels or other products. For example, the integrated hydropyrolysis and hydroconversion (IH^2) process appears to have been successful for the feedstock used (wood). Another project using wood builds on the pulp and paper industry by separating clean cellulose and hemicellulose to make nanocellulose and clean sugars for biochemicals. Still another project is developing fast pyrolysis of municipal sludge to create syngas and biochar for land remediation. All these are exploratory in nature, and some may result in value-added applications.

Biogas Processing to Advanced Fuels

There is a large and growing effort to produce and/or convert biogas or equivalent into syngas for the production of liquid fuels, particularly advanced fuels, such as SAF or diesel. Some of these projects focus on smaller conversion technologies compatible with distributed sources of biogas, such as anaerobic waste digesters or landfill gas. Novel electric reformers, cooler-operating catalytic Fischer-Tropsch reactors, and other catalytic reactors that combine several steps into significantly fewer unit operations are all being proposed and tested. Some of these processes have the potential to make a significant contribution to gas-to-liquids (GTL) options from waste gases.

RECOMMENDATIONS

The review team had a number of questions for the project leaders, and those are captured in the individual remarks by project. In addition, the review team offers a number of recommendations for consideration by BETO management in evaluating and funding future projects in this area.

Recommendation 1: Add more resources to programs designed to more effectively recover and recycle plastic waste.

One major area of opportunity that seems to be under-resourced is in the reclamation and recycling of plastics. The sources of these plastics could come from municipal solid waste (MSW) and recycle collection centers. Only a minor portion of these materials are recycled today, and there is a growing problem of microplastics in the environment, in addition to the growing use of new fossil carbon to manufacture plastics. In addition, there are decades of MSW buried in landfills, which represent a significant opportunity.

Recommendation 2: Put more resources into recovering CO_2 from concentrated sources for use as feedstocks.

Another area for GHG reduction would be to separate CO_2 from concentrated emission sources, point sources, and collection points at landfills (in addition to CH_4) and effective utilization of the recovered carbon (CO_2 and CH_4) into materials, thereby replacing those currently produced from fossil sources. There should be emphasis on using renewable electricity for these projects.

Recommendation 3: Require biomass-to-fuels programs to use real feedstocks from multiple sources and during the course of a harvest cycle.

Many of the biomass-to-fuels projects are not yet addressing the fact that biomass is highly variable and very unstable for mid- to long-term storage. All the large-scale failures for cellulosic fuels hinge in part on the fact that the feedstock had significant handling characteristics and contamination or integrity (stability) during the course of an annual operation year. It should be a requirement for future funding that these projects conduct their testing and scale-up as soon as practical on real feedstocks sourced from many different locations and of different ages.

Recommendation 4: Devise funding approaches that make national labs more affordable for smaller users.

With all the national laboratories, the full cost of using their facilities and personnel for testing is quite expensive and is a barrier for smaller startups. It is recommended that the labs use formulas based on the ability to pay to make these resources more accessible to entrepreneurs and startup companies.

Recommendation 5: Implement high-level analyses of programs and their potential impacts to enable BETO management to have a more succinct and objective view of commercial viability to assist in ongoing funding decisions.

To gain a true perspective of BETO's programs as they relate to the advanced biofuels and bioproducts being targeted, it would be helpful to see a fairly complete mapping of all of the programmatic pathways that are potentially known or are being funded. In addition to a visual map, a spreadsheet of those pathways with the current state of completion, potential impact on total GHG targets, and financial metrics, such as net present value (NPV) and internal rate of return for investments, along with a technology readiness level (TRL) status and probability of success, would be helpful to the reviewers and especially to BETO management to facilitate a clearer picture of options, status, time, and money needed to ensure commercial viability. That approach will also help make decisions about how to distribute taxpayer funds toward projects in the portfolio, with projects that have a higher probability of achieving success gaining higher priority for funding.

SYSTEMS DEVELOPMENT AND INTEGRATION – SCALE-UP PORTFOLIO PROGRAMMATIC RESPONSE

INTRODUCTION

The SDI team would like to thank the SDI-SUP review panel for providing their time and expertise throughout the 2023 Project Peer Review process, including the critical and helpful interaction with presenters at the Project Peer Review, the Review Panel Summary Report, and the valuable project comments. We appreciate the review panel's comments that the SDI portfolio has appropriately shifted to technologies producing SAF and other off-road transportation fuels. The review panel commented that there are still means of improving light-duty vehicles. Activities like light-weighting are within the DOE Vehicle Technologies Office. Other solutions, such as bio-based fuel additives and engine improvements, are presently beyond the scope of BETO. From 2016–2022, BETO worked with the DOE Vehicle Technologies Office on supporting the Co-Optimization of Fuels & Engines (Co-Optima) consortium, which identified solutions, such as boosted spark ignition engines combined with bio-blendstocks with certain properties such as high octane, that could deliver 10% engine efficiency increases; with multimode engines, an additional 14% engine efficiency could be provided. These activities have been communicated to the private sector through meetings and webinars. Ultimately, DOE has decided that, to reach nationwide net zero by 2050 and considering that there is a limited amount of sustainable biomass, the pathways for decarbonization are electrifying the light-duty sector and using biofuels along with other solutions, such as hydrogen and batteries, for the medium-duty/heavy-duty on-road and off-road sectors. The focus on electrification for light-duty vehicles has been described by the recently published *U.S. National Blueprint for Transportation Decarbonization*. As an R&D office that cannot immediately deploy commercial solutions, BETO seeks end uses for sustainable liquid fuels that have the greatest long-term opportunity.

The SDI-SUP review panel noted that there is a gap in the SDI portfolio with a limited amount of attention paid to bio-based chemicals and materials. The SDI team notes that the 2021 SDI peer review panel commented that there may be too much attention paid to specialty coproducts; however, the primary reason for the shift away from bioproducts is an intentional BETO program move to prioritize biofuels for hard-to-decarbonize sectors—specifically for aviation as the highest priority and secondarily for marine, rail, and other transportation applications. The nuance of maintaining a portfolio with the appropriate balance for fuels and chemicals has long been a challenge for BETO. FOAs typically still allow for bioproducts, but there is clearer language designating a high priority for SAF and other strategic fuels; for example, often there is a project requirement that at least 50% of the carbon from the feedstock must be converted to fuel.

The SDI team appreciates the SDI-SUP review panel's detailed analysis of portfolio features such as project risk management, biomass pretreatment equipment improvements, lignin valorization, the national laboratory PDUs, algal deployment, alcohol-to-jet (ATJ) technologies, preprocessing and pretreatment with thermochemical conversion, and biogas upgrading to liquid fuels. The SDI team will act on the SDI-SUP review panel's concerns that some cellulosic ATJ projects are not sufficiently considering feedstock variability.

Following are the SDI team's responses to the review panel's recommendations. A common theme is that the review panel would like to see a wider range of feedstocks in the SDI program's portfolio. The SDI team is attempting to focus on feedstocks with the potential for delivering the largest resulting biofuel volumes from the wide range of available feedstocks across the U.S. biomass landscape.

Recommendation 1: Add more resources to programs designed to more effectively recover and recycle plastic waste.

In the SDI program's most recent FOA, which was released in Fiscal Year (FY) 2022, with selections announced in January 2023, sorted MSW, defined as organic and plastic constituents of the MSW stream going to the landfill, was an allowable feedstock. This was not always the case. For example, the SDI program's FY 2016 FOA did not allow MSW except for post-sorted MSW, where all recyclables and non-biomass components were removed. Nevertheless, despite the trend in allowing plastic waste feedstocks, the SDI team understands that the SDI-SUP review panel would be concerned that there is a lack of program activity focused on recovering and recycling plastic waste. BETO has focused these activities in the conversion program, which stood up the Bio-Optimized Technologies to Keep Thermoplastics out of Landfills and the Environment (BOTTLE) consortium to develop bio-optimized technologies for reducing thermoplastic waste. BOTTLE presented separately from the SDI program at the Project Peer Review. The SDI team will seek more engagement with BOTTLE to understand the TRL of the technologies under development.

Recommendation 2: Put more resources into recovering CO_2 from concentrated sources for use as feedstocks.

In the SDI program's FY 2022 FOA, waste carbon dioxide produced as a byproduct from fermentation or the combustion of biomass or other biopower processes was an allowable feedstock. Nevertheless, the SDI team understands that the SDI-SUP review panel would be concerned that there is a lack of program activity focused on carbon dioxide recovery and utilization. In terms of carbon dioxide capture from non-biogenic sources, the SDI teams notes that other DOE offices have led large efforts in recent years toward these activities. For example, the DOE Office of Clean Energy Demonstrations announced plans for $2.5 billion for carbon dioxide capture from natural gas and coal power plants and industrial facilities. In terms of using carbon dioxide as a feedstock, the SDI program recently awarded a project that will use biogenic carbon dioxide from ethanol fermentation as feedstock for biological upgrading. This award was made in 2023, so it was too soon for presenting at the Project Peer Review. Further, BETO has relied on the Conversion Technologies program to stand up the CO_2 Reduction and Upgrading for e-Fuels Consortium (CO_2RUe). The SDI program will seek more engagement with the consortium to understand the TRL of the technologies under development.

Recommendation 3: Require biomass-to-fuels programs to use real feedstocks from multiple sources and during the course of a harvest cycle.

The SDI program greatly appreciates the recommendation for projects to use feedstocks with wide variability. The SDI programs notes that typically projects acquire all feedstock early in the project and then store it until use. If it is possible and pending appropriations, the SDI program will consider that future FOAs stipulate that projects acquire feedstock throughout the project lifetime and from multiple sources/sites. The SDI program is actively responding by engaging with relevant projects and facilitating more collaboration with the national laboratories. Additionally, the SDI program is working with the Feedstock-Conversion Interface Consortium (FCIC) to facilitate conversations between the FCIC and pilot and demonstration projects using agricultural residues or woody feedstocks. The FCIC is jointly managed by the Renewable Carbon Resources, Conversion Technologies, and SDI programs. The FCIC is actively conducting R&D in feedstock variability and its impact on preprocessing, pretreatment, and conversion.

In addition, the SDI program is funding a new project at the national laboratories to explore the opportunities and challenges for envisioning a cellulosic sugars depot strategy to commoditize preprocessed agricultural residues. This project will include national laboratory experts to reach out and engage with industry experts on the SOA in managing agricultural residues.

Recommendation 4: Devise funding approaches that make national labs more affordable for smaller users.

Though this is an important recommendation, there may be limits to what BETO can do about making national labs more affordable for smaller users. BETO has conducted some limited funding opportunities that provide relatively small amounts of funding to be made available to assist small companies and local government entities. Further, BETO's competitive FOAs often have clear language encouraging engagement with the PDUs at the national laboratories. If awarded, the project would then include funds awarded to the external user (applicant) as well as funds contracted to the national laboratory.

BETO also supports directed funding opportunities where funds are awarded to the national laboratory for solving a problem identified by an industry partner and where the industry partner supplies a cost share. The directed funding opportunities are often in other programs besides SDI, so the SDI-SUP reviewers did not see these projects. The SDI program will keep the directed funding opportunity approach in mind for future use.

Recommendation 5: Implement high-level analyses of programs and their potential impacts to enable BETO management to have a more succinct and objective view of commercial viability to assist in ongoing funding decisions.

In the last year, BETO supported an internal portfolio analysis led by the office's chief scientist and chief engineer. The results have not been publicly shared, but this information provided a mapping of projects supported by BETO and their features, such as feedstocks, conversion process, and TRL. The SDI program also maintains other internal analyses to track project development. The review panel recommends including metrics such as NPV, internal rate of return, and GHG reductions. Under SDI FOAs, the project recipients are required to present forward-looking *pro forma* and environmental analyses. And the SDI program will seek to have these analyses updated and reviewed as the project progresses.

MODELING FLOW BEHAVIOR IN A DISC REFINER FOR DMR PROCESS

National Renewable Energy Laboratory

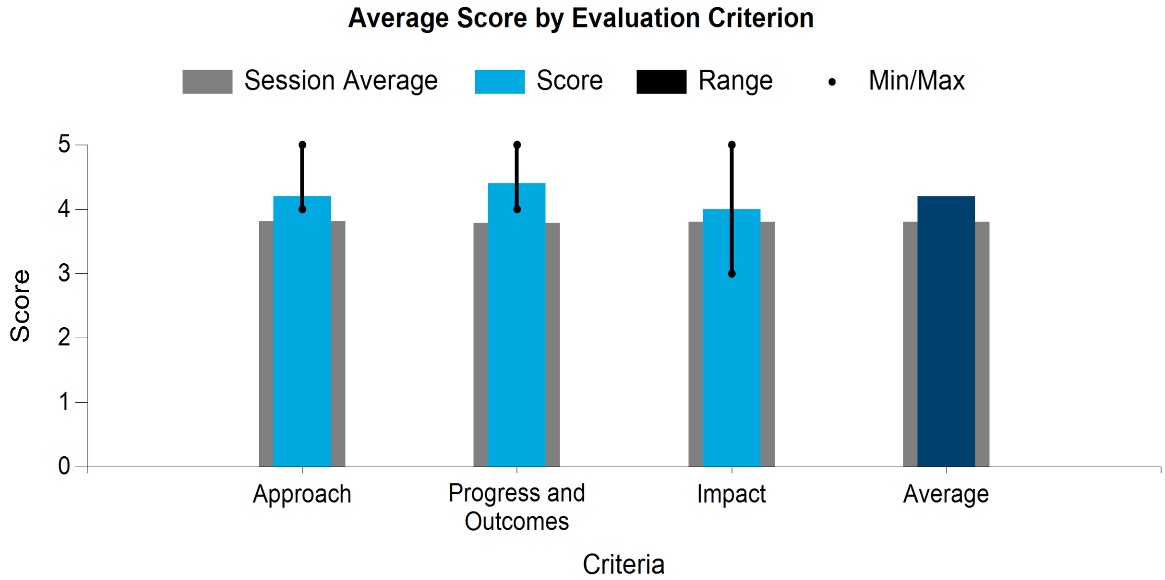
PROJECT DESCRIPTION

WBS:	3.1.1.012
Presenter(s):	Xiaowen Chen
Project Start Date:	09/03/2019
Planned Project End Date:	09/30/2023
Total Funding:	$750,000

The objective of this project is to develop 3D computational fluid dynamics (CFD) models that can accurately forecast refining power during disc refining. These models can then be used to guide future disc plate designs and process parameter selections, resulting in reduced energy consumption and GHG emissions in the DMR process; however, reducing the energy intensity of the mechanical refining-based pretreatment process while maintaining enzymatic hydrolysis sugar yields is challenging. To tackle this challenge, the research team examined the impact of different refining conditions on energy consumption, enzymatic sugar yields, minimum sugar selling price, and environmental impacts.

The team found that when changing the refiner gap, a positive proportionate correlation between specific energy consumption and enzymatic sugar yields was observed, which was consistent with other published works; however, changes in refining rotational speed and refiner plate design made the correlation between specific energy consumption and enzymatic sugar yields less straightforward. The team observed that by decreasing the rotation speed for low-consistency disc refining, specific energy consumption decreased by more than 50% without affecting enzymatic sugar yields. By changing refiner plate designs, the team achieved a 45% reduction in specific energy consumption without affecting glucose yield, although there was a negative impact on xylose yield.

Using a high-fidelity disc-refining model, the team could predict the energy consumption for different refiner plate geometry designs and operating conditions. The techno-economic analysis (TEA) and life cycle analysis (LCA) showed that the plate design and operating conditions have a direct impact on process power consumption and sugar yields, with sugar yields strongly influencing the minimum sugar selling price, the life cycle GHG emissions, and fossil energy consumption. To minimize environmental impact and maximize process economics, the mechanical refining process optimization should focus on maintaining high sugar yields while reducing refining energy consumption.



COMMENTS

- The DMR process is a promising technology NREL developed, and the disc refiner modeling work looks good. The obtained results in the modeling and the experimental results are very close; however, the DMR has not continuously worked with the DMR processing, and the difficulties of integrating two different systems (and, lately, the downstream processing) have not been considered.

  I believe that DMR is a promising technology, but NREL has not worked on the process's integration, which poses a question about the solution's scalability. I fear previous failures in scaling biomass treatment technology have not been considered. I want to encourage NREL to review what happened in the past and learn from it. The big issue is ensuring that you can process any corn stover and handle all types of impurities. Please be sure that you do not encounter the same issues as before.

  Another question is whether working with 3% solids in the disc refiner will demand high energy to separate products from the water. The disc refiner will need to work with much higher solid content.

- The project has successfully developed a CFD model that accurately predicts refining power (as shown by the validation against experimental data) and can be used to inform future disc plate designs. The impact of this project is reducing energy consumption and thus GHG emissions and economics of the DMR process for SAF/biofuels production. The CFD model will be useful for determining the optimal plate design for different feedstocks.

- This modeling approach to rotating equipment used in size reduction is unique and has produced good results, as verified by the actual enzymatic production of fermentable sugars as a function of milling energy use. A nearly 50% reduction in energy used with the same sugar production is very significant for biomass feedstock pretreatment. This modeling approach should be useful for studying different types of feedstocks being processed in different types of equipment to reduce costly and time-consuming empirical approaches, subject to experimental verification. It could also be useful to reduce noise in the processing area, assuming energy input reductions also lead to somewhat lower noise production.

- The modeling approach used in this study is unique and has resulted in a predictive model that has been validated against experimental data. Further work is encouraged to assess the model's accessibility and ease of use for a wider range of users. Friction generated during the refining process can contribute to the cooking of polymeric sugars, which may pose a challenge. Additional investigation is suggested to understand the extent of this issue. Most refiner plates have been developed for the particleboard industry, and their suitability for handling various agricultural and woody feedstocks, particularly those with high ash and silica content, remains uncertain. Additional testing will be required to assess their wear and tear under these conditions. Disc refiners have traditionally been used in the pulp and paper industry with wood chips containing up to 50% moisture as well as with softened wood; however, using corn stover with a moisture content of 15% and without precooking may impact the wear and tear of the refiner discs, and this needs to be investigated further. It is important to encourage greater industry participation in the development and implementation of biorefinery-specific plate manufacturing technologies.

- This project tackles an important component of the DMR process and involves the optimization of the disc refiner to achieve maximum sugar yields. The work that has been done has shown a clear improvement in sugar yields with an optimization and reduction in energy use. The experiments were carried out at low solids concentration (3%), which does not represent the industrial conditions under which the disc will be operated. Although it is outside the scope of the goal to model and optimize design and flow behavior, it would be very useful and informative if the operation of the disc at the optimized conditions can be tested at actual conditions, such as solids concentration, that would be used in a biorefinery. This will identify whether the improvements in sugar yield and energy consumption will still be achievable at relevant conditions. Further, although it is not part of this project, it would be useful to be provided with information on the disc deterioration and performance over lengthy periods of time.

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate and value the feedback provided by the reviewer concerning our disc-refining modeling project. We strongly agree with the majority of the reviewer's comments, which highlight the significance of this project in reducing disc-refining energy and the associated GHG emissions for SAF production through DMR processes. As the project progresses, we plan to implement the reviewer's suggestions. One comment we received was that our experiment was conducted with low solids and does not accurately represent industrial conditions. Unfortunately, due to our current 12-inch disc refiner, we are unable to increase the solids; however, the installation and commissioning of the new 22-inch disc refiner at NREL will enable us to conduct experiments at higher solids with continuous flow. This will enable us to model the process with more realistic industrial conditions. Regarding the other comment on the integration of the disc refining with other process units—we are closely collaborating with the Sustainable Aviation Fuel From [i] Renewable Ethanol (SAFFiRE) project to integrate the disc-refining process with other unit operations to establish continuous operation. This will allow us to identify and address any potential scalability issues. Addressing the issue of disc plate wear is another important aspect that we plan to tackle in future iterations of the project. To achieve this, we will work closely with the FCIC to develop solutions that characterize and mitigate the effects of ash content present in agricultural waste, which has been identified as a leading cause of wearing problems during disc refining.

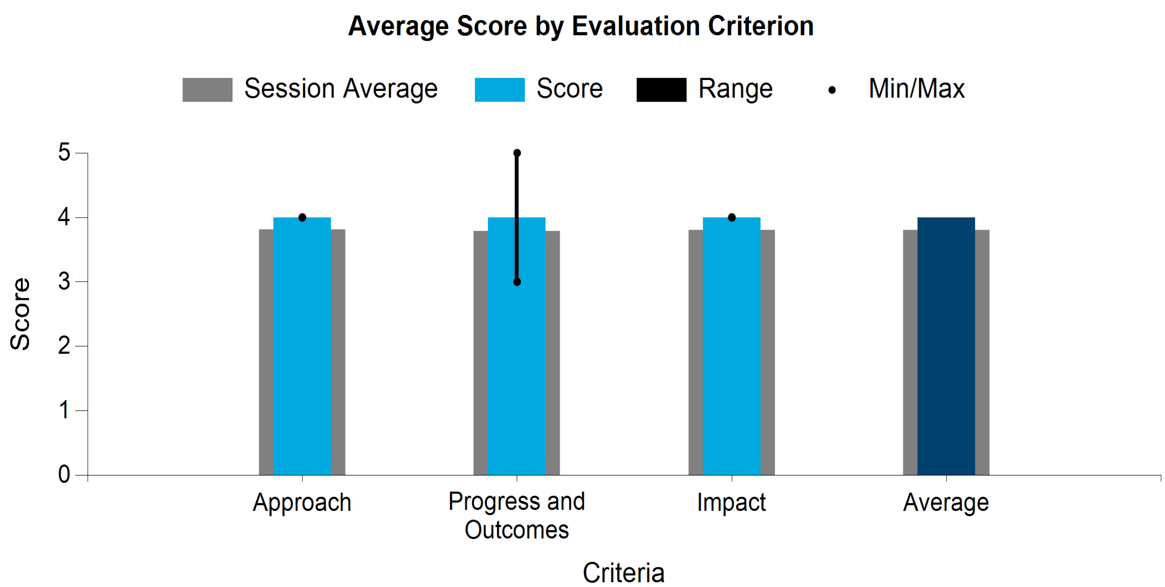
RISK MANAGEMENT PROGRAM FOR BETO SCALE-UP PROJECTS

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	3.2.4.001
Presenter(s):	Hannah Rabinowitz
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$1,400,000

Scaling up bioenergy projects presents challenges, often resulting in significant cost and schedule overruns or even project failure. Identifying risks that could lead to cost and schedule impacts is a critical part of project planning and execution to ensure proper risk handling. Based on industry consensus standards as well as many years of experience, PNNL has developed a risk management process to help scale-up projects identify and manage risks and to help BETO track and manage risks across its portfolio. To create a consistent and best-practice risk management process, PNNL developed a Risk Management Plan Guidance (RMPG) document that serves as a template for projects to write their own risk management plan (RMP). Additionally, PNNL delivered training on risk management topics as part of a technical assistance effort with one pilot BETO Phase 1 scale-up project, and a second pilot is planned for 2023. PNNL will facilitate risk elicitations to help the pilot projects identify, characterize, and capture risks in a project risk register. The Excel-based risk register is the principal tool to help the project track risks, manage risks through handling actions, and support risk reporting to BETO. Supporting the development of pilot project RMPs and risk registers will inform the finalization of the RMPG to allow its application across the BETO portfolio of scale-up projects.



COMMENTS

- Risk management is a must exercise that any project needs. The concept and approach are consistent with industry standards; however, I am afraid that the project team is developing the tool from scratch. There are many tools out there to do project risk management. The risk assessment is translated to the level of contingency. You should recommend BETO to allow a certain level of contingency in the budgets. I will not recommend requesting a full risk analysis during the FOA application because it is cumbersome and requires significant time, but it should be one of the first tasks once the project has been awarded.

- This project provides guidance and a consistent, uniform process for the risk management of BETO projects, and I am glad to see it. The overall framework looks good. From the presentation, it is not clear when projects begin the quantitative risk assessment—before or after being funded for Phase 2?

  Because budgets are developed during the proposal development, would teams perform the quantitative risk assessment during the proposal development for Phase 2 and provide their risk register and contingency budget as part of their proposal? Would project teams need to provide a contingency budget?

  Generally, in industries (nuclear, oil and gas, etc.) where risk management is a standard practice, risk management professionals are brought in to facilitate risk workshops to ensure a comprehensive, efficient, and inclusive risk assessment process and to manage any challenging personalities. Does the RMPG provide guidance on facilitating a risk workshop? Does the RMPG provide guidance on how to write good risk statements?

- The audience for a clear risk analysis should be both the project leaders as well as BETO program management. The best time to do that initial analysis is before the project even starts. The approach being developed in this project is semiquantitative, and it leans on experiences in the nuclear power and oil and gas industries, among others, which could lead to a more objective assessment of the risks and mitigation strategies being planned for each project. That analysis depends to a great extent on the background and experience of the technical advisory board members, so the choices for those roles should be consistent with the type of project being considered. It will be more useful as a managing tool if clear standards can be set for each criteria and then consistently applied. It may also be helpful to use financial metrics tempered with probability of success—for example, an NPV that is risk adjusted, as is commonly used in industry. Also, it might be useful to do a lookback on projects that underwent risk analysis to see if the analysis was useful and if the methodology can be improved in the future.

- The SDI project's success rate can be improved by implementing a uniform framework that focuses on risk identification, mitigation, and maintenance of a risk register for BETO's scale-up projects. The framework must consider various types of risks, such as technical, implementation, unforeseen events, identification, and allocation of resources, along with cost (on-budget) and timeline (on-schedule) risks. To ensure accuracy, industry standards used by the chemical, engineering, and aeronautical industries must be incorporated into the calculation methodology. Based on the risk score, only projects with acceptable risk levels should be selected for implementation. After completion of this project at PNNL, the developed tool should be made available to all FOA submitters, and funding should include a contingency budget (e.g., 15% of the requested budget) for any unforeseen risks. As identified risks are mitigated, the contingency budget could be accordingly reduced. Additionally, tasks should be included in this project for technology transfer efforts, especially to the SDI team. In conclusion, BETO would greatly benefit from the implementation of this risk management framework to ensure the successful scaling up of projects.

- Risk management is critical for project success, and this framework will assist projects to identify risks and have contingencies in place. This will be important to successfully scale up.

PI RESPONSE TO REVIEWER COMMENTS

- The project team thanks the review panel for their time and thoughtful comments. We appreciate the reviewers reinforcing the importance of conducting formal risk management for BETO's scale-up projects. In the following, we clarify several items brought up in the review panel's comments.

The review panel mentioned a concern about developing a tool from scratch given the large number of processes already available. The framework that we have put together does, indeed, follow industry standards and is not intended to reinvent the wheel. We have put together an RMPG as a template that projects can use as a starting point to create their own RMP, but the RMPG heavily draws from previous RMPs developed in a range of industries. In terms of the risk register tool, the intent for creating a risk register, Excel-based tool is to ensure that all projects have a risk register available that captures the inputs outlined in their RMP and provides outputs that can be directly used in risk reporting. By developing an Excel-based tool for BETO, this resource is available free of charge to all BETO projects and will help produce consistent results across BETO's portfolio, enabling BETO to manage its portfolio of risks. For projects that progress to a fully quantitative RMP in Phase 2, we expect that existing commercial tools would be leveraged for the risk analysis and that BETO would recommend a software tool to be used by all applicants to help ensure consistency across the portfolio.

The review panel also had questions about the timing of the semiquantitative and fully quantitative risk assessments relative to the BETO scale-up project FOA, Phase 1, and Phase 2 timelines. The intent of providing the RMPG as part of the FOA is to help projects understand the level of effort associated with risk management that they should plan for in their FOA application and budgeting for Phase 1. It is not intended that they complete a risk analysis prior to the project being awarded; rather, this risk management framework can help them to meet one of their Phase 1 milestones related to developing an RMP. The intent is that the quantitative risk assessment will be conducted during Phase 2, but training on how to conduct a fully quantitative risk assessment will be given as part of Phase 1 to enable the projects to plan appropriately for Phase 2. Although, ideally, a robust quantitative risk study would provide the basis for contingency estimates at the outset of in Phase 2, the practicality is that the type of detailed, resource-loaded schedule required to support such a study would not be in place prior to Phase 2. Instead, the anticipation is that the Phase 1 semiquantitative risk study would provide input to a preliminary contingency assessment. We also anticipate that the risk analysis will provide a robust basis for contingency estimation. As a project's methods evolve from semiquantitative to fully quantitative (in Phase 2), the robustness and completeness of the basis for contingency assessment will improve, including collecting data such as discounts that allow for calculating NPV.

In terms of risk scores being a basis for project selection, if such an approach were to be considered, it would be important that the principles of risk-informed decision making be applied and that factors such as risk model quality, detail, and completeness be accounted for so that projects are not incentivized to underreport their risks. The panel also emphasized the importance of leveraging risk professionals when conducting risk elicitations to provide a more comprehensive and efficient risk assessment process that yields a risk register populated with well-structured and well-characterized risks. Although the RMPG that we have developed does not include specifics on facilitation and writing risk statements, it is the topic of two training courses being provided to scale-up project teams. Also, we fully endorse the statement that risk professionals should facilitate risk workshops, particularly for the early sessions. This would provide hands-on training so that, ultimately, the facilitation role could be taken in-house, if desired.

Additionally, the panel noted the importance of incorporating technical advisory board members who are experienced in the industry. The risk management project has established a technical advisory board to provide bioenergy industry perspectives in the development of the risk management framework. The board includes a member of the independent engineering team that supports BETO and another industry expert. Additionally, the RMPG lays out the role for a project-specific risk advisory committee that comprises both industry and risk technical experts and can support the project in reviewing risk documentation and reporting. For the current pilot projects, the risk advisory committee comprises PNNL risk experts and the technical advisory board. It is intended that each project should create their risk advisory committee to include members with expertise relevant to their particular project, but additional guidance can be added to emphasize the types of people who should be included.

Finally, the panel noted that it could be useful to do a lookback and compare the success of projects that followed the formal risk management process with projects that did not. We agree that a lookback on project success with and without formal risk management would be useful, though that is likely to be a more successful endeavor in a few years, once several projects have implemented the risk management process and have been subsequently completed. Also, the RMP is a dynamic process with continual improvement based on experience with each project. We anticipate that BETO will play a key role in ensuring that general programmatic risk insights gained across the portfolio will be shared with all scale-up projects.

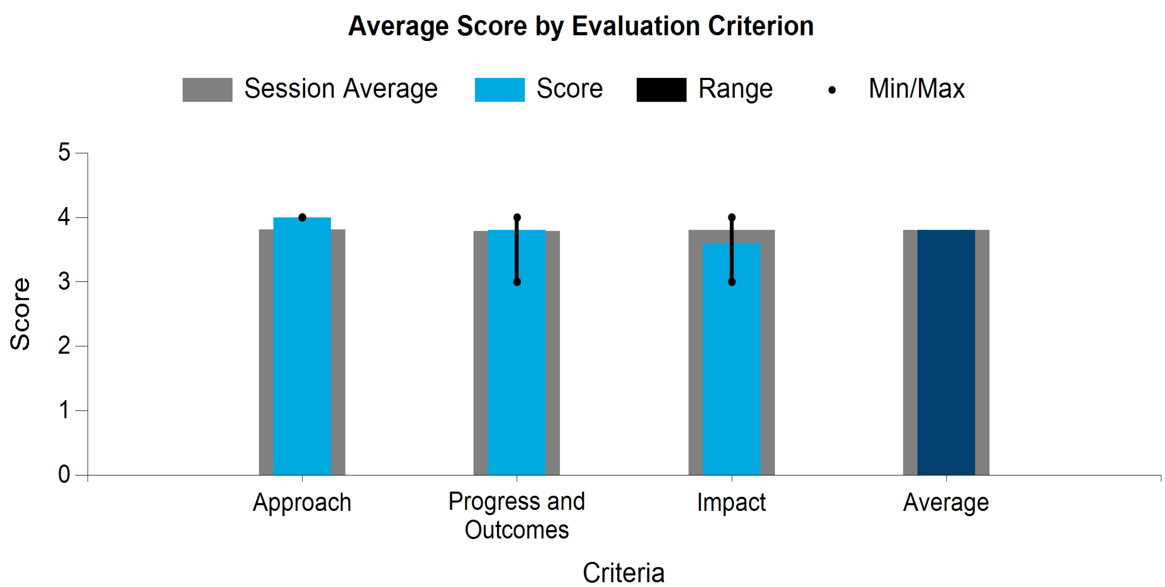
SOLID LIGNIN RECOVERY

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	3.3.4.601
Presenter(s):	Dan Schell
Project Start Date:	09/03/2019
Planned Project End Date:	09/30/2023
Total Funding:	$600,000

Valorizing the lignin residue remaining after enzymatic hydrolysis of pretreated biomass is necessary for realizing cost-effective biofuels/bioproducts from a biochemical pathway. But no clear options existed at the start of this project for achieving high recovery of dewatered and washed lignin solids at low-water-usage rates with good sugar recovery using commercially available, solid-liquid separation equipment, particularly for lignin derived from the DMR process or caustic-based pretreatments. This separation is challenging due to the lignin's small particle size (10-µm mean) and low particle settling velocities. Our goal is to find an economic solution for recovering solid lignin using either flocculation or a non-flocculated separation process. Based on a TEA completed in December 2020, both decantation (decanter centrifuge) with multiple-stage washing and cross-flow filtration produced a minimum fuel selling price (MFSP) of $0.21/gallon gasoline equivalent (GGE) and $0.03/GGE, respectively, below the flocculation-based process. This outcome generated a go/no-go decision to further explore and optimize the performance of these later non-flocculated processes. We generated enhanced data sets for cross-flow filtration and dynamic cross-flow filtration, and we will do the same for decantation in FY 2023, leading to a final economic evaluation at the end of FY 2023.



COMMENTS

- NREL tested and analyzed different alternatives to filter lignin solids coming from DMR pretreatment. It seems that the best system uses a decanter like in 1G ethanol production for thin-stillage separation.
- This project takes a sound approach to finding and evaluating solutions for recovering solid lignin to increase biomass conversion for more cost-effective SAF production. These are the types of

investigation that will enable improvements in the techno-economics of SAF production. The TEA will be important for the selection of the best method and for quantifying the economic improvements.

- Solid/liquid separations are an often troublesome unit operation in many processes. The need for lower-cost and more effective separations became obvious while evaluating the DMR enzymatic pretreatment process at increasing scale, and this study identified a few approaches that appear to be effective without the expensive addition of flocculants. When the final experimental work is completed and the data are evaluated, a TEA should elucidate the best approach for this feedstock and this pretreatment system. More work may be useful to investigate other feedstocks and their pretreatment and separations to broaden the potential applicability generally.
- The aim of this project is to improve the solid-liquid separation process in the DMR process, specifically for the separation of solid lignin. This separation process presents a significant operational challenge. When scaling up from the pilot to commercial scale, it is essential to consider the process's technical and economic feasibility. In this case, it is crucial to assess the efficiency of the separation process at larger scales and the potential cost implications of implementing the necessary equipment and infrastructure. The DMR process has shown promising results in laboratory and pilot-scale studies; however, further research is necessary to fully determine its commercial viability. This assessment should include a comprehensive evaluation of the technical, economic, and environmental aspects of the process. The separation of sugars and solids before fermentation may be necessary to optimize the fermentation process's efficiency. Solids, such as lignin, can hinder the fermentation process by binding to the microorganisms and inhibiting their growth. Additionally, sugars in the solid fraction will not be readily available for fermentation, resulting in lower product yields. Although there is a potential loss of sugar during the washing of solid lignin, efficient separation processes can minimize this loss. The concentration step following the washing can increase the sugar concentration of the feed to the fermenter, resulting in higher product yields; however, it is essential to consider the increased water load for the process due to the washing step and evaluate the process's environmental impact.
- The economics of a cellulosic ethanol facility are linked to the ability to valorize all coproducts or byproducts. Lignin valorization has been a significant challenge, and most cellulosic ethanol facilities have burned the lignin for energy generation. This project looks at lignin recovery after the DMR process (still undergoing development and optimization). The characteristics of the lignin make it challenging to separate and recover, and various methods are evaluated. The project can significantly impact the viability of cellulosic ethanol facilities based on coproducts derived from the lignin. Switching to lignin separation before fermentation makes sense to prevent the inhibition of the fermentation organism because sugars can be concentrated. There does not appear to be a clear winner among the investigated approaches, with the cost reduction against the baseline being quite small for a few alternatives. It would be useful to show the difference in wash water consumption between the most promising approaches. Which option achieves the highest sugar concentration? What is the impact of different recovery approaches on the proposed lignin valorization approaches?

PI RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' comments and their efforts reviewing this work. This project's primary goal is to ascertain if commercially available solid-liquid separation technology can effectively recover solid lignin generated after the enzymatic hydrolysis of treated biomass. Although the focus has been on DMR-derived biomass, the results should be generally applicable to any aqueous-phase pretreatment process; however, additional work could look at other pretreatment/feedstock combinations, but we have found that DMR-derived lignin is the most difficult to separate, and for this reason, this material was used in this work. TEA is being extensively used in the project to assess the relative economic performance of the various separation options being analyzed in this study. The separation performance data for each option—including wash water usage, solids and sugar recovery, and extent of solids dewatering—are being generated in pilot-scale equipment. The TEA analysis is being performed by the NREL process analysis team using previously established models. These models include DMR and lignin utilization process designs and economics as documented in NREL's 2018 design report (doi.org/10.2172/1483234), which has been reviewed and vetted by industry and other external reviewers. The TEA will identify the optimum operating conditions (e.g., water consumption) as well as the relative cost of each separation option.

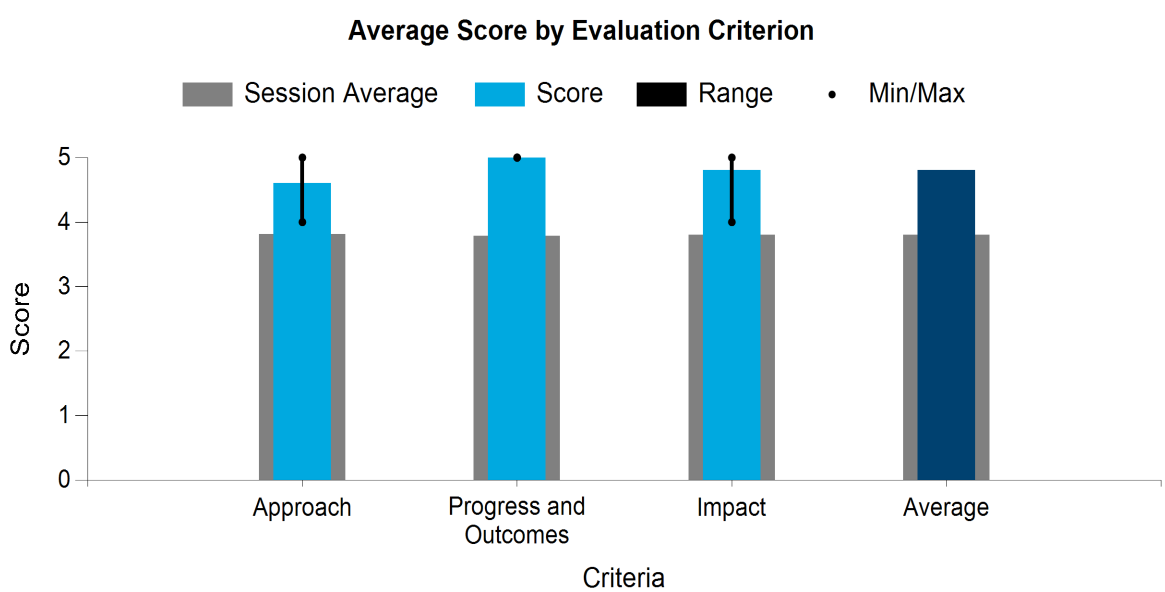
BIOMASS—FEEDSTOCK USER FACILITY

Idaho National Laboratory

PROJECT DESCRIPTION

WBS:	3.4.1.202
Presenter(s):	Neal Yancey
Project Start Date:	07/03/2008
Planned Project End Date:	09/30/2024
Total Funding:	$6,000,000

Variability for low-value carbon feedstocks continues to create challenges during storage, preprocessing, and conversion. The purpose of this project is to ensure that feedstocks are procured and prepared for all BETO-funded research projects as well as industry and academia. Part of that involves maintaining equipment and reconfiguring to meet customer needs. The project has advanced the TRL of new technologies with the aim of moving promising technological developments from the bench scale to the pre-pilot scale. Three BFNUF projects were selected to develop processing methods for corn stover, forest residue, and MSW. Each specifically addressed variability in moisture, particle size, and ash. Upgraded BFNUF equipment was used to fractionate, remove contaminants, and create a product with significantly reduced variability. The targets were met using screening, advanced milling, and contaminant-removal operations, which were also part of the BFNUF equipment upgrade. This project supplied feedstocks to more than 100 requests from industry, academia, and national laboratories during FY 2022 and will exceed that number in FY 2023. One technological challenge of this project is the integration of the BFNUF upgrade equipment, the inclusion of that equipment in the current operating system, and data acquisition. A desired outcome from this project is to increase the inclusion of underrepresented companies and individuals in the development of technology solutions.



COMMENTS

- INL is doing excellent work helping companies and other national labs to address biomass handling and pretreatment issues. They had 73 projects funded in 2022–2023 and have worked with various feedstocks, covering the whole spectrum. Keep on working as you have until now!

- Feedstock handling and preprocessing continue to be a challenge. INL's BFNUF is a valuable resource to companies and researchers in the bioeconomy to work through feedstock challenges and assess the techno-economics of different preprocessing options. It is great to see additional investment being made to expand the capabilities of the BFNUF. Because feedstock drying is often required for the conversion process, BFNUF should consider how it can support that.
- A multipurpose, multiunit operation, multi-feedstock facility to facilitate scale-up the front end of various processes has become a very useful investment. This is very attractive to industry users, as indicated by the many collaborative projects.
- Because consistent feedstock handling and feeding remain significant challenges in biomass projects, this project has the potential to make a meaningful impact. This project has made excellent progress, underscoring the critical role of producing dependable feedstocks for successful project outcomes. To leverage the expertise of engineering firms and equipment vendors, are there any plans to collaborate with them? Are there any ongoing or planned projects to improve feedstock preprocessing, particularly in the area of densification, to ensure a consistent and stable feed for end users? In addition to air classification for cleaning, is a washing step included to clean the feedstocks, similar to those used for cleaning wood chips in pulp and paper facilities? What plans are in place to share lessons learned, including dos and don'ts, with other project developers to help them avoid common pitfalls?
- INL performs a vital function in commercializing technologies for biofuel and bioproducts production. The cleanup and processing of feedstocks is critical for any biorefinery, and the expertise and equipment at INL can achieve this. The most important part of this role is the feedback to companies to translate these data into industry decisions for pilot, demonstration, and commercial-scale facilities. Based on the presentation of their work, INL has a good communication strategy, which includes the collection of data on TEA and LCA to help companies with decision making. Keep up this excellent work.

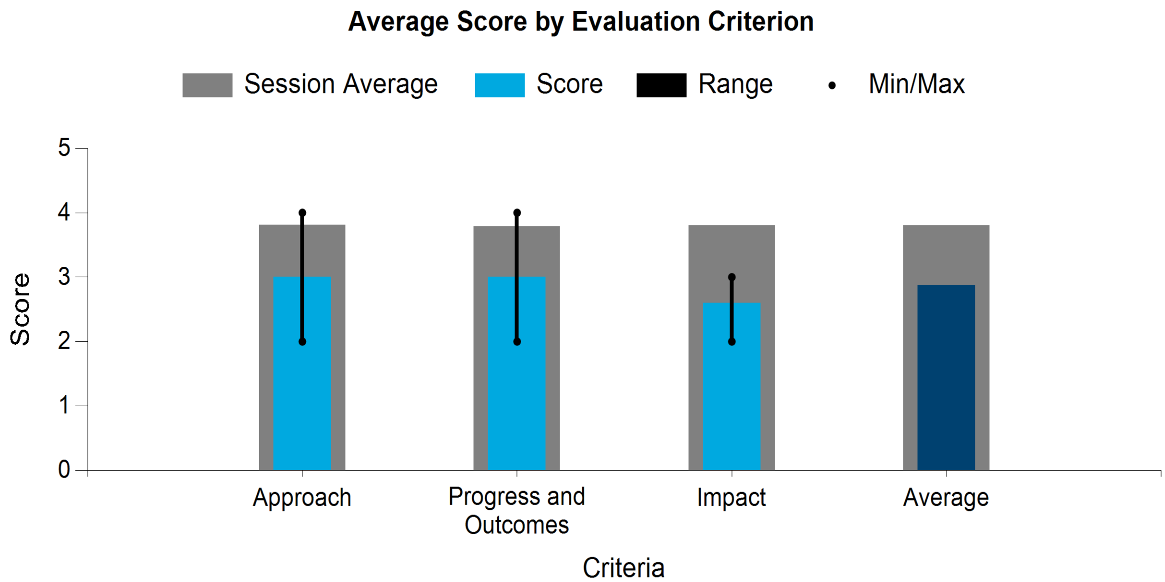
PI RESPONSE TO REVIEWER COMMENTS

- Thanks for the comments; they were beneficial and insightful. The BFNUF continually seeks engagement with equipment manufacturers. Some examples are the partnership with Warren and Baerg Manufacturing in developing the new bale processor. In May 2023, INL hosted a ribbon-cutting ceremony where university partners, industry partners, and our DOE customer came and participated in an open-house demonstration. This along with conference attendance and publications have led to added customer interactions with the BFNUF. Specifically, the BFNUF is working with air classification vendors and milling manufacturers, such as Forest Concepts. But, to your point, improvements can always be made to include more partnerships with industry and manufactures alike. We routinely seek partnerships with industry to improve preprocessing and material handling/flowability. Densification is also of particular importance; most recently, we engaged with companies such as Fulcrum, Enerkem, and Lignetics in conducting densification research. INL is in the process of establishing additional partnerships with industry in developing densification research with both MSW and corn stover as well as other feedstocks as the opportunity arises. Washing capabilities are also an ever-increasing need. The BFNUF has multiple laboratory-scale washing capabilities where research is being completed but not as much at the PDU scale. Certainly, that is an area that may increase in need in the future. INL produces many papers/publications each year to help get the word out on the research being conducted. But, to your point here, it would be beneficial to develop a lessons-learned publication on an annual basis to highlight those types of issues, both positive and negative.

SCALE-UP OF NOVEL ALGAE DRYING AND EXTRACTION UNIT OPERATIONS

Global Algae Innovations

WBS:	3.4.2.101
Presenter(s):	David Hazlebeck
Project Start Date:	10/01/2020
Planned Project End Date:	08/31/2024
Total Funding:	$5,000,000



COMMENTS

- The project we are reviewing is for drying and extraction operations; however, the presentation does not specify how the process will be done. The final product portfolio has changed from oil and meal to various higher-value products that may positively impact the project's economics. Considering that the project started very recently, I will need to wait for further development of the project to have a better assessment of its performance.

- This project aims to enable economic algae-based biofuel by developing high-value coproducts and new drying and extraction unit operations that are less energy intensive. Although the lipid coproducts are valuable bio-based chemicals, biofuels production is reduced by 66%.

  Global Algae Innovations has also selected a non-genetically modified organism (GMO) algae, which allows the algae to be produced in open ponds without concerns of GMO algae being unintentionally dispersed into the wild. The feasibility of the large-scale production of algae is still in question in regard to the land and water requirements. Water makeup needs to account for not only evaporation but also water entrained in the algae when harvested.

It is not possible to provide a technical evaluation of the project due to the lack of information on the new drying and extraction technologies.

- This algal project differs from other approaches in that they are using selected algae to produce increased amounts of lipids and proteins and employing novel unit operations to reduce the cost of algal isolation and drying, the latter dramatically reducing energy costs. The lipids and algal meal are separated, and the lipids are further separated into value-added streams for different applications. More process analytical controls are used to increase the security of the algal pond and manage nutrients for growth. A key question about the cost-effectiveness of microalgae for fuels remains, but coproduct value appears to help. Although the usual questions remain about land and water use, this seems to be a smart approach for this type of platform.

- The use of algae as a feedstock for biofuels and bioproducts has gained significant interest due to its improved growth rate, high lipid content, and ability to grow in a variety of environments; however, the cost of producing biofuels from algal biorefineries is currently prohibitively expensive, which limits the impact as well as the widespread adoption of this technology. Despite this, ongoing R&D efforts are being made to improve the efficiency and reduce the costs associated with algal biofuels. This project focuses on the use of a novel drying and extraction method for the separation of algae (lipids and meal) for downstream processing to produce algal oil and products. Several questions and challenges with respect to water use, water recycling after separation, and land use (does it impact agricultural land?) remain to be answered. To better understand the various projects from Global Algae Innovations, it would be helpful to have a clear illustration of the similarities and differences between the projects. Additionally, understanding how the project team members collaborate, particularly during the execution phase, can provide valuable insights into the success of these projects.

- The production of lipids from algae and commercialization has proven to be quite difficult over the years, and many companies have failed; however, the high demand for low-carbon-intensity lipid feedstocks will keep growing, and algal lipids have been identified as a potentially significant source.

  The project reviewed here focused on the scale-up of a novel drying and extraction technique rather than the overall process, although these are definitely some of the most critical components. We were not provided with any information on the actual technologies because patents are still pending; however, the results in terms of energy consumption and yields were very good.

  The 50% lipid production in a naturally occurring organism seems very impressive, but it is not clear whether contamination of the ponds, and therefore lipid yields overall, were a problem. At a broader level, there are some concerns about land use change and water consumption that will affect the sustainability and carbon intensity of the lipids. This should be investigated in terms of scale-up and location because it will be an important consideration for the offtake of lipids by a biofuel producer, such as Neste. The impact of fertilizer consumption (and the source of the fertilizer, likely from fossil fuels) will also be a consideration for carbon intensity.

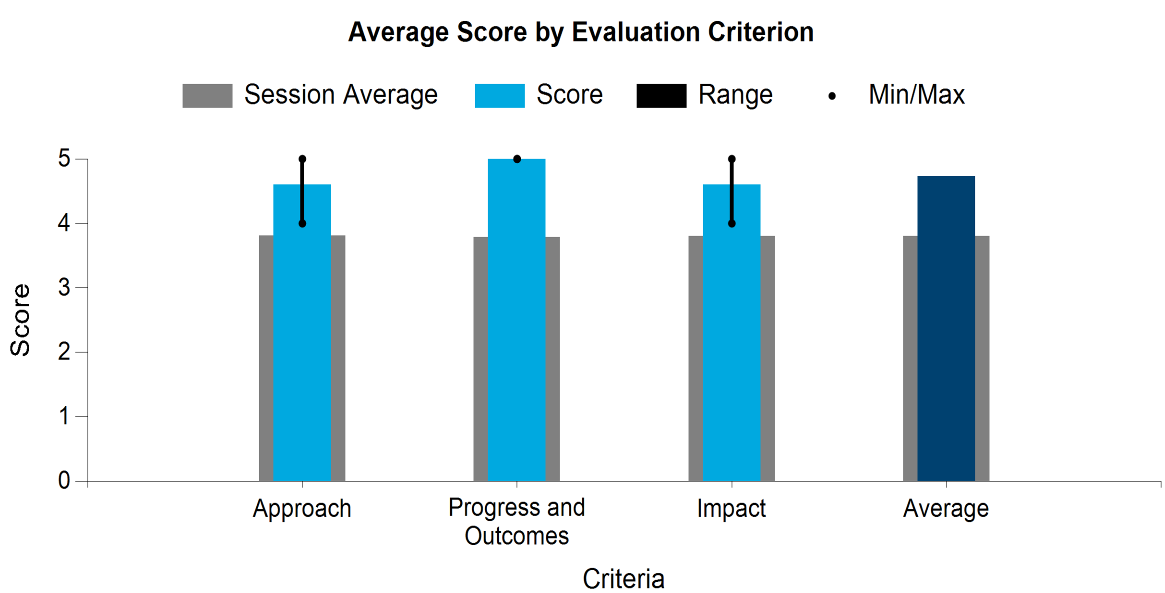
BIOCHEMICAL PILOT-SCALE SUPPORT AND PROCESS INTEGRATIONS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	3.4.2.201
Presenter(s):	Dan Schell
Project Start Date:	10/01/2018
Planned Project End Date:	09/30/2024
Total Funding:	$4,468,000

The Biochemical Pilot-Scale Support and Process Integration project's high-level goal is to help transition technology to the marketplace by providing a facility for pilot-scale performance testing and verification. To facilitate this goal, we maintain the functionality and operational readiness of the biochemical pilot plant and evolve its capability to perform process-relevant testing or integration work for BETO and industry clients. We also encounter and solve unknown scale-up issues that usually manifest only at the pilot scale prior to technology deployment; however, processing biomass feedstocks remains a challenge at the pilot scale, particularly handling a variety of raw biomass materials. In the past 2 years, we completed the modernization of the pilot plant's control software with a new automation software product that is cheaper to maintain, easier to learn, and has enhanced capabilities, i.e., automated data storage to a Structured Query Language (SQL) database. We developed and implemented a data management system that effectively captures and logs all pilot-plant sensor data associated with experimental runs into an easily retrievable format including sample tracking. This year, the plant's aging boilers and air compressors will be replaced using non-project funds, and we will install a new 22-inch disc refiner to support a new pretreatment technology. The pilot plant continues to be used by BETO projects as well as by industry clients, with 11 new industry-based projects begun in FY 2021/2022.



COMMENTS:

- NREL is known worldwide as a reference for biomass treatment, utilization, and upgrading. During the last 30 years, NREL has worked with multiple stakeholders trying to solve the intricacy of sugar liberation in biomass feedstocks. I think NREL has outdated facilities, and the $39 million they have just started will revamp and bring back their facilities to SOA. This investment is really needed.

NREL is expensive for small businesses, and it is necessary to find formulas to make it more accessible to entrepreneurs. NREL should seek more feedback and participation from the industry.

- The Integrated Biorefinery Research Facility (IBRF) provides a valuable facility for testing, scaling, and de-risking the commercialization of biochemical conversion. Continued investment to upgrade to SOA technologies is a well-spent investment to continue innovations and the commercialization of biochemical conversion.

  As with all national labs, the cost for testing at the IBRF is expensive and is a barrier for smaller startups. DOE BETO FOAs enable smaller, resource-constrained companies to partner with NREL and conduct testing, but FOAs are limited. Otherwise, access to the TCPDU is limited to large corporations and startups with early-stage venture capital funding.

- Adding data retrieval and process control management to the already existing biochemical piloting facility provides a significant improvement to its capabilities. In addition, generating process hazards analyses and procedures is very important, along with sample generation and product analysis. This is a very important tool for investigating and scaling up biochemical conversions to de-risk unit operations, provide real-time process characterization, and generate data for scale-up. As evidenced by the many industrial collaborations in these facilities, there should be strong support for continued investment to keep up with new technologies for this application area. I would like to see additional pilot unit operations for biochemical separations.

- Biochemical conversion is a promising technology used to convert biomass feedstocks into useful products. The operations involving various feedstocks have helped to modernize the IBRF, and the insights gained are being used by industry clients for process development and scale-up, tailored to their specific needs. Over the years, the IBRF has evolved into an SOA facility. What type of change management (control) mechanism is implemented to ensure that modifications made to the facility do not adversely affect its operations? This mechanism should be designed to carefully evaluate and approve any changes to the facility to ensure that they are safe, effective, and do not violate any regulations. Understanding this mechanism can help differentiate any work performed before and after modifications to the facility. Can the IBRF operate 24/7, making it feasible to conduct experiments or runs that span multiple days? This allows for a more thorough analysis of the processes and a more accurate understanding of their potential for commercial-scale deployment. In addition to tracking the utilization of the facility, does the IBRF maintain a record of projects that have been performed and have resulted in commercialization? This information is essential for understanding the success of the IBRF and the impact of its research on the industry. The results and efforts of the IBRF project are expected to significantly contribute to the successful deployment of biochemical projects at commercial scales.

- The work of the unit is important for facilitating the commercialization of biochemical technologies for biofuels production.

PI RESPONSE TO REVIEWER COMMENTS

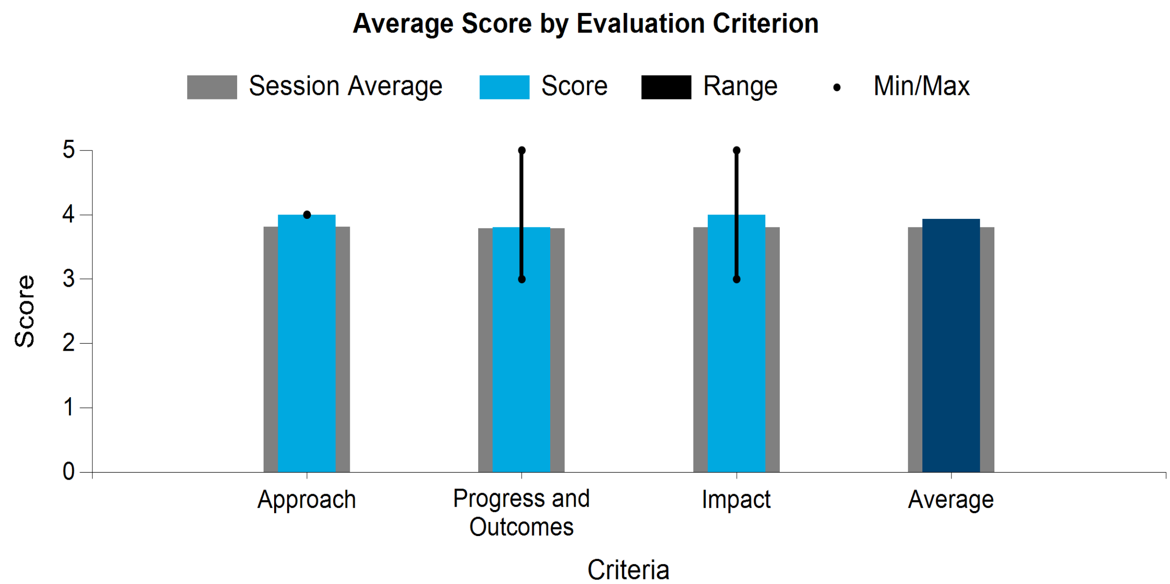
- We appreciate the reviewers' comments and their assessment of this work, and we have provided clarifications and answers to the comments in the following. The project's primary goal is to maintain a safe and process-relevant biochemical-based pilot plant that is made available to others to use including industry partnerships and BETO research projects. Regarding 24/7 operations, the facility has been used in the past and currently can conduct work requiring 24/7 operations. With respect to change management, we follow guidelines from the Occupational Safety and Health Administration and the

American Institute of Chemical Engineers' Center for Chemical Process Safety, and we document the change and its impact on operations, provide expert reviews of design and safety prior to system use, and verify that the changes were satisfactorily completed. Regarding separations, we are continuing efforts to upgrade the facility to perform biomass-to-finished fuel processing, and we will likely acquire additional separations capabilities to support this effort as well as more generic downstream processing requirements. The challenge is identifying the most versatile equipment to support multiple projects, all typically with unique downstream processing needs. We understand and share the concerns regarding the cost of doing business at NREL and other national laboratories. But beyond the FOA process and associated DOE cost sharing and other limited programs at NREL, there is currently no mechanism to reduce or provide cost shares for a project using our facility. Finally, we do not maintain good records of the fate of companies and technologies used in the plant; however, we would like to initiate work on this suggestion and develop a database to begin tracking this information and mine previous work to the extent possible.

INNOVATION AND OPTIMIZATION OF THE SZEGO MILL FOR RELIABLE, EFFICIENT, AND SUCCESSFUL UPSCALING OF THE DEACETYLATION AND MECHANICAL REFINING PROCESS FOR BIOFUEL PRODUCTION

University of Alabama

WBS:	3.4.2.203
Presenter(s):	Luke Brewer
Project Start Date:	10/01/2020
Planned Project End Date:	01/31/2026
Total Funding:	$3,816,102



COMMENTS

- The University of Alabama is performing a very thorough analysis of the metallurgy required for manufacturing the Szego Mill for biomass processing after the DMR disc refiner. The lab-scale mill has suffered corrosion and very quick degradation of the internals. The University of Alabama is trying to identify the causes and provide a metallurgical solution to avoid those problems. The University of Alabama has proven different types of stainless steel and has identified two promising alloys and two possibilities for material filling. The mill rotates at 1,200 rpm, and water with a 3% solid content is inside. I am sure the team has considered cavitation as the source of material degradation, but nothing was mentioned in the presentation. I think that this should be studied. Please keep working as you have done in the past and bring a feasible solution.

- The team has developed a sound approach to selecting better steels for the Szego Mill to address the wear and vibration issues with corn stover. The project will make the Szego Mill viable for commercial use with the DMR process. The Szego Mill improves sugar yield in the DMR process and thus enables better economics of commercial SAF production via the DMR process. A TEA should be included as part of this project to quantify the economic improvements.

- This is a very systematic approach to selecting and improving the materials of construction of the Szego Mill rollers to improve wear and corrosion resistance. The additional benefit will be noise reduction for this unit operation. A cost-benefit analysis would be helpful in making the final decisions on how to proceed. This kind of analysis would be useful for any other pretreatment unit operation that is subject to mechanical wear or corrosion damage. It might also be useful to consider other materials of construction, such as advanced ceramic composites, which are both tough and unaffected by corrosion. Several questions still remain about this unit operation, however—for example, whether the conditions of high speed and tight clearances are causing cavitation, which might impact wear and noise. A nearly horizontal configuration might allow for higher residence time, thus allowing for slower and less damaging speeds.

- The reliability and robustness of process operations using high wear-and-tear equipment for biomass applications is a crucial consideration that needs to be addressed. Equipment that shows signs of wear and tear after only 30 hours of operation is not scalable in an industrial setting. Although the Szego Mill may have been used in the pulp and paper industry with wood chips containing up to 50% moisture, as well as with softened wood, using corn stover with a moisture content of 15% and without precooking may affect the wear and tear of the equipment. Further investigation is necessary to understand the impact of these conditions on the equipment. At present, the results of this project may satisfy academic curiosity, but the commercial implementation of the findings will be limited until the reliability and robustness of the process operations are established.

- The addition of the Szego Mill to the DMR process can increase sugar yields from enzyme hydrolysis by 10%, according to the data presented. This would have a clear impact on the yield of fermentation product and potentially improve the economics of a facility based on this technology. The principal investigator (PI) presented the approach that was taken to identify problems with wear and corrosion on the metal in the Szego Mill, and the research approach is sound; however, the impact on the metal seems different for this type of feed, and it might be useful to identify the conditions under which wear and corrosion will be minimized. For example, pH adjustment before the Szego milling step to the pH required for enzyme hydrolysis might minimize the problems encountered. Moving to expensive metals or metal treatments will likely add costs to the overall process, which could be avoided or minimized. It will also be useful to include some cost data on metals and treatments to get an idea of whether the increased costs would be warranted for the inclusion of the Szego milling step.

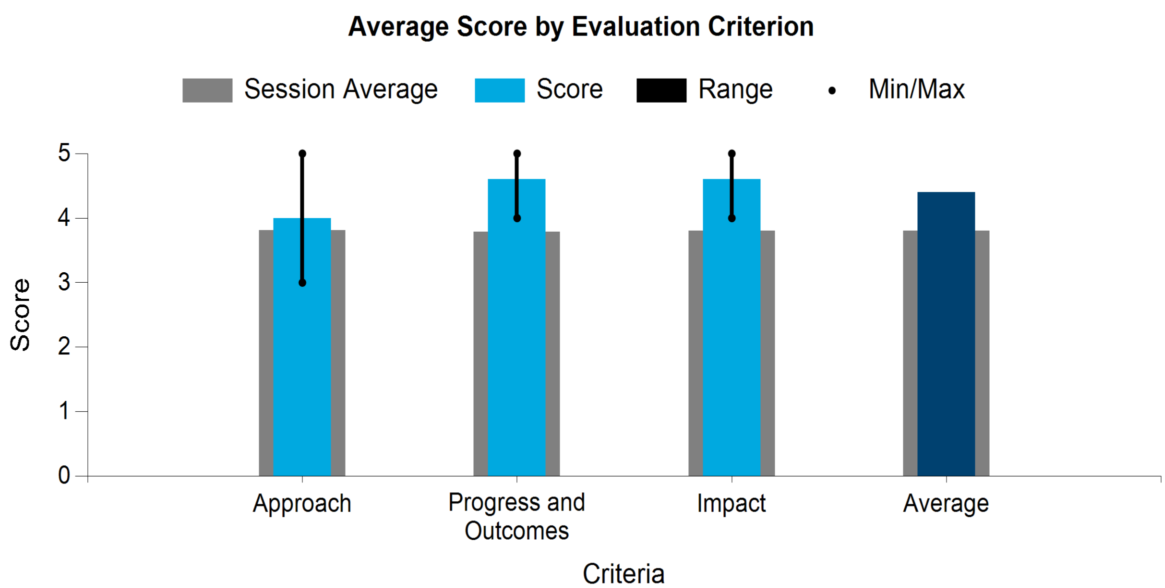
PNNL HYDROTHERMAL PDUS

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

WBS:	3.4.2.301
Presenter(s):	Mike Thorson
Project Start Date:	10/01/2018
Planned Project End Date:	09/30/2024
Total Funding:	$5,055,000

The PNNL hydrothermal PDU project is focused on adapting and applying hydrothermal PDU capabilities (hydrothermal liquefaction [HTL], catalytic upgrading, catalytic hydrothermal gasification) to produce biofuels and coproducts from wet waste feedstocks. The project has four major objectives: (1) conduct process development R&D to enable the scale-up of hydrothermal processing unit operations; (2) scale up testing and the production of fuels and coproducts from wet waste feedstocks; (3) PDU systems capability management supporting operations, maintenance, and system modifications; and (4) PDU utilization and development of industry partnerships. The PDU project is addressing engineering scale-up challenges that must be resolved to move forward with later-stage integrated pilot testing and commercialization. This has resulted in several industry collaborations, cooperative R&D agreements, the development of intellectual property for improved HTL processing and upgrading, and licensing agreements with commercialization partners.



COMMENTS:

- The PNNL has developed a promising technology to produce biocrude from wastewater biosolids. They have designed a plant, tested it at a small pilot-plant scale, and developed an engineering package for technology scale-up. The escalation factor from pilot to demonstration is 30–40 times, which is reasonable. They have addressed the fouling issues in high solid-liquid by eliminating heat exchangers. PNNL is focused on only one type of feedstock (biosolids from wastewater treatment plants), and I think they should also look at other available feedstocks. Licensing the technology is a great business concept, but the PNNL, as a national lab, should also dedicate its resources to providing feedback to other potential technology users.

- PNNL's hydrothermal PDU provides a valuable facility for testing, scaling, and commercializing HTL projects and valorizing wet waste feedstocks. PNNL has been clever in taking lessons learned from tar sands for solids separation and wastewater treatment plants for eliminating heat exchangers and associated fouling problems; however, the PDU does not have the capabilities to identify and solve contaminant issues besides for per- and polyfluoroalkyl substances (PFAS). Given that sewage sludge is the target feedstock, it seems that contaminants are an important issue to address.

- This wet waste-to-liquid fuels installation represents a good collection of feedstock sources and comprehensive unit operations. Building on collaborations involving Canadian tar sands is a good idea, and it led to the conclusion that avoiding heat exchangers makes sense when dealing with heavily fouling processes. Investing in this capability should accelerate many programs involving recalcitrant feedstocks. I would like to see more effort on in-line analytical capabilities.

- The primary focus of this project is to develop processes for HTL, scale up unit operations, and build industry partnerships. These efforts have a direct impact on the commercialization of HTL projects. HTL is an appropriate technology, especially for processing feedstocks with high moisture content. The project is well managed, with clear goals and accomplishments; however, note that achieving GHG emissions reduction greater than 81% compared to fossil sources depends on the feedstocks used. Regarding the production of biocrude, it is important to address the potential presence of PFAS. If PFAS are detected, what measures will be taken to handle and mitigate their impact? Additionally, what assistance does this project aim to provide to end users in tracking biogenic carbon in the final product? This methodology will enable end users to accurately report the carbon footprint of the biocrude produced and biogenic carbon in the final product, contributing to the overall sustainability of the project.

- HTL is an important technology for the production of drop-in biofuels, and the commercialization of this technology is a priority. As a process that can, uniquely, use wet feedstocks, HTL can access niche feedstocks and can be used for the treatment of waste. The work done at PNNL is therefore very important. The only comment/concern is that there is a focus on sewage sludge alone. Many projects and research efforts also focus on solid feedstocks that may contain high moisture content, and these feedstocks can pose unique challenges but make a significant contribution in the biofuel sector to expand the access to feedstocks without the energy inputs associated with drying that is needed with pyrolysis or gasification. As a national lab, advancing a broader feedstock utilization would be beneficial to industry and research efforts.

PI RESPONSE TO REVIEWER COMMENTS

- We would like to express our appreciation for the valuable feedback and thoughtful comments on our project. We are pleased to hear that the reviewers have recognized the potential and significance of our efforts in developing HTL technology for producing biocrude from wastewater biosolids. We appreciate the following positive feedback: "PNNL has developed a promising technology to produce biocrude from wastewater biosolids," "PNNL's Hydrothermal PDU provides a valuable facility for testing, scaling, and commercializing HTL projects," "Investing in this capability should accelerate many programs involving recalcitrant feedstocks," "The project is well managed, with clear goals and accomplishments," and "Hydrothermal liquefaction is an important technology for the production of drop-in biofuels."

  Diversification of feedstocks: We appreciate the suggestion to explore other available feedstocks beyond wastewater biosolids. Although our current focus has been on advancing the robustness of HTL using biosolids from a water resource recovery facility as the design case, we understand the importance of considering a broader range of feedstocks, and we have carried out extensive work on a variety of feedstocks, ranging from woody material, to algae, to a variety of organic wet waste. We agree that by diversifying our feedstock sources, we aim to enhance the versatility and economic viability of HTL for different waste materials.

Addressing contaminant issues: We appreciate the concern raised regarding the identification and mitigation of contaminants, particularly beyond PFAS. As part of our ongoing conversion R&D, we are addressing contaminant destruction around PFAS/perfluorooctyl sulfonate species, we and have historically looked at the destruction of a wider range of contaminants.

In-line analytical capabilities: We agree with the reviewers regarding the importance of in-line analytical capabilities for real-time monitoring and process optimization. This is a valuable area of consideration, and we will assess options for the integration of advanced in-line analytical techniques within our HTL processes. Such capabilities would enable us to enhance process control, improve product quality, and ensure the efficient conversion of wet waste feedstocks into valuable biofuels.

GHG emissions reduction and carbon footprint tracking: We appreciate the reviewer's acknowledgment of HTL as an appropriate technology for reducing GHG emissions. Addressing the specific feedstock-dependent GHG reduction potential is indeed a critical aspect of our research. Regarding the carbon footprint tracking, we are partnered with Argonne National Laboratory (ANL) for detailed LCA analysis that models GHG reduction exceeding 80%. Again, we sincerely appreciate the reviewer's feedback. We remain committed to collaborating with industry partners and to actively engaging in knowledge sharing to ensure the broadest impact of our work. We are dedicated to advancing the field of biofuels production, improving sustainability, and contributing to a more environmentally friendly energy landscape.

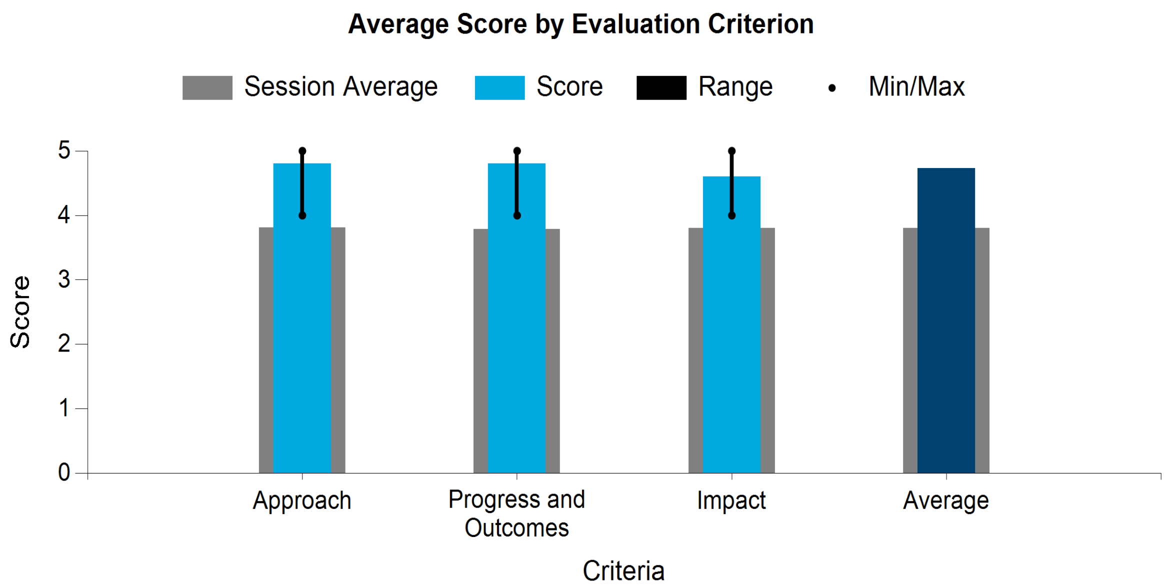
TCPDU - CATALYTIC CARBON CONVERSION CENTER OF PILOTING AND EXCELLENCE (C4PE)

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	3.4.2.302
Presenter(s):	Mark Still
Project Start Date:	10/01/2018
Planned Project End Date:	09/30/2024
Total Funding:	$5,307,000

The Catalytic Carbon Conversion Center of Piloting and Excellence (C4PE) maintenance and upkeep project supports facilities that address key technical and economic risks of biofuels production. The industrial relevance of these facilities is maintained through industry engagement, internal evaluation, and implementation. Maintenance and upkeep of C4PE facilities helps generate industry partnerships and accelerate progress toward BETO's renewables production goals.



COMMENTS

- NREL is known worldwide as a reference for biomass treatment, utilization, and upgrading. During the last 30 years, NREL has worked with multiple stakeholders trying to solve the intricacy of sugar liberation in biomass feedstocks. I think NREL has outdated facilities, and the $39 million they have just started will revamp and bring back their facilities to SOA. This investment is really needed. NREL is expensive for small businesses, and it is necessary to find formulas to make it more accessible to entrepreneurs. NREL should seek more feedback and participation from the industry.

- NREL's TCPDU is a valuable resource that enables R&D for developing, de-risking, and scaling thermochemical conversion processes, which are capital intensive. Continued investment to maintain the TCPDU as an SOA facility is a key component of developing large-scale biofuels and the biochemicals industry. Interviewing industry experts and holding bioeconomy listening sessions are great approaches to ensuring that additional investments and improvements align with industry interest and needs; however, the cost for using the TCPDU is expensive and is a barrier for smaller startups. DOE/BETO

FOAs enable smaller, resource-constrained companies to partner with NREL and conduct testing, but FOAs are limited. Otherwise, access to the TCPDU is limited to large corporations and startups with early-stage venture capital funding.

- This facility is a valuable resource to de-risk multiple pathways from the bench scale to piloting for commercial basic data. It has many essential elements—from heat and mass transfer data collection, to solids handling, to data collection for TEAs, to modeling and sample generation. It is a very good example of how government and industry can work together to collaborate on big challenges. I support continued funding to keep up with the SOA on new technologies.
- Thermochemical conversion is a vital technology for converting biomass feedstocks into valuable products. This project is making excellent progress toward its defined goals, with significant achievements and industry participation and collaboration. The project's primary focus is on conducting R&D for process development, scaling up unit operations, and fostering industry partnerships. The project's methodology should include a robust system for tracking biogenic carbon in the final product, ensuring the sustainability and environmental integrity of the process. I suggest the allocation of resources to process modeling work, particularly in the development of reaction kinetics. These models are essential for simulating the process, and they help to optimize operations, increase efficiency, and reduce costs. By using process simulators, the project team can evaluate different scenarios and identify areas for further improvement, leading to more effective and profitable thermochemical conversion processes.
- The NREL TCPDU performs an important function in the advancement of thermochemical technologies, such as pyrolysis, catalytic pyrolysis, and upgrading. Continuous upgrading of the facilities is critical to provide advances in the area and a relevant service to industry.

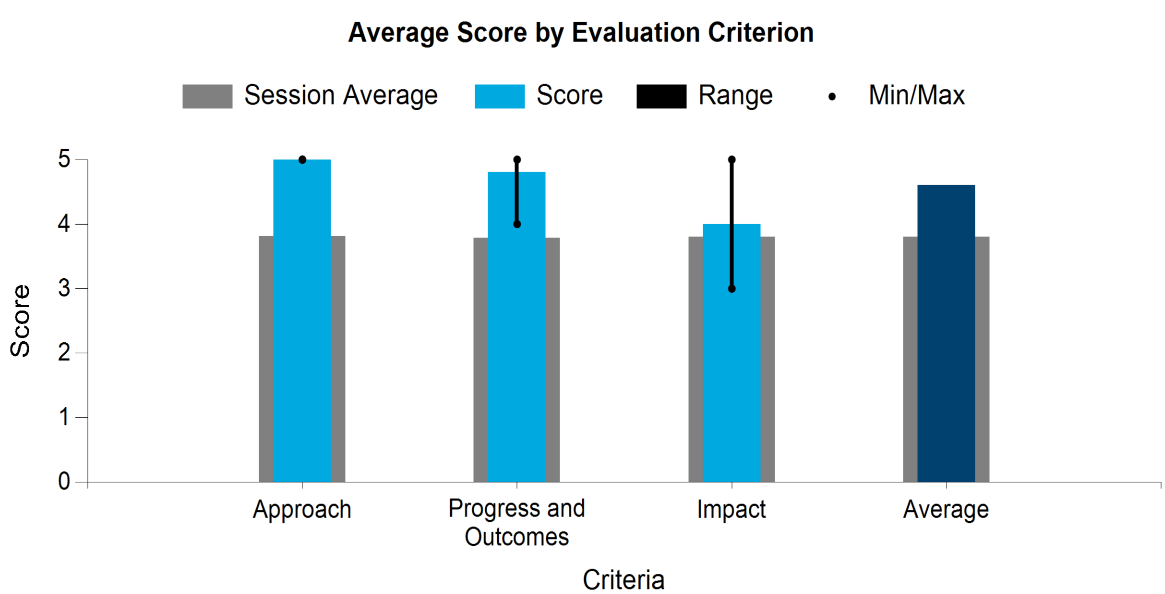
CONVERSION OF 2,3-BUTANEDIOL TO BIOJET FUEL: SCALE-UP AND TECHNO-ECONOMIC ANALYSIS OF ENERGY-EFFICIENT SEPARATIONS AND FERMENTATIVE DIOL PRODUCTION

Georgia Institute of Technology

PROJECT DESCRIPTION

WBS:	3.4.2.501
Presenter(s):	Sankar Nair
Project Start Date:	10/01/2020
Planned Project End Date:	09/30/2024
Total Funding:	$3,754,356

This project targets key process scale-up, modeling, detailed evaluation, and TEA LCA issues in the conversion of 2,3-BDO to kerosenic biojet fuel blendstocks. This goal will be achieved by collaborative advancement of five project elements:. (1) We will demonstrate the scale-up of BDO enrichment to 85+ wt % from clarified fermentation broths by a continuous adsorption pilot plant to produce 100 kg BDO at more than 1 kg/day. (2) We will demonstrate the construction and operation of a pervaporation membrane module for the last-mile dehydration of BDO. Each scaled-up system will be operated for 500 hours cumulative and 100 hours continuous on-stream time. (3) We will demonstrate the scale-up of fermentative BDO production at the 1,000-L scale to obtain at least 100 kg BDO with at least 100-g L concentration. (4) Laboratory-scale catalytic conversion work will optimize catalyst properties and conditions for enriched BDO feeds and produce biojet fuel samples that meet ASTM biojet blendstock standards. (5) The entire project will be tied together by a process modeling, TEA, and LCA framework that will produce accurate, well-parametrized separation process models, and we will integrate them with an overall process TEA to meet (modeled) throughput, MFSP, and CO_2 emissions reductions. The separation and fermentation technologies scale-up levels will be 100–1,000 times the present bench scale, and they would constitute the highest scale-up for BDO production to date.



COMMENTS

- The project will produce SAF from corn stover using 2,4-BDO as the sugar fermentation product (instead of ethanol). The novelty is that BDO can be separated from water without boiling it, and it is already a C4, which improves the oligomerization process. Extensive work is required in all aspects of the process: (1) BDO production, (2) BDO-water separation and purification, (3) BDO dehydration, and (4) olefines oligomerization. This is not an easy process, and it requires that various subsystems that have not yet been developed are integrated and can economically produce the fuel. The project has been ongoing for almost 3 years, and the presenter has reported good results in BDO fermentation and bench-scale BDO-water separation. The catalytic conversion of BDO to olefins still needs significant in-catalyst screening, kinetic modeling, and characterization. It is a high-risk project because of its complexity.

- The project had a sound, systematic approach to developing the conversion of BDO from corn stover to SAF. The team understands the technical challenges to be addressed. The team seemed to work together and coordinated well. Given the complexity of the process, the TEA and LCA will be important to evaluate the commercial feasibility.

- The approach used by this team is classic applied chemical engineering. Experimental work, modeling, and TEA are used to guide the selection of process conditions and evaluate outcomes. Communications between member organizations across the country are seamless and are clearly moving the project along. Already the team is seeing improvements to adsorption media stability, BDO isolate concentrations, and the reactivity of metal/zeolite catalyst for BDO-to-olefin conversion. The result is lower energy consumption, higher=quality intermediates, and improved separations. Although it remains to be seen if 2,3-BDO to SAF is the preferred route, this is an excellent team effort.

- The project team consists of highly experienced members from academia, national labs, and industrial companies who are working in excellent coordination to ensure that the project progresses smoothly. Please explain the reasoning behind using pervaporation membranes for BDO dehydration? When it comes to producing jet fuels, how does the BDO process compare with the ethanol route? Additionally, what is the justification for producing jet fuels from BDO instead of other bioproducts? Note that although the jet fuel produced from ethanol is ASTM certified, producing jet fuel from BDO would require a new certification from ASTM before it can be used in airplanes.

- This project targets the production of 2,3-BDO as an alternative to ethanol as an intermediate for conversion into SAF. A novel separation method is proposed using adsorption and enrichment of 2,3-BDO, thus avoiding energy-intensive methods required for ethanol removal from the fermentation broth. Comparing this process with an ethanol production and conversion process will be useful based on titer, yields, productivity, energy inputs, economics, etc. Specifically, the comparison should be assessed for the production of ethanol/BDO, the separation process, and the ATJ process. The BDO-to-jet process will require more steps, which would impact the economics of this stage. It is not clear whether any jet fuel has been produced from BDO and the characteristics of the jet fraction, and this should be provided. ASTM approval for BDO to jet will need to be obtained.

PI RESPONSE TO REVIEWER COMMENTS

- Overall, the five reviewers have given very positive comments on this project. In the following, we have excerpted the questions/concerns of the reviewers and answered them. Similar comments from different reviewers have been grouped.

  Comments: The catalytic conversion of BDO to olefins still needs significant in-catalyst screening, kinetic modeling, and characterization. It is a high-risk project because of its complexity. Response: The catalytic conversion element in this project involves bench-scale work only, targeted at proving the entire corn stover-to-SAF process flow. Our latest results (available after the peer review and included in the most recent quarterly report) show excellent performance of zeolite-based catalysts for both the BDO dehydration and oligomerization steps. We have thus successfully completed the catalyst screening and initial characterization, which greatly de-risks this project element. This project element will now focus on improving the SAF blendstock fuel quality and collecting systematic reaction data on the specific selected catalysts for use in updating our process model and TEA/LCA.

Comments: Given the complexity of the process, the TEA and LCA will be important to evaluate the commercial feasibility. Response: We agree. TEA/LCA update tasks are continually present in the project. Two iterations of the TEA/LCA have already been performed and show a positive delta NPV with respect to the prior state of technology. We will continue to refine the TEA/LCA using the detailed experimental data being generated in the project.

Comments: Although it remains to be seen if 2,3-BDO to SAF is the preferred route, this is an excellent team effort. When it comes to producing jet fuels, how does the BDO process compare with the ethanol route? Additionally, what is the justification for producing jet fuels from BDO instead of other bioproducts? Response: The project is responsive to the DOE goal of reducing the MFSP of bio-based aviation fuels to less than $3/GGE, and preferably less than $2.5/GGE, by 2030. Our current TEA indicates that the proposed route can meet these targets with comparable modeled costs to other routes based on ethanol. The catalytic conversion processes for BDO versus ethanol are somewhat different, including effects on catalyst longevity and efficacy in producing the required hydrocarbon slate. Our hypothesis is that starting from a C4 intermediate will have positive impacts on the catalytic processes. These aspects are not as easily captured in TEA and will require further detailed catalyst testing (which is planned in our project), which will then enable a better comparison with ethanol-based routes.

Comments: Note that although the jet fuel produced from ethanol is ASTM certified, producing jet fuel from BDO would require a new certification from ASTM before it can be used in airplanes. ASTM approval for BDO to jet will need to be obtained. Response: Our project, which proposes to produce SAF blendstock (ASTM D7566), has specific tasks in Budget Period 3 and Budget Period 4 to assess and continually improve the fuel quality using ASTM D7566 tests. Detailed hydrocarbon product analysis is being conducted (and the first results were reported in our most recent quarterly report). This work will be performed in close collaboration with our industry partner.

Comments: Please explain the reasoning behind using pervaporation membranes for BDO dehydration? Response: The adsorption (simulated moving bed) process and the vacuum distillation column together remove the vast majority of the water (mainly the simulated moving bed) and recycle the ethanol desorbent (vacuum distillation). This produces a stream of approximately 85% BDO and 15% mostly water. The pervaporation membrane downstream performs last-mile dewatering of this stream to 90%–95% (this can be controlled); therefore, it is an important de-risking operation and is electrified (uses very little thermal energy). For example, if water content is found to have a significant long-term impact on downstream catalyst function, then the capability to control the last-mile water removal independently of the simulated moving bed and vacuum distillation will be a significant factor.

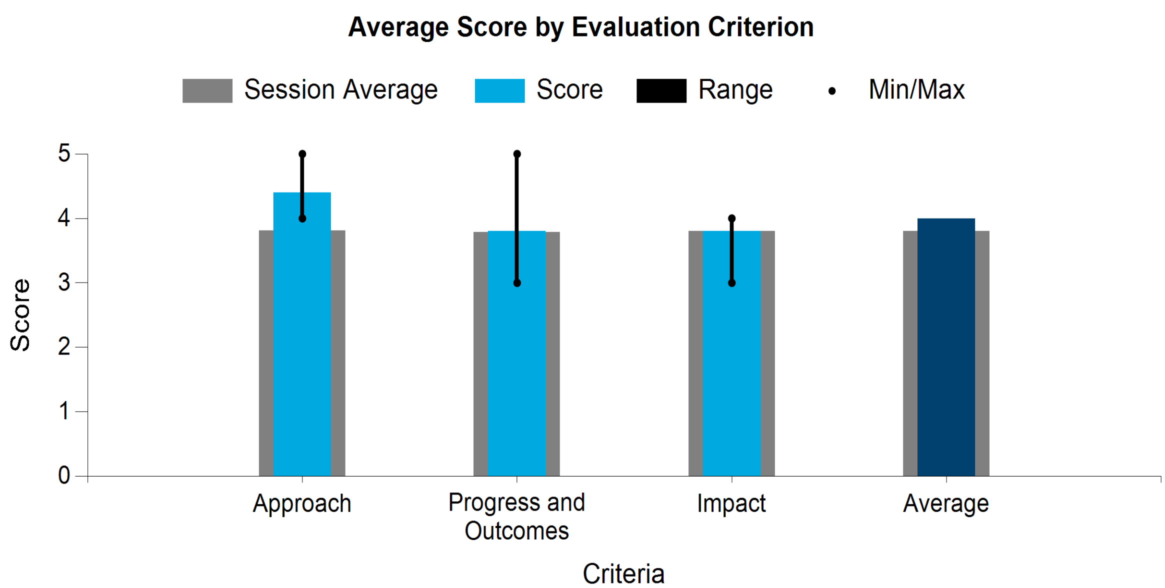
SCALE-UP OF THE PRIMARY CONVERSION REACTOR TO GENERATE A LIGNIN-DERIVED CYCLOHEXANE JET FUEL

University of North Dakota

PROJECT DESCRIPTION

WBS:	3.4.3.501
Presenter(s):	Wayne Seames
Project Start Date:	10/01/2020
Planned Project End Date:	06/30/2025
Total Funding:	$4,778,359

The goal of this project is to translate lab-scale reaction technology to produce cyclohexanes from corn stover-derived reactive lignin to the engineering scale and to determine the technical, economic, and environmental feasibility of producing jet fuel and byproducts from this technology. Corn stover is preprocessed by INL and shipped to NREL, where the deacetylation step of NREL's dilute alkali DMR process followed by evaporation is used to generate 10 wt % reactive lignin in a 10+ pH NaOH/water solution and shipped to the University of North Dakota. The lignin is then non-catalytically fragmented. The fragments are recovered by solvent extraction and hydrogenated into cyclohexanes using an Ru-based catalyst developed at Washington State University and pelletized by Advanced Refining Technologies. The conversion system is being optimized at the bench scale and then upscaled to the engineering scale, where it will be demonstrated with operation for at least 100 continuous hours and 500 total hours. Secondary objectives are to develop a less expensive, more efficient hydrogenation catalyst and improved analytical methods for comprehensive reaction product evaluation, plus production/testing of the prototype jet fuel. The technology is also being assessed via TEA and sustainability analyses.



COMMENTS

- Interesting concept, and the project progresses. Good work so far. There are a lot of challenges in the future, but the teams have demonstrated their capabilities. The project was not presented at the Project Peer Review; the presenter was not able to travel due to weather. This evaluation is based only on a review of the slides. The team has taken a sound, systematic approach to scaling from the lab scale to the engineering scale and evaluating the technical, economic, and environmental feasibility of the technology to produce SAF. So far, the team has been able to address multiple challenges as well as coordinating the work to meet tight schedules during the constraints of the pandemic. Biomass-derived cyclohexanes jet fuel/blendstocks would provide a renewable solution for the seal swell requirement and enable higher renewable content in jet fuels, especially Fischer-Tropsch jet fuels. The TEA will be important for evaluating the commercial viability, given that the preliminary TEA showed that the original process is not commercially feasible.

- The presenter was not able to be present for this review. The comments are based on the published charts. This seems like a comprehensive approach to experimental testing and modeling of the reaction conditions leading to catalyst improvement opportunities, including TEA to guide choices. Although the optimum set has not yet been identified, this approach holds promise to find a set of conditions that allow lignin in alkali media to be directly converted to cyclohexane that can be used to make jet fuel. This approach may also be useful to explore other feedstocks and other pathways to advanced biofuels.

- The following comments are solely based on the information obtained from the slide deck because the presenter was unable to attend the Project Peer Review. The main objective of this project is to produce cyclohexanes, which can be used as fuels, from the lignin fraction obtained during the biochemical processing of corn stover. The project team has demonstrated excellent coordination and has successfully modified the execution strategy to overcome challenges encountered during the implementation phase. The modified approach identified for the conversion of lignin to cyclohexanes holds promise; however, the efficient recovery and reuse of ethyl acetate may dictate the economics of this approach. It is unclear, however, if the team has revised the TEA to account for the alternative strategy identified. It is also uncertain how feasible it is to scale up the fragmentation of lignin and the extraction of solubles for conversion into jet fuel for commercial operations. Further analysis will be necessary to determine the commercial viability of this process.

- This project produces cyclohexanes from phenolic compounds in the lignin fraction of corn stover after DMR. If this can be done economically, it can have a very favorable impact on lignin valorization in cellulosic ethanol production while providing an important blending component for SAF in place of aromatics. Only preliminary results were shown, and the crucial TEA and LCA were not completed at the time of the presentation and will be critical to evaluate the potential success and commercialization potential. Switching to a multistep process will likely result in increased costs and added complexity. What is the hypothesis regarding the inability to hydrodeoxygenate the pH 10 NaOH solution? Is removal of the Na required? Is reduction of the pH required, or is the NaOH used as a basis for decomposition of the lignin? How is the lignin non-catalytically decomposed, and how effective is recycling of the non-decomposed lignin for achieving greater decomposition?

PI RESPONSE TO REVIEWER COMMENTS

- Thank you to the reviewers for their thoughtful and encouraging comments. In reference to Comment 4, we have demonstrated that more than 96% of the organics can be extracted from the fragmentation reactor outlet NaOH/water solution, that more than 99% pure ethyl acetate can be recovered by a single-stage distillation, and that the resulting organics have less than 0.1% ethyl acetate. A more comprehensive TEA is being prepared based on the current process scheme and the preliminary data obtained. This TEA will help us to focus future lab- and bench-scale research tasks while we are scaling up the process to the engineering scale. In reference to Comment 5, although the multistep process will be more complicated, the quantity of Ru-based catalyst is reduced by more than an order of magnitude, so we do not expect this version to be more expensive than the original single-step reaction scheme. We postulate that at high hydroxide concentrations, as the hydrogen disassociates, it quickly reacts with the hydroxide to form water instead of hydrogenating the lignin fragment compounds. The purpose of the NaOH is to increase the pH to increase the solubility of lignin in water. Other bases will also work and may eliminate this effect. These will be explored at the lab scale in the upcoming year. Complex organics like lignin are too large to fit in the pore of most catalysts, so the first step in any complex organic decomposition is most likely non-catalytic even when a catalyst is present. This is also when oligomers and other tarry compounds are formed that can foul catalysts. By separating the fragmentation and hydrogenation steps, these issues will be minimized, which may be more important operationally than having to use more unit operations. Preliminary results suggest that once the leftover lignin solution is concentrated back to its original concentration, that fragmentation comparable to the initial fragmentation can be achieved. We will be exploring this in more detail during the upcoming year.

FIELD-TO-FUEL PRODUCTION OF CARBON-NEGATIVE SUSTAINABLE AVIATION FUEL FROM REGENERATIVE-AGRICULTURE BIOMASS

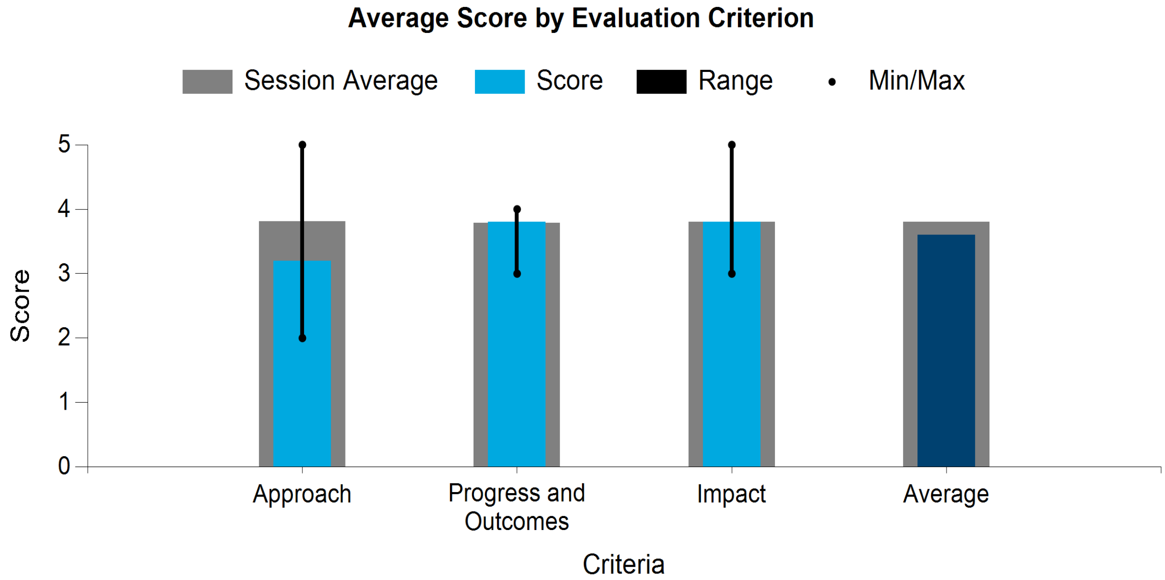
Alder Energy

PROJECT DESCRIPTION

WBS:	3.4.3.603
Presenter(s):	Derek Vardon
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2024
Total Funding:	$5,920,596

This project will scale Alder Energy's proprietary Alder Renewable Crude (ARC) technology to convert 0.5 tons per day (TPD) of biomass and produce SAF with negative carbon intensity from regenerative-agriculture miscanthus. Alder's ARC technology addresses the challenge of refinery hydrotreater plugging with commercial fast pyrolysis oils (FPOs) by employing solvent fractionation to generate two process streams for downstream upgrading. This allows ARC to undergo continuous hydrotreating to produce high C-yields of SAF that meets ASTM specs. We will evaluate regenerative-agriculture miscanthus biomass as the feedstock, which has the potential to produce SAF with negative carbon intensity due to the net carbon sequestered in the soil during cultivation. This project will provide key data to baseline woody biomass ARC performance against miscanthus ARC and conduct hydrotreating with iterative SAF fuel property testing for meeting ASTM specs. Success will provide the data needed to accelerate Alder's SAF commercialization.

To advance Alder's ARC technology, our team brings together world-class expertise across the entire SAF value chain. Our expertise includes FPO fractionation technology into ARC, regenerative-agriculture miscanthus field trials and carbon intensity quantification by AGgrow Tech and the University of Illinois, biomass preprocessing know-how by INL, commercial fast pyrolysis expertise by Biomass Technology Group (BTG), ARC hydrotreating and refinery integration expertise by Honeywell UOP and RPD Technologies, SAF fuel property testing expertise by Washington State University, TEA and LCA skill sets by NREL and the University of Illinois Urbana-Champaign (UIUC), commercial and business aviation industry insight for SAF by United Airlines and Gulfstream, and SAF flight test capabilities by United Airlines and Boeing. As the capstone, if target metrics are successful, we will conduct the world's first carbon-negative flight demonstration on Alder SAF produced from regenerative-agriculture miscanthus. If realized, this technology will spur the creation of new U.S. jobs for decarbonized energy and regenerative agriculture.



COMMENTS:

- The project has a significant number of participating partners. Managing them is complex and requires great effort. The company has not explained how they are handling it and whether they are having issues with the coordination. It is unclear why the team is using miscanthus when it seems to work with woody biomass. The presence of ashes in the feedstock may represent a very significant problem downstream and could prevent the use of pyrolysis oil in a hydrotreater. The company has not provided either TEA data to evaluate the economic feasibility of the technology and check the targeted production cost of \$2.75/gallon or any LCA data.

- Alder is expanding its feedstock options to miscanthus, which has the potential to play an important role in regenerative agriculture. The presentation identified major risks for the project and provided sound risk mitigation strategies. Due to the higher nitrogen content in miscanthus, the miscanthus greencrude would have a higher nitrogen content than a wood greencrude. Does Alder plan to remove the nitrogen from the miscanthus greencrude? Could miscanthus greencrude and wood-based greencrude be processed together into SAF at the same refinery? The presentation has only a high-level overview of the process. What does Alder's core technology consist of?

  For the go/no-go decision in FY 2023 Q4 on slide 9, if metrics are not met for miscanthus, pivoting to wood-based pyrolysis oil is proposed. Has Alder and/or Honeywell UOP conducted the remaining project campaign with wood-based pyrolysis oil? If so, what new information would be gained?

  Feedstock harvesting, handling, processing, storing, and feeding are often overlooked and not given appropriate attention. What challenges in miscanthus handling and processing has the team encountered or anticipate that would require solving to successfully operate a continuous process at a commercial plant?

- The proposed process uses a relatively smaller biomass supply (miscanthus, which is usually grown on marginal land) as the feedstock, does a fast pyrolysis to a biocrude, then solvent extracts the lighter products from the heavier products. It seems that a hydrotreating step should follow that fast pyrolysis to remove oxygenates. After extraction, the lighter products proceed to another hydrotreating step for conversion to a mix of fuels. The heavier fraction goes to a cracker to make lights and heavies. It uses fairly well-proven unit operations, and the team has a lot of experience with those unit operations. Concerns include the feedstock not being a larger agriculture byproduct like corn stover, the multiple processing steps with their capital charge, and the usual concerns about feed composition variability. A detailed TEA and LCA needs to be done to determine if the claimed economic benefits are sustainable as the process is scaled up. The approach has merit if the feedstock mix can be expanded and the value of products offsets the cost of equipment and operation.

- The challenge for this project will be to coordinate a number of diverse partners and successfully deliver their deliverables. This will require effective communication, collaboration, and project management skills to ensure that everyone is working toward the same goals. The proposed approach for this project is the ARC pilot, which aims to leverage the conditions established with wood pyrolysis oil. A go/no-go decision will be made to determine whether to move forward with wood pyrolysis oil if necessary; however, if miscanthus were to replace woody biomass as the commercial feedstock, it would likely require significant modifications to the project plan and potentially result in a different project altogether. One potential issue with using nitrogen-rich feedstock is that it could increase the nitrogen content in SAF when the biocrude is inserted into the hydrotreater. To address this, the project team may need to explore different processing methods to reduce the nitrogen content or consider using a different feedstock altogether. It is unclear from the provided information how deoxygenation will be performed to remove the oxygen present in the ARC. This will need to be further explored and defined as part of the project planning process to ensure the successful implementation of the project.
- The expansion of SAF production will have to shift to lignocellulosic feedstocks that are more abundant, and pyrolysis-type technologies will play a very important role to deliver SAF volumes, provided that SAF production can be successfully commercialized and ASTM approval can be obtained. Commercialization of the Alder technology will play an important role in this regard. Although I have several concerns about the technology approach, this project is limited to an evaluation of miscanthus as a feedstock and an assessment of the carbon intensity of the feedstock. The development of energy crops for SAF production will be critical to deliver the high SAF volumes required to meet the climate targets for the sector, and this project is very relevant. Although the carbon intensity of a feedstock is critical, the overall sustainability based on Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) sustainability criteria should also be assessed. Carbon intensity and LCA must also be assessed based on CORSIA methodology, which will be relevant for SAF. This may differ from an assessment based on Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET), and differences could provide important information to the improvement of the CORSIA method. The higher ash content in miscanthus (structural) will have an impact on the yield of the bio-oil (ARC and residual pyrolysis oil [RPO]) and impact the techno-economics. The miscanthus will likely also impact the fractionation of the bio-oil to ARC and RPO, and this will be relevant for the future suitability of miscanthus as a feedstock for this process. “Careful” harvesting of miscanthus to limit nonstructural ash content was proposed (in addition to winter harvesting to reduce ash from leaves), but the potential for these approaches to work at a commercial scale should be considered. Harvesting and processing at a small scale will not expose logistics and supply chain challenges such as storage to the scale-up of feedstock use.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The project has a significant number of participating partners. Managing them is complex and requires great effort. The company has not explained how they are handling it and whether they are having issues with the coordination. It is unclear why the team is using miscanthus when it seems to work with woody biomass. The presence of ashes in the feedstock may represent a very significant problem downstream and could prevent the use of pyrolysis oil in a hydrotreater. The company has not provided either TEA data to evaluate the economic feasibility of the technology and check the targeted production cost of $2.75/gallon or any LCA data. Response: We thank the reviewer for their comments.

This project leverages partnerships and diverse expertise from leading institutions across the bioenergy value chain to advance critical goals for the realization of carbon-negative SAF from regenerative agriculture. Joint milestones are used to ensure data integration and achieve project goals through coordinated contributions from all partners. Further, the communication strategy consists of project team meetings every 2 months to track progress, monthly small-group discussions centered on upcoming deliverables (e.g., field-to-gate miscanthus LCA), in addition to six-month project review meetings that include feedback from original equipment manufacturers and industry partners. Alder aims to enable process flexibility for feedstocks beyond woody biomass, and this project explores a regenerative-agriculture feedstock, miscanthus, and its potential for carbon-negative SAF production. Miscanthus holds significant promise for soil organic carbon sequestration relative to woody residues or annual crops like corn stover and sugarcane. Higher-ash-content biomass was identified as a key risk factor with possible impacts to pyrolysis, ARC, and SAF quality in this project. With this in mind, and with guidance from AGgrow Tech partners, the project team leveraged supply chain opportunities for managing feedstock quality, employing approaches for miscanthus harvest and timing to limit ash accumulation from soil contamination (nonstructural ash). In this study, structural ash content (inherent to biomass) was measured at approximately 0.7%, with accumulated ash at approximately 1.5% (dry matter). Ash content in corn stover often exceeds 5% (ranging from 5%–25%), with some reports of soil-derived, nonstructural ash exceeding 7%. In addition, preprocessing approaches were employed through the BFNUF housed at INL to further reduce feedstock ash content with selective preprocessing and fines removal of particles less than 500 microns. We appreciate the reviewer's feedback, and we will continue to closely track ash propagation and metal contaminants from feedstock through conversion to pyrolysis oil and fractionation to ARC and RPO to assess the impacts on hydrotreating and the final SAF product. The field-to-biorefinery gate LCA is currently underway and will combine high-quality data collected from field research sites with geospatial mapping and data-driven approaches developed by UIUC for evaluation of the miscanthus footprint. Miscanthus harvested from field research sites was characterized through compositional analysis and used for the production of FPO and fractionation to ARC at the bench and 10-gallon batch scales for hydrotreating and SAF production. During the next 6 months, the project team will scale to 20-metric-tons miscanthus for the production of FPO and continuous operations for ARC production at the barrel-per-day scale. These data will inform the TEA and LCA, allowing for the refinement of the final SAF product cost and field-to-fuel carbon intensity.

Comments: Alder is expanding its feedstock options to miscanthus, which has the potential to play an important role in regenerative agriculture. The presentation identified major risks for the project and provided sound risk mitigation strategies. Due to the higher nitrogen content in miscanthus, the miscanthus greencrude would have a higher nitrogen content than a wood greencrude. Does Alder plan to remove the nitrogen from the miscanthus greencrude? Could miscanthus greencrude and wood-based greencrude be processed together into SAF at the same refinery? The presentation has only a high-level overview of the process. What does Alder's core technology consist of? For the go/no-go decision in FY 2023 Q4 on slide 9, if metrics are not met for miscanthus, pivoting to wood-based pyrolysis oil is proposed. Has Alder and/or Honeywell UOP conducted the remaining project campaign with wood-based pyrolysis oil? If so, what new information would be gained? Feedstock harvesting, handling, processing, storing, and feeding are often overlooked and not given appropriate attention. What challenges in miscanthus handling and processing has the team encountered or anticipate that would require solving to successfully operate a continuous process at a commercial plant? Response: We thank the reviewer for their comments. Miscanthus harvest timing occurred after plant dry down and senescence—during which a significant translocation of nutrients, including N, occurs from the plant tissue back to the soil. Miscanthus used in this study had a measured N content of approximately 0.3%, comparable to softwood feedstocks evaluated in the ARC process. Experiments to date have not encountered high nitrogen, which is attributed to these steps taken during feedstock harvesting. It is anticipated that miscanthus and wood-derived ARC/greencrude can be processed in the same refinery.

Alder's core technology for renewable transportation fuel production links commercial fast pyrolysis technology with existing refinery infrastructure. Alder's proprietary technology fractionates FPO into two streams for renewable energy production: (1) ARC/advanced pyrolysis oil that can be shipped off-site for cohydroprocessing with fats, oils, and grease in existing refineries and (2) RPO that has the potential to be used as a boiler fuel for renewable electricity, upgraded to biogas, or hydrocarbon fuels via fluid catalytic cracking. Honeywell UOP has completed the first phase of development for ARC first-stage hydrotreating with woody biomass. Also, Alder has worked closely with partners at AGgrow Tech, UIUC, INL, and BTG to identify and mitigate challenges related to feedstock variability and supply chain and impacts to conversion. As discussed, miscanthus was harvested in late winter/early spring 2022 after plant dry down, senescence, and leaf fall to reduce moisture and limit ash content, improve feedstock quality, and provide material to meet pyrolysis infeed specifications. Moisture at harvest was approximately 10%–12% to ensure storage stability, and miscanthus was harvested with a standard forage chopper and blown directly into a wagon, so stems never touch the ground, further limiting ash contamination from soil (as discussed). Chopped miscanthus was stored in Ag-Bags (like silage bags) to preserve material at less than 15% moisture until further processing. The team has encountered minor challenges related to material feeding and handling of miscanthus biomass for pyrolysis. Alder is working with partners at BTG and INL to identify size reduction approaches that offer more uniform particle size distributions and a reduced particle aspect ratio to improve flowability, feeding, and handling and facilitate conversion. The team is also working to identify opportunities to reduce the carbon intensity of biomass size reduction required for pyrolysis infeed specifications. In batch studies, lower ARC mass yields were obtained due to the reduced lignin content in miscanthus relative to woody biomass. For successful operation at the commercial scale, reductions in ARC yield must be balanced by RPO, which can be upgraded to value-added fuels and chemicals.

Comments: This proposed process uses a relatively smaller biomass supply (miscanthus, which is usually grown on marginal land) as feedstock, does a fast pyrolysis to a biocrude, then solvent extracts the lighter products from the heavier products. It seems that a hydrotreating step should follow that fast pyrolysis to remove oxygenates. After extraction, the lighter products proceed to another hydrotreating step for conversion to a mix of fuels. The heavier fraction goes to a cracker to make lights and heavies. It uses fairly well-proven unit operations, and the team has a lot of experience with those unit operations. Concerns include the feedstock not being a larger agriculture byproduct like corn stover, the multiple processing steps with their capital charge, and the usual concerns about feed composition variability. A detailed TEA and IRR (internal rate of return) needs to be done to determine if the claimed economic benefits are sustainable as the process is scaled up. The approach has merit if the feedstock mix can be expanded, and the value of products offsets the cost of equipment and operation. Response: We thank the reviewer for their comments. Please see the brief description of Alder's proprietary fractionation technology in the response to Reviewer 2. Alder's technology separates the "bad actors" and reactive components, including small oxygenates, from FPO into an aqueous phase, and it significantly reduces the reactive oxygenates in ARC prior to hydroprocessing. The aim of this project is to evaluate ARC yields achievable through regenerative-agriculture miscanthus and integrate field-scale carbon flux data with modeling approaches to quantify the carbon intensity of the ARC-SAF pathway and potential for carbon-negative SAF. The results of this project will be directly compared with more abundant feedstocks that are also being assessed by Alder, such as woody biomass sources. This project does not consider a first-generation feedstock like corn stover given its variable feedstock quality, high ash content (see response to Reviewer 1) exceeding limits for pyrolysis, and requirement for intensive agricultural practices, which are not carbon neutral. With a purpose-grown feedstock like miscanthus, there are fewer sources of variability inherent to the biomass given the homogeneity in the vegetative portion of the plant and harvest timing after leaf fall and senescence, further reducing the ash content (see response to Reviewer 1). This project can also contribute insights to how harvest timing and agricultural practices are used in feedstock quality management for sustainable and profitable SAF production. The project is partnered with BTG bioliquids to produce pyrolysis oils, which has processed more than 75,000 tons of biomass into FPOs and evaluated more than 50 biomass feedstocks. Alder is leveraging BTG's vast expertise in feedstock composition variability impacts on both pyrolysis to gain deeper insight into potential impacts on the ARC process and upgrading to SAF. This project began Budget Period 2 execution on Dec. 12, 2022, and a preliminary TEA and LCA for the field-to-gate process will be reported in the FY 2023 Q3 milestone on June 30, 2023. During the next 6 months, the project team will scale to 20 metric tons of miscanthus for FPO production and continuous operations for ARC production at the barrel-per-day scale. These data will inform the TEA and LCA, allowing for the refinement of the final SAF product cost and field-to-fuel carbon intensity. We appreciate the reviewer's feedback regarding the current scale of miscanthus production. Projections from a recent study show promise for miscanthus to contribute 30 billion gallons per year of SAF from marginal lands in the rain-fed United States. This project will combine high-quality field data with geospatial mapping tools to refine estimates for miscanthus yields and sequestration potential under various environmental scenarios. The outcomes of this project can be used as a market pull for regenerative agriculture to produce carbon-negative SAF.

Comments: The challenge for this project will be to coordinate a number of diverse partners and successfully deliver their deliverables. This will require effective communication, collaboration, and project management skills to ensure that everyone is working toward the same goals. The proposed approach for this project is the ARC pilot, which aims to leverage the conditions established with wood pyrolysis oil. A go/no-go decision will be made to determine whether to move forward with wood pyrolysis oil if necessary; however, if miscanthus were to replace woody biomass as the commercial feedstock, it would likely require significant modifications to the project plan and potentially result in a different project altogether. One potential issue with using nitrogen-rich feedstock is that it could increase the nitrogen content in SAF when the biocrude is inserted into the hydrotreater. To address this, the project team may need to explore different processing methods to reduce the nitrogen content or consider using a different feedstock altogether. It is unclear from the provided information how deoxygenation will be performed to remove the oxygen present in ARC. This will need to be further explored and defined as part of the project planning process to ensure the successful implementation of the project. Response: We thank the reviewer for their comments. Alder has extensive experience dealing with complicated team structures. Alder's chief technology officer, Dr. Derek Vardon, formerly led a team within the CO-Optima initiative, and our research director, Dr. Allison Ray, is formerly of the FCIC. Our team is well experienced with multi-institution project management. In our ARC R&D activities related to woody biomass, we have created tools for sample management, executed tolling production runs, and coordinated analysis in collaboration with national lab, domestic, and international business partners. This project leverages diverse expertise from leading institutions across the bioenergy value chain to advance critical goals for the realization of carbon-negative SAF from regenerative agriculture. Joint milestones are used to ensure data integration and achieve project goals through coordinated contributions from all partners. This requires a collaborative, communication strategy that consists of project team meetings every 2 months to track progress, monthly small-group discussions centered on upcoming deliverables (e.g., field-to-gate miscanthus LCA), in addition to six-month project review meetings that include feedback from original equipment manufacturers and industry partners. As noted, miscanthus N content was measured at approximately 0.3%, comparable to softwood feedstocks evaluated in the ARC process. Alder did not identify high nitrogen levels in miscanthus-derived FPO or ARC at the 2-metric-ton scale and batch processing. Miscanthus FPO contained 0.1% N, and advanced pyrolysis oil contained 0.2% N (analysis precision is approximately 0.1%). Alder's proprietary fractionation technology separates the bad actors and reactive components, including small oxygenates, from FPO into an aqueous phase, and it significantly reduces oxygenates in ARC prior to hydroprocessing. Alder collaborates with partners at Honeywell UOP and RPD Technologies for deoxygenation via hydrotreating ARC to fuel products.

Comments: The expansion of SAF production will have to shift to lignocellulosic feedstocks that are more abundant, and pyrolysis-type technologies will play a very important role to deliver SAF volumes, provided that SAF production can be successfully commercialized and ASTM approval can be obtained. Commercialization of the Alder technology will play an important role in this regard. Although I have several concerns about the technology approach, this project is limited to an evaluation of miscanthus as a feedstock and assessment of the carbon intensity of the feedstock. The development of energy crops for SAF production will be critical to deliver the high SAF volumes required to meet climate targets for the sector, and this project is very relevant. Although the carbon intensity of a feedstock is critical, the overall sustainability based on CORSIA sustainability criteria should also be assessed. Carbon intensity and LCA must also be assessed based on CORSIA methodology, which will be relevant for SAF. This may differ from an assessment based on GREET, and differences could provide important information to improvement of the CORSIA method. The higher ash content in miscanthus (structural) will have an impact on the yield of the bio-oil (ARC and RPO) and impact the techno-economics. The miscanthus will likely also impact the fractionation of the bio-oil to ARC and RPO, and this will be relevant for the future suitability of miscanthus as a feedstock for this process. “Careful” harvesting of miscanthus to limit nonstructural ash content was proposed (in addition to winter harvesting to reduce ash from leaves), but the potential for these approaches to work at a commercial scale should be considered. Harvesting and processing at a small scale will not expose logistics and supply chain challenges, such as storage to the scale-up of feedstock use. Response: We thank the reviewer for their comments. As discussed in our previous responses, high ash content was identified as a key risk factor for miscanthus-derived SAF. CORSIA’s default life cycle emissions values, which have been produced partly in GREET, are not yet available for hydrotreated depolymerized cellulosic jet fuels, such as the ARC-derived SAF; hence, we are following the CORSIA methodology for calculating actual life cycle emissions values using GREET. Based on an in-house assessment of the CORSIA sustainability criteria, we expect the ARC-derived SAF from miscanthus to be certified as a CORSIA eligible fuel by an approved Sustainability Certification Scheme in the future. Also, we agree with the reviewer that ash content is a key consideration related to feedstock quality for pyrolysis-based pathways and can significantly impact FPO yields. The impacts of ash content on FPO yield will be dependent on the elemental composition, in particular the concentration of alkali and alkaline earth metals relative to inert species (like silicon). Detailed characterization of miscanthus for this project has revealed that ash was significantly reduced (approximately 2%) when compared to agricultural residues like corn stover. In the first phase of the project, batch experiments with miscanthus (approximately 2 metric tons) resulted in FPO yields comparable to previous experiments with woody feedstocks. We agree with the reviewer that the scale-up of feedstock logistics and supply chain challenges are an important consideration for technical feasibility and economic viability in de-risking ARC technology with miscanthus regenerative agriculture for SAF. Given that feedstock quality and availability are central to this project, Alder has established key partnerships with industry, academia, and national laboratories to address the intersections of the feedstock supply chain with conversion to ensure alignment of the technical approach with commercial relevance. Alder is working with a commercial partner, AGgrow Tech, a leader in renewable agriculture that is implementing innovative and sustainable agriculture solutions with miscanthus farms in 11 states and has 8,000 acres under management. UIUC is the world leader in sustainable agriculture analysis and bioenergy crops science, including miscanthus cultivated using regenerative agricultural practices. UIUC efforts also include the Center for Advanced Bioenergy and Bioproducts Innovation, whose goal is to develop and deploy technologies and crops that are economically and ecologically sustainable. INL and NREL are leading national laboratories funded by BETO in feedstock and conversion technologies, respectively, and are the lead labs in BETO’s FCIC to address challenges posed by feedstock variability, material handling, and preprocessing. INL is the lead lab for feedstock and preprocessing technologies, while NREL is DOE’s premier biofuel research laboratory. As noted in the response to Reviewer 3, the team hopes that broader project outcomes can be used as a market pull for regenerative agriculture to produce carbon-negative SAF.

INTEGRATION OF IH² WITH THE COOL REFORMER FOR THE CONVERSION OF CELLULOSIC BIOMASS TO DROP-IN FUELS

Gas Technology Institute

PROJECT DESCRIPTION

WBS:	3.5.1.101
Presenter(s):	Terry Marker
Project Start Date:	10/01/2019
Planned Project End Date:	12/31/2023
Total Funding:	$1,596,065

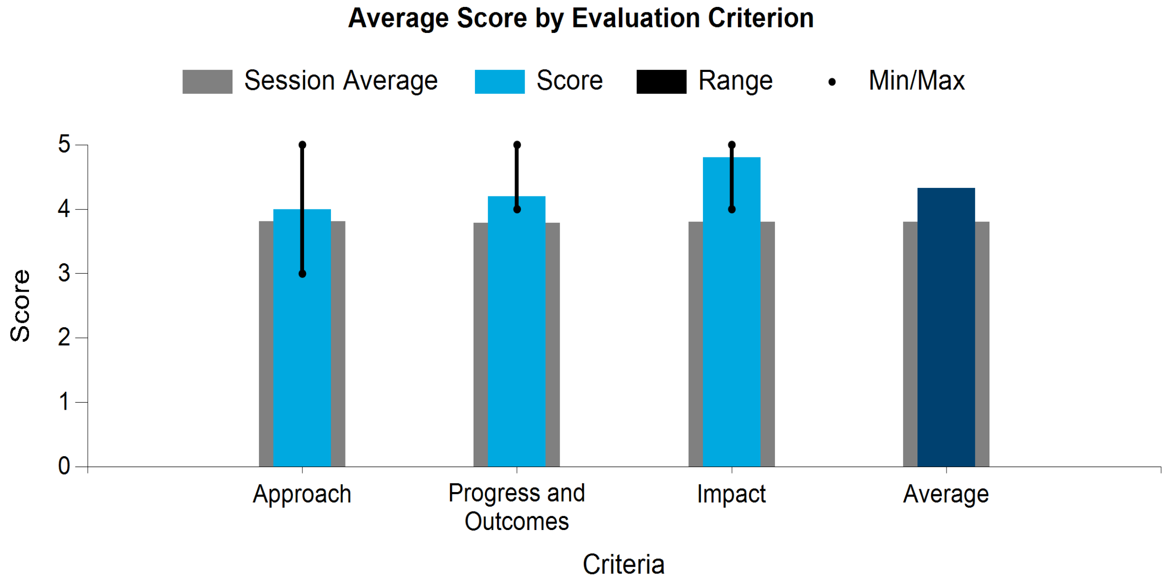
In this project, we will integrate the IH^2 pilot plant with the Cool Reforming pilot plant to show that the IH^2 process is hydrogen self-sufficient and that the systems can be integrated in a simple, low-cost way. The goal of the project is to:

- Make drop-in fuels from cellulosic biomass for less than $2.5/GGE.
- Show that the integrated system is hydrogen self-sufficient.
- Show that the integrated system is simple and low cost.
- Run the integrated system for more than 1,000 hours and more than 100 continuous hours, and produce more than 100 gallons of drop-in biofuel with less than 0.4% oxygen.
- Demonstrate that the integrated system can convert more than 50% of the biogenic carbon from a wood feed into biofuel.
- Develop a skid-mounted modular design for IH^2 based on the Cool Reformer integration along with innovative new technologies for all peripheral equipment, and reduce the capital cost by more than 30% and the operating cost by more than 40%.
- Confirm that the improved design reduces GHG emissions by more than 70% compared to petroleum fuels.

The IH^2 process uses hydropyrolysis followed by hydroconversion to convert cellulosic biomass directly to high-quality drop-in fuel. The IH^2 process produces 86 gallons per ton of high-quality gasoline and diesel from wood. Cool reforming can convert the biogas from the IH^2 process to make all the hydrogen required in the IH^2 process in a simple, low-cost process.

This project will lead to the rapid commercialization of the IH^2 process in compact modular plants. These modular plants will be used to produce bio-renewable drop-in fuel for less than $2.5/GGE.

Major participants in the project are Gas Technology Institute (GTI) Energy, Shell Catalysts and Technologies, KBR, Michigan Technological University, and SynSel Energy.



COMMENTS

- The project's objective is to demonstrate that there is no need for makeup hydrogen. Shell owns all the rights to IH^2. The catalyst is provided by Shell (ICR). The project is almost finished and has demonstrated its main objective: Show H_2 self-sufficiency with the integrated Cool Reformer, and verify there is no need for makeup hydrogen in the integrated process. The IH^2 process consists of biomass hydropyrolysis and a hydroconversion to produce liquid fuel. The current project will use the incondensable gases produced in the hydrocracking reaction to generate hydrogen in the Cool Reformer to demonstrate that both integrated systems can self-produce enough hydrogen for the IH^2 process. The project has demonstrated its feasibility in a short-term run, and in its final step, it will run for 250 hours continuously. GTI invented the IH^2 technology, but Shell has purchased all rights to commercialize it.

- The project has successfully demonstrated short-duration integration of the IH^2 with the Cool Reformer and reduction of the number of unit processes, which should reduce capital expenses (CapEx), operating expenses (OpEx), and operational complexity. It is good to see slide 26 identify specific process improvements that provide for improved techno-economics. The presentation did not provide any information on feedstock used in the testing and the preprocessing requirement for biomass feedstock. For forest residue, would bark and needles/leaves need to be removed?

- Combining hydropyrolysis and hydrogenation to make up the IH^2 process appears to have been successful for the feedstock used (wood). The program needs to demonstrate this with corn stover and other biomass to mitigate the concern that those might be much less clean and consistent, especially over storage time. The partner (Shell) is bringing expertise on fluid bed reactor and catalyst design to the hydropyrolysis step, a significant unit operation in the process. It looks promising, but I would like to see the TEA and IRR work.

- This project, the first of its kind of the integration of the IH^2 process with reforming, has shown promising progress toward achieving its objectives. To fully evaluate the success of this project, a comprehensive table outlining the final cost and TEA, environmental impact, and GHG reduction achieved should be presented as the project nears completion. Additionally, a section detailing lessons learned and how unanticipated changes were effectively addressed during the project's execution would be beneficial. To better understand GTI's various projects, it would be helpful to have clear illustrations that highlight similarities and differences between them. This will allow stakeholders to better evaluate the potential impact of each project and identify best practices that can be applied to other initiatives. Moreover, learning how project team members from different departments collaborate during the execution phase and how they share learnings from various projects can provide valuable insights into the success of these projects.

- The IH^2 process has significant potential to advance drop-in biofuels production through the hydropyrolysis of cellulosic biomass. This project demonstrates the potential to use the gas from the IH^2 process to produce hydrogen for upgrading the liquid product (presumably to remove oxygen and produce saturated hydrocarbons). This could potentially reduce the production cost of the IH^2 fuels and reduce the carbon intensity. This information needs to be provided. One of the project objectives is stated as a reduction in the cost of gasoline, jet, and diesel to less than $2.50/GGE; however, no TEA results were shown to demonstrate that this will be achieved. What is the current cost of gasoline, jet, and diesel with the IH^2 process, and how much does this integration reduce the cost?

PI RESPONSE TO REVIEWER COMMENTS

- GTI has tested the IH^2 process for a variety of feedstocks, including some that include bark and corn stover. Corn stover and bark have lower liquid yields than wood, but they are acceptable feeds for IH^2 as well. The final project report will include the techno-economics for this improved reformer system; however, the techno-economics for the current IH^2 were done previously, which were very promising. Because of limited funding, we were unable to include an LCA analysis in this project; however, earlier studies of IH^2 LCA have also shown a very favorable LCA, with more than a 70% CO_2 reduction.

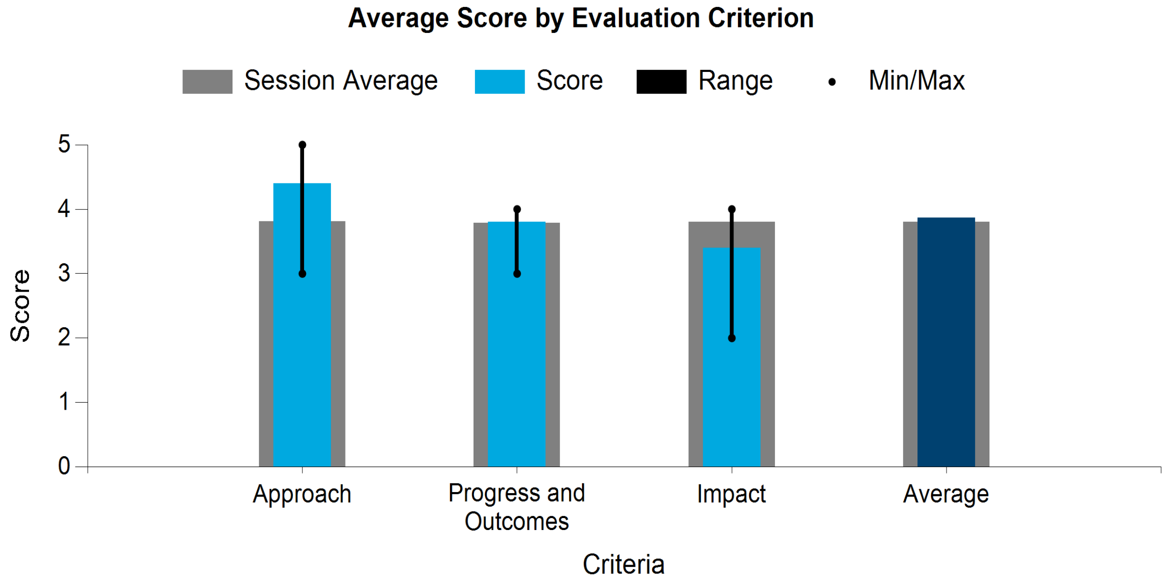
TRIFTS CATALYTIC CONVERSION OF BIOGAS TO DROP-IN RENEWABLE DIESEL FUEL

T2C-Energy

PROJECT DESCRIPTION

WBS:	3.5.1.201
Presenter(s):	Devin Walker
Project Start Date:	10/01/2019
Planned Project End Date:	09/30/2023
Total Funding:	$2,909,698

There are 2,451 landfills, 1,241 wastewater anaerobic digester facilities, and 282 agricultural anaerobic digester facilities in the United States. These sites generate more than 800,000 standard cubic feet per minute (scfm) of biogas representing a fuel equivalent of 3.7 billion GGE/year. The biggest challenge to this industry is its largely decentralized nature. Existing biogas projects include direct heating, electricity generation, and enrichment of methane for pipeline use or for natural gas-powered vehicles. T2C-Energy has developed and patented a novel catalytic technology that we have trademarked TRIFTS for the direct conversion of biogas to drop-in transport fuels. This project is focused on optimizing this new TRIFTS technology at a relevant engineering scale capable of using both the CO_2 and CH_4 portions of biogas and incorporating them into the hydrocarbon backbone of the final product of the process (renewable drop-in diesel). This renewable source of diesel resembles its petroleum counterpart both physically and chemically, and it can be used in current-day engines with no engine modifications necessary. Heavy equipment and waste-hauling trucks can therefore unload and refuel at the same landfill or anaerobic digester site with a renewable diesel fuel derived from the very waste they hauled; thus, a closed-loop process is created from feedstock to end point user. We have previously collaborated with DOE to build a mobile pilot facility for the purpose of testing the technology on-site at multiple landfills and anaerobic digesters. The unit was designed to convert a 9- to 24-scfm slipstream of raw biogas into renewable transport fuel. Successful demonstrations and testing at engineering scales are a proven pathway to commercialization and provide confidence to all stakeholders for scale-up. This project focuses on rigorously testing our TRIFTS technology at the engineering scale to convert a diverse range of biogas feedstocks derived from MSW, wastewater, animal waste, food waste, and crop residues into high-quality renewable, drop-in diesel fuel. These feedstocks present variations in biogas feed compositions and varying levels of impurities that offer unique challenges. We therefore seek to prove the robustness of the TRIFTS process over this broad biogas range and efficiently convert them into middle-distillate hydrocarbons in a highly profitable manner and at scales that were traditionally not thought economically feasible. The biogas variations, catalytic parameters, process dynamics, system performance, process LCA, and fuel product quality will all be monitored and studied over sufficiently long-term periods (more than 500 hours per site) to optimize the efficiency, productivity, and economics of the TRIFTS process and to incorporated into the scale-up of the TRIFTS plant designs. Economic opportunity; job creation; production of drop-in renewable fuel, fertilizer, and freshwater; and the creation of circular economies within the United States at the rural and metropolitan levels are direct impacts of this project.



COMMENTS

- This is a good presentation. There is a lot of good data. It includes credible information and is a good business concept. It can survive with no subsidies. Well done. I have concerns about the catalyst life. The presenter said it would last at least 6 months, but no proof was provided. There is very little information about the type of catalyst, cost, and regeneration procedures. It is not clear how the company is going to deploy the technology. Will it be in large biomass-producing sites, building large facilities, or installing mobile units and running campaigns?

- This project presents an investigation of a new catalytic process that removes five unit processes and thereby simplifies the GTL process platform while also using the CO_2 to maximize production. The capture and use of waste heat and Fischer-Tropsch synthesis (FTS) water helps to create a self-sufficient process and is a best practice for sustainability, and it may be key to making this process economically feasible at the commercial scale. The project seems to replicate actual commercial operation conditions by using raw biogas as the feedstock and using the FTS water in the process (with results showing a lack of impact on the process and products).

  Slide 8 shows that the TRIFTS system produces the jet fraction. A distillation system, which is a well-proven technology, would be needed. The project team has chosen to produce only renewable diesel to minimize the number of unit processes and associated costs and to keep the number of products to one.

  The presentation indicated an MFSP of $2.91/GGE without subsidies or credits, validated by an independent engineer, which is commendable. At what scale was the MFSP of $2.91/GGE calculated? It would be helpful to see at what scale this process is economically feasible, given that FTS is generally economic at large scales.

  Can the catalysts (for tri-reforming and FTS) be regenerated, and if so, how many times? How long does it take to regenerate? Would the catalyst be regenerated in place, or would it be removed from the reactors and regenerated off-site? How would the catalyst be disposed? Does the catalyst contain anything that would make it a hazardous waste that would require treatment or special disposal methods?

  What does the waste industry scale translate to in terms of the range of production volumes of the renewable diesel (in gallons or barrels)?

- The rationale to have biogas to reformers and syngas-to-liquid fuel at small and distributed scales is not elucidated well, if at all. Conceptually, this project can make a significant contribution to the decarbonization of rail and heavy transportation fuels, but success depends both on the widespread use of biomass digestion to biogas and the aggregation to clustered conversion facilities to ensure economy of scale. In addition to the pending verification trials, a TEA and risk assessment is needed to better understand the economic impact and ability to reach the goal $/GGE without renewable identification numbers (RINs).
- Additional data on experimental runs besides the 4 days in October 2021 that were highlighted in the slide deck should be included to provide a more comprehensive picture of the project's performance. Please provide details on how the small-scale FTS operates and if any challenges were encountered during its operation at a smaller scale? Because this project is coming to an end, it would be beneficial to have a summary table that includes information on the final costs, LCA, GHG reductions achieved, and any other relevant economic data. In addition, it would be helpful to compare the actual completion dates of tasks and milestones with the original proposed dates and to get insights on lessons learned and how unexpected changes/challenges were addressed. Finally, a risk register should be integrated into the project deliverables to ensure that all completed projects include an assessment of potential risks that might adversely affect the project's goals and objectives.
- This is an excellent project, and the approach is thorough and comprehensive. The technology has been demonstrated based on different sources of biogas and the quality of the renewable diesel meets standards. The modular approach for testing is very interesting and has potential to access smaller volumes of biogas at multiple locations, a resource that is underused. Although the potential for licensing modular units for small-scale production was stated as one approach in the business plan, it is questionable whether this type of sophisticated technology could be operated without highly skilled technicians. An analysis of the fuel product characteristics versus ASTM specifications should be included. Has the pathway been approved by the U.S. Environmental Protection Agency (EPA) for RIN generation? What are the GHG reductions achieved, and was this measured using GREET?

PI RESPONSE TO REVIEWER COMMENTS

- Catalyst and process longevity studies were done during a seven-month continuous pilot study on-site at the Citrus County central landfill using the raw biogas produced at this MSW landfill. During this pilot demonstration, the plant consistently achieved methane conversions of 88%–92%, at times approaching the theoretical maximum conversions of 99%. CO_2 conversions were consistently between 30%–40%, at times reaching 50%–60% conversions. Conversion efficiencies during the long-term pilot demonstration aligned with bench-scale results as we proved the ability to maintain high conversions throughout the entirety of the demonstration. During the entirety of the demonstration, the reformer was able to produce the ideal syngas composition, with an H_2:CO ratio of 1.7–2.2. This is one of the unique aspects of our tri-reforming capabilities to tune the syngas H_2:CO ratio as needed throughout the demonstration. During this pilot demonstration, the plant consistently achieved CO conversions of 50%–70%. During the pilot demonstration, we intentionally limited the CO conversion to 60%–70% because it is known that higher conversions can lead to high partial pressures of H_2O and deactivate the FTS catalyst; however, there were little to no signs of FTS catalyst deactivation throughout the entirety of the demonstration, and, in fact, we achieved our greatest conversions toward the last few weeks of the demonstration. Typical industrial GTL have lifetimes of approximately 4–5 years. Based on the long-term pilot data at the Citrus County landfill, the catalyst used in this project would meet or exceed industrial catalyst lifetimes. The reformer and FTS catalysts used in this project were produced in-house using a T2C-Energy patented catalyst. Currently, T2C-Energy manufactures the reforming and FTS catalyst at $20.44/kg and $85.59/kg, respectively. Current manufacturing capabilities allow us to produce approximately 10 kg/hour of catalyst. During the pilot demonstration, regenerative studies were performed using two techniques. The first technique involved regenerating the reforming and FTS catalyst while remaining online (*in situ* regeneration). Higher steam flows are fed to the reformer to oxidize the carbon deposits on the catalyst surface. This increases the H2:CO ratio of the syngas product while also removing carbon in the form of methane. The elevated H2:CO ratios feeding the FTS facilitate carbon removal and shift the FTS products to a lighter boiling point fraction, allowing for continuous operations as the FTS catalyst bed is regenerated. This regeneration cycle typically takes approximately 2–4 hours to complete and return to steady-state conditions. The second regeneration technique requires the feed to both reactors to be removed and replaced with a steam/air feed, effectively oxidizing coke deposits on the catalyst surface. This is done over a 1-hour period, followed by a reduction gas mix of hydrogen and nitrogen to reduce the active metal of the catalysts. This second regeneration cycle takes approximately 24–30 hours to complete and return to steady state. The second regeneration technique is more rigorous and done approximately every 2,000 hours of run time or if the catalyst activity drops 10% below the desired conversion efficiencies. Both regeneration methods are performed within the respective reactors for reforming and FTS. Spent catalyst are disposed of according to EPA solid waste regulations (K171). This includes utilization to produce new catalysts and other useful materials, recycling through recovery of metals, and treatment of spent catalysts for safe landfill disposal. The full-scale TRIFTS modular system is designed to accommodate biogas production facilities generating 123–1,750 scfm. This is T2C-Energy's short-term serviceable available market because most commercial technologies struggle to remain profitable within this range. Larger centralized facilities with traditional construction methodologies will be deployed once confidence within the waste-to-energy sector is gained through proven full-scale operational data within the biogas range from 123–1,750 scfm. The average biogas flow rates of an anaerobic digester facility and landfill in the United States are 210 scfm and 1,380 scfm, respectively. At these biogas flow rates using the TRIFTS process, the average size anaerobic digester would produce 230,000 gallons of renewable fuel annually, while an average size landfill would produce 1,470,000 gallons of renewable diesel fuel annually. The MFSP of $2.91 validated by an independent engineer was calculated based on a biogas feed rate of 1,500 scfm and excludes environmental attribute revenues. T2C-Energy has specifically targeted landfills producing more than 300 scfm of landfill gas, farm-based anaerobic digester's producing more than 123 scfm of biogas, and wastewater anaerobic digester's producing more than 275 scfm of biogas. Sites flaring the majority of their biogas and sites producing electricity from biogas with expiring electrical power purchase agreements meeting these biogas flow rate capacities are T2C-Energy's short-term market focus. Stranded facilities where the natural gas pipeline infrastructure does not exist are of particular interest for TRIFTS biogas-to-diesel projects. T2C-Energy has gained interest from these "stranded" facilities and also from developers wanting to avoid the costly gas connection/distribution fees of natural gas pipeline owners. Liquid fuel production simplifies logistics in that it can be stored and transported under ambient conditions; therefore, current freight and rail distribution channels are used, and the project location becomes less relevant than renewable natural gas (RNG) types of projects. TRIFTS landfill projects generate a carbon intensity score of -36 gCO_2e/MJ fuel, and therefore for the project to break even, the flow rate of landfill gas needed is 300 scfm. Whereas TRIFTS farm-based anaerobic digester projects have carbon intensity scores of less than -500 gCO_2e/MJ, and therefore for the project to break even, the flow rate of biogas needed is 123 scfm. Carbon intensity scores are based on the ANL GREET module that was completed under this project for the TRIFTS fuel production pathway.

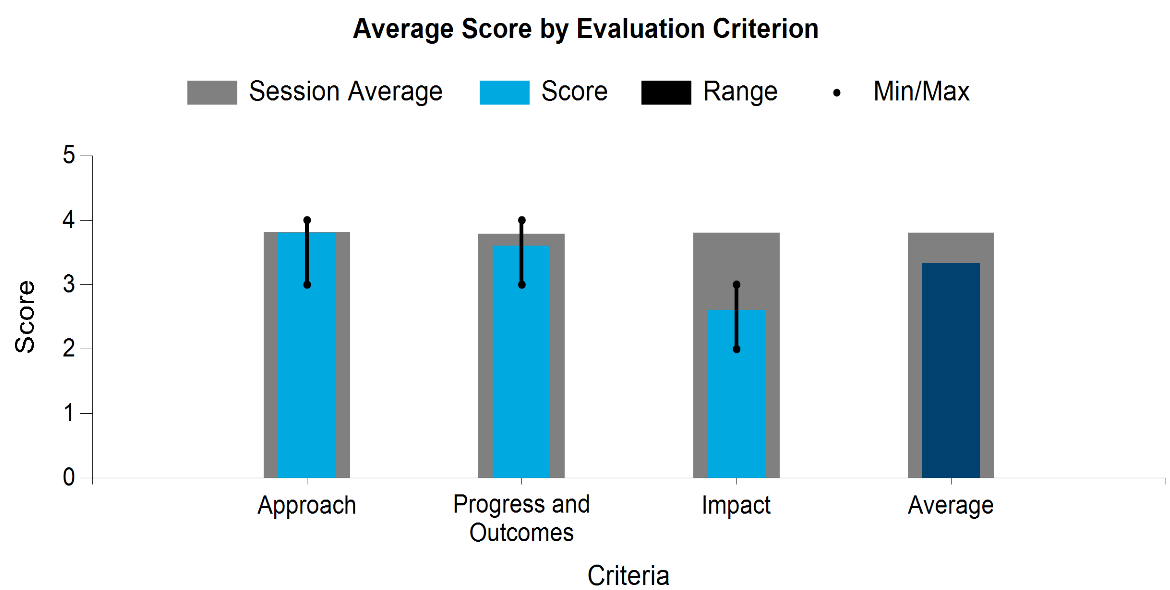
PRODUCTION OF LIQUID HYDROCARBONS FROM ANAEROBIC DIGESTER GAS

OxEon Energy LLC

PROJECT DESCRIPTION

WBS:	3.5.1.203
Presenter(s):	Jessica Elwell
Project Start Date:	10/01/2019
Planned Project End Date:	12/31/2023
Total Funding:	$2,494,236

OxEon proposed a process for the conversion of both CO_2 and CH_4 in anaerobic digester GTL transportation fuels containing three elements. A solid oxide electrolysis cell (SOEC) system converts steam and CO_2 to synthesis gas (CO and H_2) by high-temperature electrolysis. A plasma reformer converts methane to synthesis gas using the plasma to catalyze the reaction of methane with steam and oxygen supplied as oxygen-enriched air. The oxygen enrichment is the result of byproduct oxygen from the electrolysis system. The syngas from the plasma reformer and electrolysis systems are combined to produce liquid fuels in the Fischer-Tropsch reactor. Each subsystem has undergone and completed verification to key targets, and the full system fabrication and integration is underway.



COMMENTS

- The project uses four expensive block components to convert biogas to liquid fuels:

  1. CO_2-CH_4 gas separation
  2. SOEC for CO_2 to syngas
  3. Plasma reactor for CH_4 conversion to syngas
  4. Fischer-Tropsch reactor for the production of liquid biofuels.

This is a very complex approach, and it is difficult to understand if the project economics make sense and whether the technical approach is feasible. The company should clarify if they have worked with real biogas and how they manage impurities that may affect the SOEC. Working with bottled gas is not the same, and they may face big challenges down the road. There have been problems with the Fischer-Tropsch catalyst, but the company has not explained the issues and how they are trying to solve them.

- OxEon seems to have the appropriate approach to developing its three proprietary process units and their integration; however, the combination of the three technologies (SOEC, plasma reformer, and Fischer-Tropsch) into one process platform seems complex and expensive. The technical and market advantages of this process platform are not clear. Has the plasma reformer been tested with biogas or only natural gas? What contaminants and impurities are the processes sensitive to?
- This project relies on large-scale biogas availability and delivery to a conversion plant for success, as do several other similar projects. The conversion technologies envisioned are, to a large extent, relatively unproven at scale, especially in an integrated process, although individually at the pilot scale they appear to be capable. Linking these technologies together into an integrated process at a reasonable scale will be essential to prove that the approach is viable versus other syngas-to-advanced fuels concepts. Of key concerns are the plasma reactor and the electrolysis steps and integrating those with Fischer-Tropsch with high recycle ratios. The hot-gas-side stream is not fully integrated into the process for making fuels. In addition, the team needs to understand the effects of contaminants and composition variability of RNG on catalyst performance and life. A detailed TEA is planned and recommended.
- This project is quite complex because it involves the integration of three unique technologies with recycle streams. Each technology has been independently tested, making this integration project a first of its kind. The process involves separating CO_2 and methane before using them in the solid oxide co-electrolysis and plasma reformers, respectively; however, it raises the question of whether it is necessary to separate them. Is it possible to reform the combined CO_2 and methane instead to produce the necessary syngas for the downstream Fischer-Tropsch reactor? The inclusion of results from the verification tests of individual components has been helpful to understand this project. It has aided in ensuring that each component is properly functioning before integrating them. The biggest risk could be how the recycle streams would impact the performance of the electrolysis cell and plasma reformers when all components have been integrated together.
- This project focuses on the production of liquid hydrocarbons from anaerobic digestion gas, and the goals align with BETO's goals. The project includes multiple steps with novel and complex (expensive) technologies that have been developed by the applicants, and the project goal is the integration of these units for the production of hydrocarbons. Successful operation of individual units has been demonstrated, and integration will be challenging. But overall, the techno-economics derived from data in this stage will be a critical determinant of the potential of this pathway. Three specific items came to my attention that need to be addressed. As part of the integration, the syngas going into the Fischer-Tropsch reactor may have contaminants that could cause catalyst inhibition in the Fischer-Tropsch. It is not clear whether the syngas has been analyzed and whether a strategy is in place to address this. The current approach is to flare gases after the FTS, which will reduce product yield, and recycling of the gases for syngas production should be considered as part of the integration. Though not specifically important for the integration, the future commercial viability of the technology must address the following: The FTS produces a wide range of fuel products and will require separation and perhaps further upgrading. Although this is not the target of the project, it is very relevant for the future commercialization potential of the technology. At a small scale, this might not be economic. A profile of the hydrocarbons based on carbon chain length should be provided. A strategy and future business approach to product upgrading and separation will be needed. Fischer-Tropsch catalyst development has

been targeting bifunctional catalysts to produce a narrower range of hydrocarbon products, and this could be explored to minimize the number of products.

PI RESPONSE TO REVIEWER COMMENTS

- OxEon appreciates the valuable feedback on this project. We agree that SOEC and Fischer-Tropsch technologies are currently costly at scales matching biogas resources. Recent E.U. mandates for SAF include power-to-liquids SAF, and the expectation is that costs will be substantially reduced through plans currently in development at OxEon (increase in power density of the cells, automation of assembly process for SOEC, etc.). The power-to-liquids SAF approach uses the electrolysis of CO_2 and steam to produce synthesis gas (CO, H_2; commonly “syngas”) and then Fischer-Tropsch to fuels. Combining CO_2 and CH_4 to fuels will have better economics for two reasons. First, the biomethane reformation process requires almost no additional energy input (1%–2% electric for plasma), and the reformer is relatively inexpensive to fabricate. Second, the Fischer-Tropsch plant for a combined CO_2 and CH_4-to-liquids process will be close to double the size, giving the opportunity for economies of scale. The separation of biogas CO_2 and CH_4 is widely practiced to upgrade the CO_2-CH_4 mixture from anaerobic digesters to attain the quality of natural gas required for pipeline injection to claim RIN credits. The CO_2 is at a concentration of 30%–40% coming from the digester and needs to be reduced to less than 1% to meet the pipeline standards. The plasma reformer is relatively low cost to build and operate. OxEon demonstrated and the low energy requirement was verified during the verification phase. We have tested the reformer on biogas from an anaerobic digester from a dairy. The reformer is insensitive to sulfur and has shown it can reform heavy, dirty fuels that are high in sulfur and aromatics, such as NATO F-76 (1% S spec. limit). We have also shown that the SOEC, operating as a fuel cell, can be operated with 1,000 ppm of H_2S. We have not tested the cells/stacks in SOEC operation with H_2S, but we anticipate similar performance. Fischer-Tropsch is known to be sensitive to sulfur down to approximately 20–50 ppb, so although the reformer, and possibly the SOEC, are not sulfur sensitive, the Fischer-Tropsch is and will require a sulfur trap. The project will be sited and tested at a digester site to address any impacts of running on biogas (CO_2 and CH_4). There are current gas (methane)-to-liquids systems operating at a profit (e.g., the Shell Pearl plant in the United Arab Emirates). There is a great push in the European Union for CO_2-to-liquids systems. Where both biogenic CO_2 and CH_4 are available, projections are that the combined system will be lower cost than two separate systems. The interfaces between them are of a type and complexity that are believed to be within the bounds of normal industrial practice: Cooling the exothermic Fischer-Tropsch reaction raises steam for SOEC, the SOEC byproduct O_2 is used by the reformer to enhance the amount of oxygen available for the reforming reaction, a small amount of Fischer-Tropsch-produced water is also used in the reformer, and the combined syngas streams from the reformer and SOEC are compressed and supplied to the Fischer-Tropsch. Fischer-Tropsch catalyst development is a highly specialized blend of art and science that has been seeking to improve the distribution of hydrocarbons generated by the Fischer-Tropsch for nearly a century. OxEon has presented data on the product distribution from its systems and has confirmed that this product follows the well-established and accepted Anderson-Schulz-Flory distribution model. Globally, nearly 400,000 barrels/day of Fischer-Tropsch liquids are produced, refined, and sold at a profit into existing markets otherwise served by petroleum. The synthesis of hydrocarbons using the Fischer-Tropsch process has been commercially practiced since its development in Germany before World War II. The difference between biogas-to-liquids Fischer-Tropsch products and the Fischer-Tropsch liquids produced by these existing plants is feedstock. The vast majority of the approximately 400,000 barrels/day of current production uses fossil-based feedstocks that also contain sulfur and other contaminants. These feedstocks are primarily associated gas from oil wells and coal (in South Africa). The challenge is scaling the technology down to a size matched to the disperse and distributed nature of bio-feedstocks. The use of the bio-CO_2 nearly doubles the product potential from biogas, and it at least doubles the potential from biomass gasification. The application of SOEC to bio-CO_2 to produce energy-dense fuels provides an extremely efficient and compact means of storing renewable electric energy. In effect, it shifts the renewable energy from the time and location it is available to when and where it is needed. Once the Fischer-Tropsch liquids have been produced, they constitute a storable and energy-dense material that is transported to refineries as easily as crude oil. This program has been scoped to provide outputs that would feed a TEA in a follow-on effort. The TEA of the integrated system would be used to establish the commercial potential for the technology and provide a cost basis for comparison to other comparable sources of energy on both a capital and operating basis.

COOL GTL FOR THE PRODUCTION OF JET FUEL FROM BIOGAS

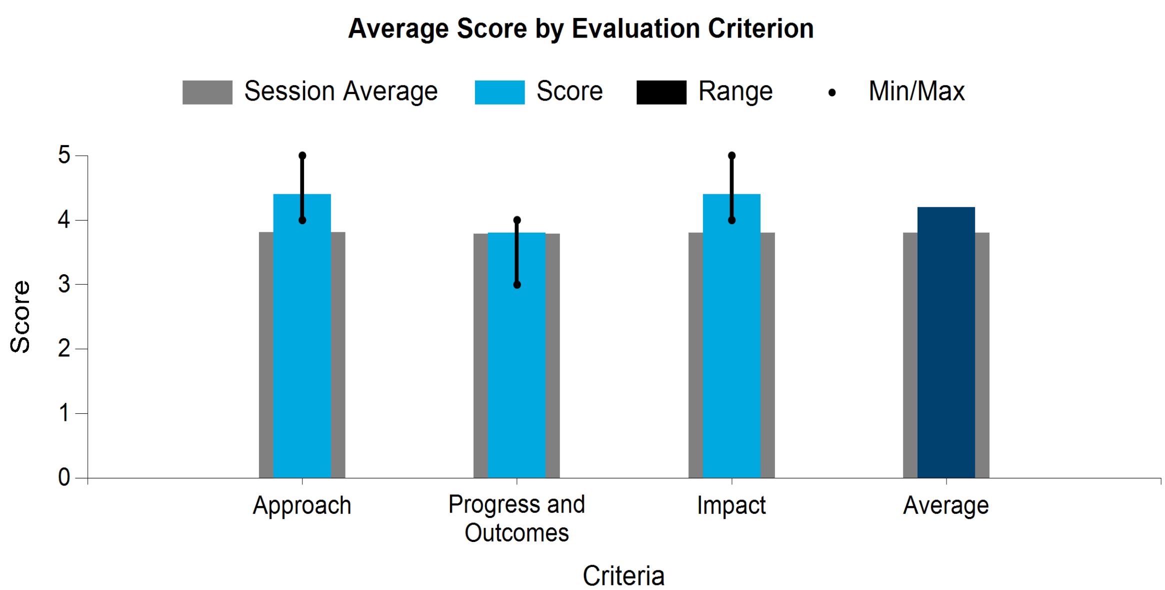
Gas Technology Institute

PROJECT DESCRIPTION

WBS:	3.5.1.405
Presenter(s):	Terry Marker
Project Start Date:	10/01/2018
Planned Project End Date:	07/31/2023
Total Funding:	$3,839,596

Cool GTL is a new gas-to-liquids technology that directly converts high CO_2 and CO-containing C1–C3 gases to jet fuel, diesel, and gasoline. Cool GTL can be used to convert biogas from digesters, IH^2, or gasifiers, so it has a wide range of applications. Cool GTL uses a unique new catalyst for CO_2/steam reforming in the first stage and a unique new catalyst and fluid bed reactor for Fischer-Tropsch plus wax cracking and isomerization in the second stage to directly make jet fuel from biogas.

The goal of this project is to develop the Cool GTL technology for biogas conversion to jet fuel by making 100 gallons of high-quality jet fuel. In this project, we expect to show that the Cool GTL technology can produce drop-in jet fuel for less than $3/gallon and reduce the GHG emissions of jet fuel by more than 60%. As a result of this program, the Cool GTL technology should go from a TRL of 3 to 5. The major participants are GTI, Hatch Engineering, Particulate Solid Research Inc. (PSRI), Michigan Technological University, SynSel Energy, and Veolia Environmental Services Inc. The major participants are GTI, Hatch Engineering, PSRI, Michigan Technological University, SynSel Energy, and Veolia Environmental Services Inc.



COMMENTS

- The project is about to finish, and GTI has performed very good work. It has developed a very promising process that is flexible and can use different feedstocks. The presenter has provided TEA data and LCA. CapEx for the demonstration unit is substantial. The cost of production using digestor biogas is $6.2/GGE. GTI should do further analysis to try to reduce this cost of production.

- GTI has conducted a good project and has successfully demonstrated the Cool GTL and its unique catalysts for reforming and FTS. The wax cracking is indicated as being in an "integrated trailing reactor." This seems to indicate that the Fischer-Tropsch wax does not need to be separated for the wax cracking step, which simplifies the process.

  Has catalyst regeneration been conducted? What are the main lessons learned on this project that inform the next scale-up? Biogas sources tend to be smaller, distributed systems. What is the minimum scale at which the Cool GTL process is economically feasible?

- Fischer-Tropsch technology has been around for decades, and generally it is considered a high-capital-cost route to liquid fuels, so economy of scale is critical. A new reactor concept that can effectively operate at a smaller scale and lower temperatures and still crack wax formed during synthesis would be of high interest, provided the right catalyst and conditions can be proven. Key criteria for adoption in a biomass-to-fuels process are the feedstock cost and suitability for the gasification step, and whether the syngas produced can be effectively converted to liquids and at a low capital cost. This conceptual reactor uses an "ebullated" catalyst bed, so the demonstration should include catalyst physical integrity along with catalytic performance, coking, and life. A TEA and IRR will help determine the benefits, if any, to conventional Fischer-Tropsch.

- It will be helpful to understand how this project's approach to electric reformer technology differs, if any, from that of WBS 3.5.2.701, which also employs this technology. The preliminary LCA data provided are encouraging. Can the proposed Fischer-Tropsch slurry reactor technology be modularized for commercial plant scales? At small scales, do Fischer-Tropsch reactors operate as economically and robustly as commercial-scale Fischer-Tropsch reactors? To gain a more comprehensive understanding of GTI's diverse range of projects, it would be useful to have illustrations that highlight similarities and differences between them. Additionally, it would be beneficial to learn about how project team members from various backgrounds collaborate during the execution phase and share knowledge from different projects.

- The project demonstrates the production of jet fuel from biogas using a novel electric reformer to produce syngas followed by Fischer-Tropsch using novel catalysts to produce syncrude. Wax cracking takes place within the Fischer-Tropsch reactor to maximize the jet fraction. Further work is required to achieve the freeze point requirement for the jet fraction. If a novel bifunctional catalyst is used, it may not comply with ASTM D7566 Annex 1, and this should be investigated. From the analysis, there is still 1.1% oxygen in the diesel, indicating that further hydrotreatment will be needed. What is the strategy for upgrading? Because the jet fraction is only approximately 50%, will distillation and fractionation be part of the demonstration unit? Slide 26 shows only separation of the liquid and gas fractions. From slide 23, it seems that the break-even price is \$6.2/gallon without the RINs for digestor biogas, whereas it is \$3.2/gallon for IH^2 biogas. Presumably, the claims made for the production of jet at less than \$3.5/gallon are therefore based on using IH^2 biogas. The integration between the two processes was not shown. The IH^2 biogas will not deliver the same emission reductions achievable with digestor biogas, and the difference between the two sources must be shown.

PI RESPONSE TO REVIEWER COMMENTS

- So far, our Cool GTL Fischer-Tropsch and trailing reactor have not really deactivated enough for regeneration. In Budget Period 3, we will see if regeneration is necessary. We have a procedure developed for this if it becomes necessary. The smallest scale at which Cool GTL is economically viable will significantly depend on RIN credits; however, with the current renewable fuels credits, we believe it can be economically attractive at small biogas scales. Fractionation would be part of any demonstration unit. We do believe we will be able to make drop-in fuels requiring no further upgrading, and that is our goal in the Budget Period 3 testing. We also believe we can reduce costs for the biogas size unit by incorporating the electric reforming in the economics. This was not done in the initial Budget Period 2 economics, but the electric reformer will be included in the Budget Period 3 economics. An electric reformer provides the most cost savings for small-size equipment.

ULTRA-LOW-SULFUR WINTERIZED DIESEL

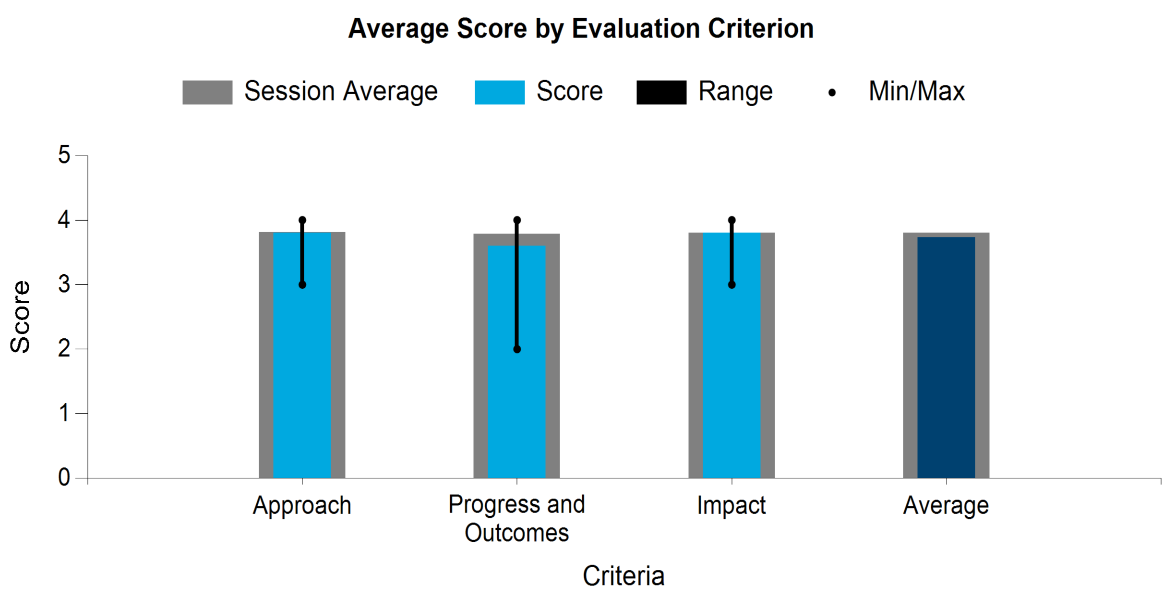
LanzaTech Inc.

PROJECT DESCRIPTION

WBS:	3.5.1.406
Presenter(s):	Rick Rosin
Project Start Date:	10/01/2018
Planned Project End Date:	03/31/2023
Total Funding:	$3,130,327

LanzaTech and PNNL are collaborating to develop and validate a robust, flexible alcohol-to-diesel (ATD) process for producing drop-in renewable diesel fuel with superior low-temperature performance from biomass-derived ethanol. PNNL is conducting R&D to understand the relationships among catalyst/process parameters and diesel product characteristics to enable diesel properties to be tuned to match the specifications for each diesel application. The technology will be validated through the production of hundreds of gallons of synthetic paraffinic diesel and engine testing.

By using an ethanol intermediate, the ATD process will enable renewable diesel to be produced from any ethanol that meets customer and application requirements. This feedstock flexibility will allow a commercial ATD refinery to minimize the cost of production by selecting the lowest-cost ethanol source that satisfies the needs of each market. Synthetic paraffinic diesel (SPD) from the ATD process will be a drop-in diesel fuel, fully compatible with existing fueling infrastructure and engines, suitable for use in each target market at any blend level. The SPD will have low sulfur content and superior low-temperature performance. The life cycle GHG reductions of the SPD fuel are expected to be 60% or higher, depending on the source of ethanol feedstock.



COMMENTS

- In the previous project presentation, LanzaTech indicated that they could change the process conditions to vary to the percentage of SAF or diesel in the final product. This project elaborates more on that possibility, but LanzaTech does not explain how they plan to do it. It seems they are using the same process and catalyst and are only slightly changing the oligomerizing reactor process conditions.

Currently, the ATJ process can produce 75% diesel without losing overall product yield. With this project, LanzaTech wants to achieve 90% diesel yield. The oligomerization will start with bottled ethylene, not produced upstream. This will not consider potential contaminants from the ethanol-to-ethylene process. LanzaTech includes a slide with unreadable information, which prevents me from properly evaluating the results. Despite its simplicity, the project is quite delayed. Very little has been accomplished during the 2 years the project has been running. LanzaTech has not provided any data regarding technical performance, TEA, or LCA, and it is using bottled petrochemical ethylene for its testing.

- The project aims to adapt the ATJ process to increase renewable diesel production and to produce a renewable diesel that has a sufficiently low cloud point to meet winter diesel specs. Winterizing the diesel is important to make it widely applicable across seasons and geographic regions and to expand the market. The project seems to be taking the thorough steps needed to ensure proper process development for commercial deployment and to ensure a consistent product that meets specs; however, the presentation does not provide details on the changes required to adapt the ATJ process to the ATD process.

  Activities in Budget Period 3 include building an ATD production unit. Is the design of the ATD production unit different from an ATJ production unit? Waste gas ethanol does not qualify for RINs. If sugarcane ethanol is to be used, what is the GHG reduction of the resulting SAF? Is sugarcane ethanol an economically feasible feedstock for renewable diesel at the commercial scale?

- This project builds on the ethanol-to-SAF approach under a separate project, and it seeks to optimize the catalyst used in the oligomerization and hydrogenation steps to increase diesel output to 90% versus jet fuel. If these unit operations can be proven to be robust in feedstock-to-ethanol production (i.e., not sensitive to variations in composition or quality), then it would allow any source of ethanol to be used to make diesel. The product will be validated as suitable for diesel engines, which should include cylinder sleeve wear, a critical step for commercialization. If the TEA and IRR prove sustainable, the impact would be large. A major concern is the mass loss because oxygen is eliminated from the ethanol during reduction.

- Slide 5 mentions “jet range hydrocarbons” even though the project’s current focus is on producing diesel from alcohol. This is confusing because the range of carbon numbers for diesel (C11–C23) is higher than that of jet fuel (C8–C18). This ATD project is similar to the ATJ project except the final product contains a higher proportion of diesel. Can you discuss the major challenges and differences that are expected to be encountered in this project compared to the already developed ATJ project? It is not clear how the production process will change from ATJ to ATD. Will two separate catalysts beds (one specific for jet fuel and the other specific for diesel) be used, or will the process be modified in some other way? Can you provide more information about the changes in the production process? Economic information (similar to WBS 3.5.2.403) was not available. The project aims to produce diesel, but it is not clear to which market this diesel will be targeted. Given that heavy-duty vehicles are moving toward compressed natural gas, what market is being addressed for this diesel? There is a mass loss associated with the dehydration of ethanol, which may affect the viability of the process. Can you discuss the economic feasibility of producing diesel from ethanol accounting for the mass loss associated with the process?

- This project uses ethanol as the starting material to produce diesel. It is the same technology pathway as for SAF production, but the product slate is shifted toward diesel production. Although the ATJ process includes a diesel fraction, this project proposes to optimize catalyst and operating conditions for diesel production. The approach is sound, and progress has been made that aligns with the project timeline. As the ATJ process is near commercialization, the technical challenges are limited and achievable; however, producing diesel using this process rather than maximum SAF is, in my opinion, not the most beneficial use of ethanol feedstocks. The biggest strength of the LanzaTech's ATJ technology is the high SAF fraction that can be achieved. No information is provided to support the stated claims for production cost.

PI RESPONSE TO REVIEWER COMMENTS

- *Subject to disclaimers on the associated presentation*

How is the ATJ process being changed? LanzaTech and PNNL optimized the structure-function properties, process design, and operational parameters to achieve 90% selectivity to diesel. Although major unit operations are the same, particular aspects of equipment have been optimized for the ATD process. The performance will be reviewed by DOE's independent engineer at the next verification. The details, including the data and the engineering design of the ATD production unit, are confidential and not available outside of DOE and the independent engineer.

Source of ethylene: All variations among ethanol sources, including contaminants, are removed before or during the ethanol dehydration (ethanol-to-ethylene) step, and the resulting ethylene is of very high purity, comparable to commercial ethylene. The ethanol-to-ethylene process has been demonstrated to be equivalent across a wide range of ethanol sources in prior projects and during the initial validation of the ATJ process on WBS 3.5.2.403; therefore, there was no need to include ethanol-to-ethylene here.

Impact of mass loss during ethanol to ethylene: The most important factor in feedstock utilization is high carbon yield to products, which is not affected by water elimination in the ethanol-to-ethylene step. Under energy-based incentive programs, such as the Renewable Fuel Standard, the increase in energy density of the resulting renewable diesel and SAF relative to the ethanol feed mean that essentially no economic value is lost due to dehydration.

Why diesel, not SAF? The intent of this project was to maximize product flexibility to provide optionality to producers. Although SAF is clearly an important market, diesel will continue to play a significant role in the fuel pool, even as some transport applications shift to compressed natural gas. Relevant factors include the longevity of vehicles in legacy and near-term fleets, even as production and sales of compressed-natural-gas vehicles increase as well as the logistics of compressed natural gas distribution on the necessary scale and to all locations. Diesel is also used outside of transport, and there is demand for renewable diesel in applications such as data centers' backup power generation, as evidenced by recent announcements from Kohler (biomassmagazine.com/articles/19120/kohler-approves-use-of-renewable-diesel-in-its-diesel-generators) and Cummins (www.biobased-diesel.com/amp/cummins-high-horsepower-diesel-generator-sets-approved-for-use-with-hvo).

TEA/LCA: Initial TEA and LCA were provided in the proposal and are to be updated later with the final results from Budget Period 2. The GHG reduction (and cost) of renewable diesel is comparable to that of the SAF product. The GHG footprint of the products is largely determined by the ethanol source. LCA results for SAF were presented during the last peer review of WBS 3.5.2.403 for five different ethanol sources. The EPA has approved the ATJ pathway for the generation of D4 RINs (biomass-based diesel) with at least 50% GHG reductions when using sugarcane ethanol feedstock (www.epa.gov/renewable-fuel-standard-program/approved-pathways-renewable-fuel). The cost of production is not impacted by the ratio of renewable diesel to SAF. We agree with the reviewer that waste-based ethanol is the preferred feedstock as cost and availability allow.

Reference to "jet range hydrocarbons" (slide 5): The reviewer is correct that this should have been changed to diesel.

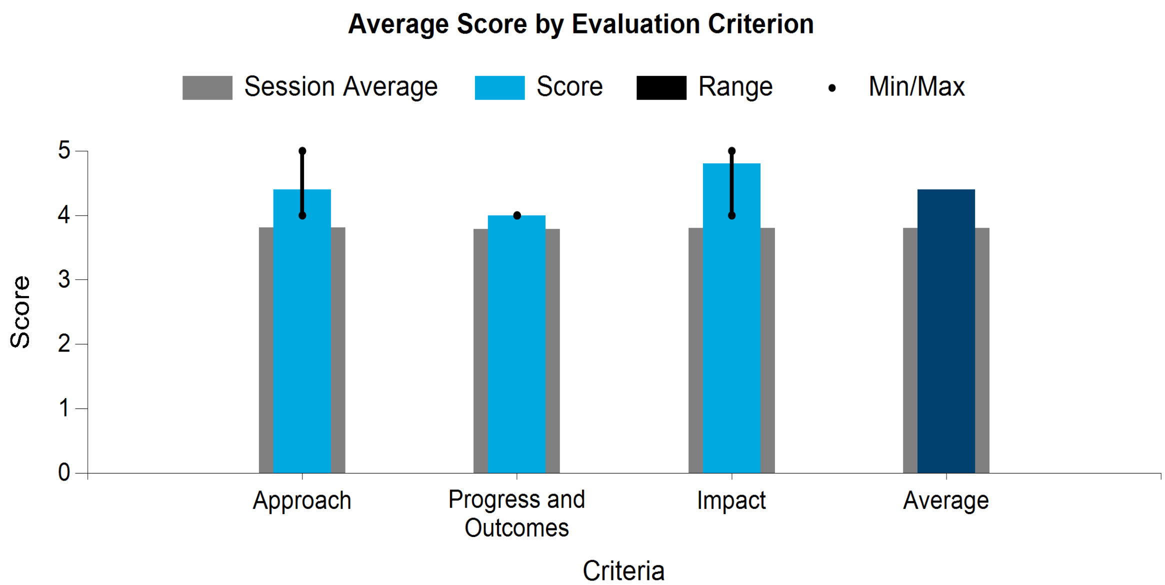
PILOT-SCALE BIOCHEMICAL AND HYDROTHERMAL INTEGRATED BIOREFINERY (IBR) FOR COST-EFFECTIVE PRODUCTION OF FUELS AND VALUE-ADDED PRODUCTS

South Dakota School of Mines and Technology

PROJECT DESCRIPTION

WBS:	3.5.1.502
Presenter(s):	Rajesh Shende
Project Start Date:	02/15/2018
Planned Project End Date:	01/14/2023
Total Funding:	$2,317,995

The main objective of this project is to demonstrate the production of selected high-value products from the unhydrolyzed solids (UHS) recovered after biochemical processing of corn stover at a pilot-scale level with a throughput of 1 TPD. An additional goal is to understand the revenue stream that can be generated from high-value products and the GHG emissions. An integrated technology approach was developed to convert UHS into selected high-value products, such as biocarbon (graphitic carbon) and carbon nanofibers, via HTL processing followed by graphitization and electrospinning, respectively. The key activities included were: (1) preprocessing of corn stover at a pilot scale, (2) UHS processing and optimization, (3) HTL plant design and fabrication, and (4) graphitization of hydrochar and analysis. The carbon materials were found to be suitable for battery and supercapacitor energy storage applications. Their specific surface area, porosity, and specific capacitance exceeded the target metrics.



COMMENTS

- The South Dakota School of Mines and Technology (SDSMT) has developed an HTL process to convert UHS into biochar. HTL can handle a liquid stream with up to 20% in solids, whereas the PNNL process cannot go beyond 8%. This is a great advantage, coupled with a much simpler process design. In addition, the SDSMT team has been able to produce biochar that actually works as an energy storage material and as a capacitor. Why is the SDSMT working with UHS rather than raw preprocessed biomass? It seems that this also may work and will simplify the process. Overall, the SDSMT has done an excellent job as the team has developed a new HTL process and produced good-quality biochar.

- The team has successfully designed, fabricated, and tested a pilot-scale HTL plant that produced high-value biocarbon and carbon nanofibers, thus valorizing the unhydrolyzed waste from the biochemical processing of corn stover. The team seems to have investigated the entire process—from feedstock preprocessing in collaboration with INL, to biocarbon and carbon nanofiber characterization, to commercialization and partnerships. The TEA and LCA will be useful in determining the economic and GHG reduction impacts of the project and in determining the size of a commercial project.

  The HTL process can handle wet feedstock streams with up to 20% solids, which is higher than the 8% solids that PNNL's HTL PDU can handle. What range of solids content can the process handle? What other feedstock streams will work? Are there any process waste streams that are toxic or hazardous that pose a challenge for disposal?

- It is not clear if this approach (HTL) to processing post-hydrolysis solids will apply to all types of feedstocks and to other types of pretreatment. For the alkaline pretreatment of corn stover, it seems to offer a way to add significant value as coproduct streams. The supply-versus-demand balance for graphitic carbon may affect the value of that stream as this technology is implemented commercially, but it appears to be a growth market. The installed capacity of electrospinning equipment is small, so the TEA should determine if there are reinvestment economics for carbon nanofibers as well. The performance of those fibers appears promising based on early results. The properties and value of heavy bio-oil are not discussed, but they should be compared to No. 6 bunker oil as a start. Overall, extracting high-value products from leftover lignin solids is certainly helpful to the economics of an integrated biorefinery (IBR).

- It is encouraging to learn that the 2021 Project Peer Review has led to a more focused approach with two high-value products: biocarbon (Product 1) and carbon nanofibers (Product 2). These products can significantly enhance the economics of a biorefinery. We are curious to know why the team at South Dakota chose to develop a new HTL system instead of using PNNL's HTL equipment. It would be valuable to understand the decision-making process and the differences between the two systems. Further, it would be beneficial to learn about the lessons learned and how the team overcame any challenges during the project. As the project approaches its end, it would be useful to have a table outlining the final economic figures as well as the LCA and GHG reductions achieved. Additionally, we would like to inquire about the possibility of collaborating with PNNL in synergistic activities.

- The project's main objective is to explore the production of high-value products from the UHS after pretreatment and enzymatic hydrolysis of corn stover. The solids are processed through HTL, and the biochar is used to make biocarbon and carbon fiber mats. The project has substantial merit and could have significant commercial impact for the valorization of UHS (lignin) during cellulosic ethanol production. This fraction has generally been burned for energy generation, but upgrading to high-value products could improve the financial viability of cellulosic ethanol facilities. As illustrated on slide 9, the process shows alkaline pretreatment of corn stover, enzymatic hydrolysis with Cellic CTec2, pH adjustment with sodium citrate, and separation of the UHS. Based on this process, the solids are expected to still contain cellulose and hemicellulose because the alkaline pretreatment alone is insufficient to achieve high sugar yields. The Cellic CTec2 enzyme preparation is not as effective as the Cellic CTec3, and residual cellulose and hemicellulose will remain in the solids. The extent of cellulose/hemicellulose remaining in the solids could impact the chemistry of the biochar, and this must be considered. It might be beneficial to obtain UHS from a more realistic, near-commercial cellulosic ethanol process (e.g., DMR with CTec2 hydrolysis) because the two processes could have significant commercialization potential when used together. Because this project is close to completion, it might not be realistic to make changes at this stage, but further progression to a larger scale may consider these suggestions and potential collaboration with a cellulosic ethanol commercialization process for the valorization of the lignin fraction. Obtaining a realistic assessment of the techno-economics of the HTL will also need valorization of the bio-oil, and potential future collaboration could investigate the characteristics of the bio-oil and potential upgrading.

PI RESPONSE TO REVIEWER COMMENTS

- Comments: The SDSMT has developed an HTL process to convert UHS into biochar. HTL can handle a liquid stream with up to 20% in solids, whereas the PNNL process cannot go beyond 8%. This is a great advantage, coupled with a much simpler process design. In addition, the SDSMT team has been able to produce biochar that actually works as an energy storage material and as a capacitor. Why is the SDSMT working with UHS rather than raw preprocessed biomass? It seems that this also may work and will simplify the process. Overall, the SDSMT has done an excellent job as the team has developed a new HTL process and produced good-quality biochar. Response: Originally, this proposal was funded for the valorization of UHS from bioethanol/biochemical processing of corn stover, and therefore we focused on UHS; however, the HTL process is also applicable to corn stover (both low ash and high material). Experiments performed with corn stover indicated that the biochar is equally well suited for the energy storage application—supercapacitors and batteries.

  Comments: The team has successfully designed, fabricated, and tested a pilot-scale HTL plant that produced high-value biocarbon and carbon nanofibers, thus valorizing the unhydrolyzed waste from the biochemical processing of corn stover. The team seems to have investigated the entire process—from feedstock preprocessing in collaboration with INL, to biocarbon and carbon nanofiber characterization, to commercialization and partnerships. The TEA and LCA will be useful in determining the economic and GHG reduction impacts of the project and in determining the size of a commercial project. The HTL process can handle wet feedstock streams with up to 20% solids, which is higher than the 8% solids that PNNL's HTL PDU can handle. What range of solids content can the process handle? What other feedstock streams will work? Are there any process waste streams that are toxic or hazardous that pose a challenge for disposal? Response: SDSMT and INL are currently pursing TEA/LCA with specific system boundaries. Initial TEA estimates suggest that the scale of 880 TPD of corn stover processing produces the fuel at a cost of approximately $2/GGE with an approximately $50 million grassroot cost for the plant with recovery of 20%–30% oil and approximately 25%–40% biochar products. The process can handle up to 25 wt % solids in water. We successfully tested the process with this slurry concentration. Also, the system is capable of processing corn stover powder and pellets, pinewood, switchgrass, cardboard, paper waste, and food waste. As such, the gas stream is only 4%–5%, whereas the aqueous waste stream generally contains oxygenated hydrocarbons. We recycle the aqueous waste multiple times after the recovery of valuable products, such as phenols and substituted phenols and lactic acid. Alternatively, the carbon in the aqueous waste stream can be oxidized to meet the discharge standards. Solid hydrochar (approximately 40%) can be processed into energy storage material. So, we do not anticipate any disposal challenge.

  Comments: It is not clear if this approach (HTL) to processing post-hydrolysis solids will apply to all types of feedstocks and to other types of pretreatment. For the alkaline pretreatment of corn stover, it seems to offer a way to add significant value as coproduct streams. The supply-versus-demand balance for graphitic carbon may affect the value of that stream as this technology is implemented commercially, but it appears to be a growth market. The installed capacity of electrospinning equipment is small, so the TEA should determine if there are reinvestment economics for carbon nanofibers as well. The performance of those fibers appears promising based on early results. The properties and value of heavy bio-oil are not discussed, but they should be compared to No. 6 bunker oil as a start. Overall, extracting high-value products from leftover lignin solids is certainly helpful to the economics of an IBR. Response: We fully agree. The alkaline pretreatment adds value in terms of the coproducts, such as phenols/substituted phenols and carboxylic acids (e.g., lactic acid). For the commercial UHS and lab UHS, the hydrochar yield was 29.4 wt %, and 29.8 wt %, respectively, which suggests that the approach of HTL is applicable. The graphitic carbon market is continuously growing because of continuous demand for sustainable carbon electrode materials for reducing the carbon intensity. We fully understand that the electrospun carbon nanofibers were made on a small scale; therefore, we will determine reinvestment economics for carbon nanofibers through TEA. On average, we generate 20% viscous oil with higher heating values of 35 MJ/kg with sulfur content less than 0.1%

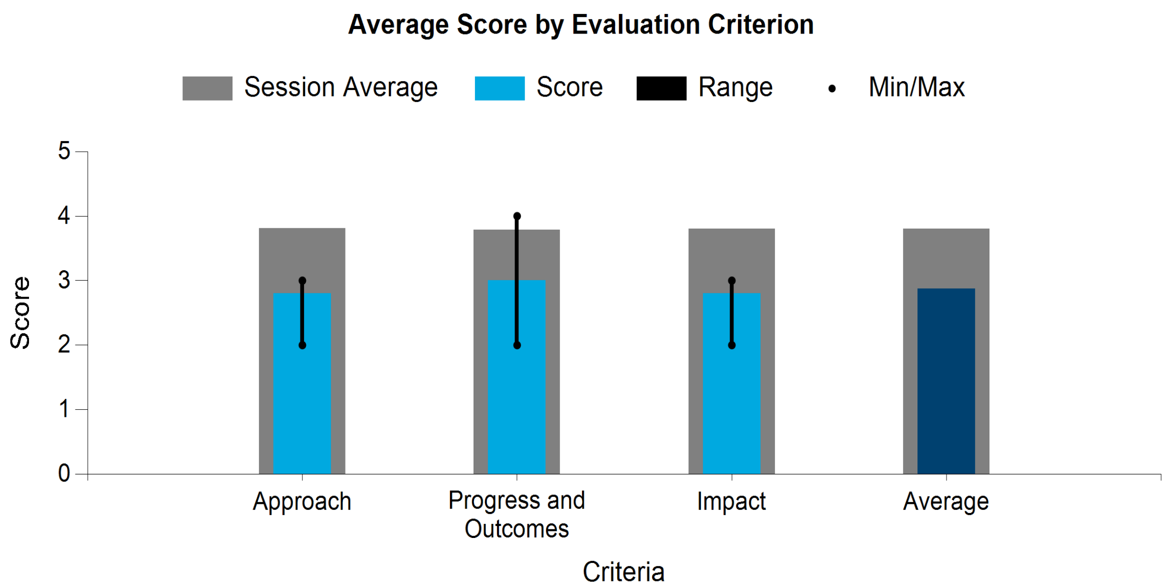
Comments: It is encouraging to learn that the 2021 Project Peer Review has led to a more focused approach with two high-value products: biocarbon (Product 1) and carbon nanofibers (Product 2). These products can significantly enhance the economics of a biorefinery. We are curious to know why the team at South Dakota chose to develop a new HTL system instead of using PNNL's HTL equipment. It would be valuable to understand the decision-making process and the differences between the two systems. Further, it would be beneficial to learn about the lessons learned and how the team overcame any challenges during the project. As the project approaches its end, it would be useful to have a table outlining the final economic figures as well as the LCA and GHG reductions achieved. Additionally, we would like to inquire about the possibility of collaborating with PNNL in synergistic activities. Response: There are two specific reasons that prompted us to design and build a new HTL system: (1) No pump characteristics are available in the literature, especially for slurries with higher solids loading; and (2) continuous pumping of slurries with higher solids loading has maintenance issues. Technical challenges were addressed by the inclusion of a digestor tank before the main HTL reactor and operating in a semicontinuous/batch mode. The SDSMT and INL are working on the TEA/LCA, and we will include all numbers, including GHG reductions. The SDSMT and the team will be extremely delighted to collaborate with PNNL on synergistic activities.

Comments: The project's main objective is to explore the production of high-value products from the UHS after pretreatment and enzymatic hydrolysis of corn stover. The solids are processed through HTL, and the biochar is used to make biocarbon and carbon fiber mats. The project has substantial merit and could have significant commercial impact for the valorization of UHS (lignin) during cellulosic ethanol production. This fraction has generally been burned for energy generation, but upgrading to high-value products could improve the financial viability of cellulosic ethanol facilities. As illustrated on slide 9, the process shows alkaline pretreatment of corn stover, enzymatic hydrolysis with Cellic CTec2, pH adjustment with sodium citrate, and separation of the UHS. Based on this process, the solids are expected to still contain cellulose and hemicellulose because the alkaline pretreatment alone is insufficient to achieve high sugar yields. The Cellic CTec2 enzyme preparation is not as effective as the Cellic CTec3, and residual cellulose and hemicellulose will remain in the solids. The extent of cellulose/hemicellulose remaining in the solids could impact the chemistry of the biochar, and this must be considered. It might be beneficial to obtain UHS from a more realistic, near-commercial cellulosic ethanol process (e.g., DMR with CTec3 hydrolysis) because the two processes could have significant commercialization potential when used together. As this project is close to completion, it might not be realistic to make changes at this stage, but further progression to a larger scale may consider these suggestions and potential collaboration with a cellulosic ethanol commercialization process for valorization of the lignin fraction. Obtaining a realistic assessment of the techno-economics of the HTL will also need valorization of the bio-oil, and potential future collaboration could investigate the characteristics of the bio-oil and potential upgrading. Response: We fully agree with the reviewer that instead of burning biochar for energy generation, valorization of UHS into biocarbon as well as carbon nanofibers will have more financial viability for cellulosic ethanol production. Commercially, this approach would be more impactful. We also believe that the Cellic CTec3 processing would be more effective than Cellic CTec2 and that the extent of the cellulose/hemicellulose remaining in the solids could impact the chemistry of the biochar. We have tested untreated corn stover for biochar production, and still we could achieve a highly porous biocarbon, which was found to be suitable for energy storage application. The HTL process was originally developed for the UHS solids that were commercially available from Glydia Biotech, Georgia, and later it was employed to the UHS derived from corn stover using Cellic CTec2. Although the hydrochar yield was almost similar (29.4% for commercial UHS and 29.8% for Cellic CTec2-derived UHS), we did observe difference in oil yields; therefore, we also believe that the use of UHS produced at a near-commercial cellulosic ethanol facility for biocarbon and carbon nanofibers will be commercially more significant. The SDSMT team will be happy and willing to join collaborative efforts with commercial cellulosic ethanol producers for valorization. At the laboratory scale, we have started valorization/upgradation of bio-oil to develop some understanding; however, this was not the focus of the currently proposed efforts. We are interested in collaborating on bio-oil upgradation. Currently, the SDSMT and INL are working on TEA/LCA, and we will include all numbers with GHG reduction in our reports.

PILOT-SCALE ALGAL OIL PRODUCTION

Global Algae Innovations

WBS:	3.5.2.201
Presenter(s):	David Hazlebeck
Project Start Date:	01/15/2017
Planned Project End Date:	06/30/2022
Total Funding:	$4,471,580



COMMENTS

- The presenter has not provided many details regarding the FEL-3 package. We do not know if this work has been done, and it is unclear whether the company has executed any pilot-plant construction yet. I question whether the company will execute the 160-acre plant or if it will be reduced to just two ponds. The 160-acre cost estimate is $73.9 million, and the production per acre is estimated at 22 tons of algae. The plant will use fresh water. The presenter did not provide the water consumption data, which represents a big concern, especially in areas like central California, where water is scarce. An industrial-scale facility will need 5,000 acres and an investment between $500 million–$1 billion. The economics of oil production are tight; water consumption in the ponds is a big environmental challenge.

- The presentation was confusing in regard to the scope of the funded project and the path to the commercial scale (slide 17). How many acres is the raceway for this pilot project? Slide 20 shows that the next scale-up for the raceways is 6 acres, then 18 acres. What is the anticipated acreage for each raceway in a commercial-scale farm targeted for design and construction in 2026–2027?

- The addition of nutraceuticals to enhance the return on investment seems useful but was not elaborated. Different conditions and sources for CO_2 and nutrients to enhance performance were also not fully explained, nor was contamination control. These seem to be critical to the overall cost and operability performance, as well as the higher percentage of lipids and protein, which were mentioned. Two-times productivity improvement, 10-times lower energy demand, and two-times higher product value are significant, but we need to understand how much that advances the technology versus other biomass-to-advanced fuels options. It would be helpful to put the statistics for the fertilizer and kilowatt-hours per metric ton of oil and meal into context relative to the other technologies and versus targets for this approach. In addition, it would be helpful to know how the estimated capital per pond acre per metric ton measures up to the national goals to understand what the land and water use impacts are to meet the goal $/GGE and GHG reduction.

- The influence of weather effects, such as wind velocity and hurricane impact, on the site selection and design considerations for algal cultivation has not been clearly understood. Further research is needed to determine their influence. There are concerns about the potential indirect land usage change resulting from commercial-scale algal projects. It is important to carefully evaluate the potential environmental impacts of these projects, including their effects on land use. The claim that a 100% increase in biomass value can be achieved for a product spectrum commensurate with 7 billion gallons of algal biofuel per year is ambitious and requires further investigation to determine its feasibility. Algal cultivation presents several challenges related to water use, water recycling after separation, and land use. These challenges need to be addressed to ensure that the industry is sustainable and does not negatively impact other sectors, such as agriculture. To better understand the various projects from Global Algae Innovations, it would be helpful to have a clear illustration of the similarities and differences between the projects. Additionally, understanding how the project team members collaborate, particularly during the execution phase, can provide valuable insights into the success of these projects.

- Does only the Nitzschia strain produce oils? If spirulina production is targeted for 75% of the time, lipid production will be negligible. Please provide an analysis of the lipids produced (chain length, etc.). What is the breakdown of the saturated, monounsaturated, and polyunsaturated lipids? What is the expected production of saturated lipids for biofuel applications (in volume per acre)? It is indicated that offtake agreements are in place for all the products—is there a specific offtake for lipids for biofuels production? Based on the information presented, the production of lipids for biofuels does not seem financially viable, although the project may be viable for other products.

PI RESPONSE TO REVIEWER COMMENTS

- This design project was for a 160-acre pilot plant based on being large enough that the revenue from the oil and protein products would cover the operational cost, so if the capital were paid by moving to Phase 2 of the award, the operations would be self-sustaining. The project was not started until after the downselection to Phase 2, so moving to Phase 2 to cover the capital was not an option. The size was fixed by the original proposal, so based on the business assessment, the design was based on operating part-time for nutraceuticals to provide a return on investment and part-time for oil and protein to prove out the technology for moving on to the commercial scale for these products. One hundred sixty acres are not needed to prove the technology and obtain offtakes for the commercial scale, so the likely path to commercialization for biofuel is to build out the initial 18 acre of the design, including a 12.5-acre individual raceway. This leaves an 8- to 16-times scale-up remaining to reach a full commercial-scale farm that includes 100- to 200-acre individual raceways. Global Algae currently has three other awards related to scale-up. This first is to build out the initial 2-acre cultivation and harvest, including a 1.3-acre individual raceway. The second is to add a 4-acre raceway and harvest system expansion with an option for a 12-acre raceway and harvest system expansion. The third is to scale up a novel drying and extraction system to approximately the 4-acre scale.

  For the Nitzschia strain, approximately 50% of the ash-free dry weight is lipid. The lipid is approximately 5% 14:0, 40% 16:0, 40% 16:1, and 15% omega-3 (primarily EPA0). The oil production is approximately 3,200 gallons per acre per year. The planned product spectrum is 1,600 gallons/acre of saturated oil fraction for biofuel feedstock, 1,300 gallons/acre of monounsaturated oil fraction for polymer feedstock, and approximately 300 gallons/acre of omega-3 fraction as an ingredient for feed. The oil is upgraded through the hydroprocessed esters and fatty acids (HEFA) process to SAF and renewable diesel. This product spectrum results in approximately $1.60/kg of oil on average, which is projected to provide a good return on investment at the commercial scale. The markets for these three products could support approximately 7 billion gallons/year of algal biofuel. Because of supply constraints relative to demand in the United States, the current price for oil for HEFA upgrading is approximately $1.6/kg, so all 3,200 gallons/year could go to biofuel with a good return on investment at the current pricing. We currently do not have offtakes for the commercial scale. Our plan is to operate at the pilot scale to validate the products so that offtakes can be obtained to enable financing the first commercial-scale farm.

Similar to any other food or biofuel crop, algal water use depends on the location. The evaporation of water per acre from algal raceways is similar to the loss of water from evapotranspiration per acre in land crops; however, algae produce approximately 24 times more protein than the most productive land plant at the same time that it is producing approximately 3,200 gallons/acre of oil. During the oil production, the algal farm reduces the total water use for protein production for feed by approximately 90%; thus, algal biofuel will reduce the water use for agriculture by 100 to 500 gallons of water per gallon of biofuel. The actual amount of water added from surface waters, underground water, or reduced water recharge through the use of rainwater is dependent on the location, just as with conventional agriculture. Global Algae's harvest system removes all biological components, so the water from harvesting is fully recycled without any issues. Compared to other biomass-to-advanced fuel options, the metrics are: land use: cellulosic ethanol approximately 600 gallons/acre versus algal oil approximately 3,200 gallons/acre; water use: cellulosic ethanol approximately 600 to 1,200 gallons of water use/gallon of fuel versus algal oil, which saves 100 to 500 gallons of water/gallon of fuel; GHG: cellulosic ethanol—at least 60% GHG reduction; algal oil 60% reduction with conventional drying and extraction or 90% with advanced drying and extraction. For all options, the key is economic biofuels production. For algal oil, the combined oil price needs to be approximately $1.60/kg for the composite price with the current technology for a high return on investment. Our current plan is to sell 50% of the oil at approximately $0.80/kg for biofuel, 40% of the oil at $2/kg for the polymer feedstock, and 10% of the oil at $4/kg as an omega-3 feed ingredient. After the first approximately $5 billion gallons/year of biofuel, additional technical and operational advances will need to be achieved to reduce the cost so that all the oil can go into biofuel and consumer markets to replace palm oil at less than $1/kg.

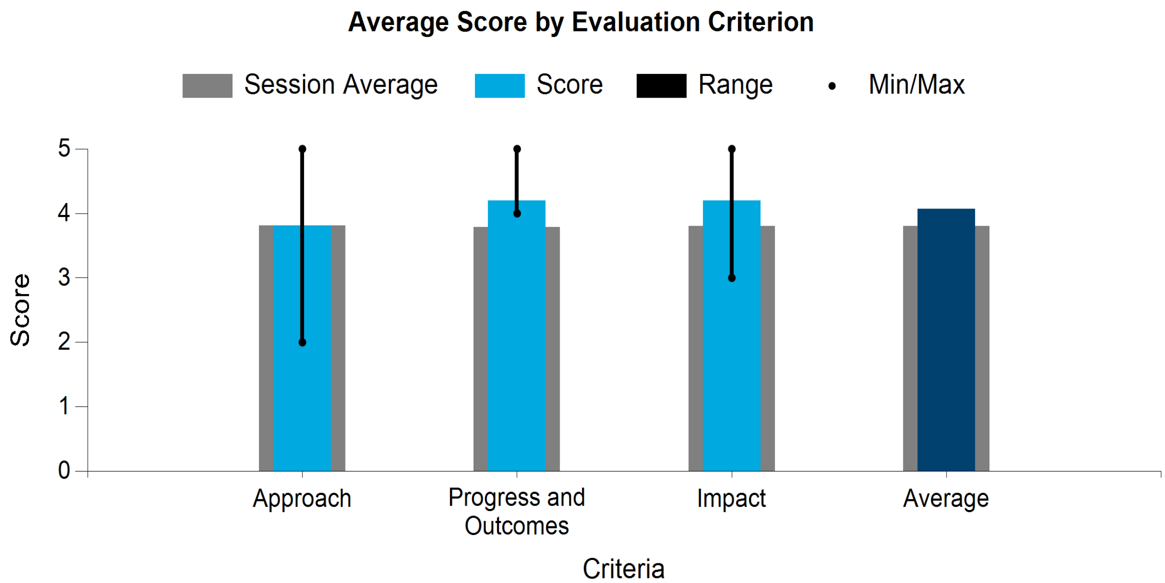
LOW-CARBON HYDROCARBON FUELS FROM INDUSTRIAL OFF-GAS

LanzaTech Inc.

PROJECT DESCRIPTION

WBS:	3.5.2.403
Presenter(s):	Laurel Harmon
Project Start Date:	01/15/2017
Planned Project End Date:	09/30/2023
Total Funding:	$37,317,103

LanzaTech and its partners are implementing a 10-million-gallon/year facility to demonstrate the production of low-carbon jet and diesel fuels from ethanol using the ATJ that originated at PNNL and was scaled by LanzaTech. The technology will be demonstrated using ethanol from steel mill off-gas and other sources. The ATJ facility, Freedom Pines Fuels, is a project entity owned and operated at LanzaTech's Freedom Pines Biorefinery by LanzaJet, a company formed by LanzaTech to commercialize the ATJ technology. During Phase 1, LanzaTech completed the design and engineering required to achieve a −5%/+15% cost estimate, and two independent engineering reviews were completed. National Environmental Policy Act approval was secured for the project. All technology and engineering, procurement, and construction partners have been selected. Now in Phase 2, the project is in construction, with mechanical completion expected in Q4 of 2023.



COMMENTS

- The project seems to be on track, with much preliminary work already performed. What is unclear to me is whether this technology has been proven at the pilot/demonstration scale and what have been the results. The presenter has not provided any technical or performance data to allow me to evaluate their results. LanzaTech changed the project's scope, eliminating the integration of ethanol produced by gas fermentation with SAF production because they say that the ethanol production had already been demonstrated; however, it is unclear if the integration of both processes may have an impact or how synergetic it can be. Now it is not clear what ethanol they are going to use and whether they can achieve the goals of GHG reduction and the cost of production. They did not share any information about the cost of the plant, operational cost, or carbon footprint. LanzaTech claimed that all this information was confidential and had been shared with DOE. I cannot make any project review, or assessment, or provide an opinion on the project.

- The project has taken a sound approach to scaling and seems to be achieving the target progress and outcomes at a high level. Technical details and results are not presented. What challenges have been solved and proven by the demonstration project? Waste gas ethanol does not qualify for RINs. If sugarcane ethanol is to be used, what is the GHG reduction of the resulting SAF? Is sugarcane ethanol an economically feasible feedstock for a commercial plant?

- This project assumes that gas fermentation of mainly CO_2 off-gas from industrial sources to ethanol is an economic reality. Otherwise, this facility would need to use existing ethanol sources that may or may not be acceptable under the current guidelines for feedstocks. It focuses on dehydrating that ethanol to ethylene, then oligomerization and hydrogenation to paraffins as advanced biofuels—mainly SAF. The participants in this project have good expertise and experience with these unit operations, thus increasing the chance of success. One concern is that the initial feedstock is an off-gas of undisclosed composition, and it is not clear how broadly applicable the process will be for other off-gas feedstocks. Another question is how this approach compares to other syngas-to-SAF approaches, such as the Honeywell UOP technology. A TEA and IRR would be useful to understand the economics. Assuming those concerns are mitigated, this approach has strong merit for scale-up.

- It is not obvious how the project plans to source the ethanol feedstock. Could you provide more information on the intended source of the feedstock? The project's end-of-milestone goal is to demonstrate that its products meet the Renewable Fuel Standard 2 requirements for advanced or cellulosic biofuels. Given that the project's scope has changed, could you explain how the project plans to achieve this goal? Although specific cost numbers and economic analyses were not provided, it would be useful to have at least a range of the project's estimated costs. This information can help in determining the financial viability of the project. It would be helpful to know about any lessons learned during the project's execution and how the project has addressed any unanticipated changes that have occurred. This information can be used to improve the project's efficiency and effectiveness and to inform future projects.

- The aviation sector faces significant challenges to achieving net zero by 2050, and SAF is considered the most important solution to contribute approximately 60% of emissions reductions; however, delays in the commercialization of additional pathways (other than HEFA) are one of the challenges that must be addressed because waste lipid feedstock volumes are limited. The ATJ pathway is one of the most promising technologies because it can use multiple sources of ethanol to produce SAF. The Freedom Pines facility will pave the way for this technology to become fully commercial and deliver significant volumes of SAF through multiple facilities worldwide. Completion of this pioneer facility is an important and exciting milestone, and this project will have a significant impact on the SAF sector.

PI RESPONSE TO REVIEWER COMMENTS

- *Subject to disclaimers on the associated presentation*

  Data and results from prior-scale work: Technical and performance data were generated in previous efforts with both DOE and private funding. The data are confidential and were provided to DOE during the application for this project and to the DOE independent engineer during validation. The purpose of the current project is to finalize the design and construct the facility; new data will be generated during initial operation.

Integration of ethanol production and ATJ: The project was designed from the outset to use multiple sources of ethanol (a hub-and-spoke model); therefore, potential synergies between gas fermentation and ATJ are out of scope here but are being assessed in other projects.

Ethanol source and GHG reductions: The GHG footprint of the products is largely determined by the ethanol source. LCA results were presented at the last Project Peer Review for five different ethanol sources. The EPA has approved the ATJ pathway for the generation of D4 RINs (biomass-based diesel) with at least 50% GHG reductions when using sugarcane ethanol feedstock (www.epa.gov/renewable-fuel-standard-program/approved-pathways-renewable-fuel). The facility will initially use sugarcane ethanol feedstock while working to build a supply of waste-based ethanol from gas fermentation and other technologies.

Waste gas feedstocks—feasibility and applicability: Three commercial gas fermentation plants are operating now, a fourth is in commissioning, and two more are in construction—all with differing feed gas compositions. Many millions of gallons of waste gas-based ethanol have been produced from these plants (www.biofuelsdigest.com/bdigest/2021/01/31/commercial-ccu-plant-using-lanzatech-tech-receives-rsb-advanced-products-certification/, www.forbes.com/sites/erikkobayashisolomon/2021/09/21/lanzatechs-paradigm-shifting-plan-to-create-carbon-negative-industrial-chemicals/?sh=2e7a9e573bdf); therefore, the feasibility of producing ethanol from waste gas has been well-established. The ethanol produced is independent of the waste gas source, so gas composition does not affect the ATJ process. Although not part of this project, gas fermentation can also produce ethanol from the syngas generated by gasifying biomass or municipal waste. A reviewer asked about the comparison to “other syngas-to-SAF approaches, like the Honeywell UOP technology.” We note that Honeywell UOP does not have a commercialized syngas-to-SAF process but has commercialized HEFA technology using lipid feedstocks to produce SAF. Fischer-Tropsch is the primary alternative process for producing SAF from syngas. Limitations of Fischer-Tropsch were included in the presentation; they include lower overall yield to high-value products (SAF, diesel) and less selectivity to SAF. As noted by one reviewer, fuels from waste gas do not yet qualify for RINs.

Costs (CapEx, OpEx): Details of the facility cost have been shared with DOE and the DOE independent engineer, including regular updates during the project development. Responding to one specific question, the cost of production from sugarcane is economically attractive for a commercial plant.

TEA/LCA: As noted, LCA results were presented at the last Project Peer Review and were recently approved by the EPA for sugarcane ethanol feedstock. Both TEAs and LCAs specific to individual regions and feedstocks are continuously updated in confidential discussions related to new projects and project finance.

Challenges and lessons learned: One key challenge was the need to raise capital for a first-of-a-kind plant, which was exacerbated by the pandemic. This was addressed in part by developing multiple creative financing mechanisms, including the involvement of strategic investors with commitments to implementing follow-on plants. In addition, both the pandemic and the war in Ukraine created significant supply chain challenges. Although such events cannot be anticipated or part of the planning process, that experience highlights the importance of maintaining supply chain flexibility to mitigate unforeseen gaps. These challenges can be mitigated in large part by good partnering, close attention to details, and the continuous consideration of alternative sources of supply.

ADVANCED BIOFUELS AND BIOPRODUCTS WITH AVAP

AVAPCO

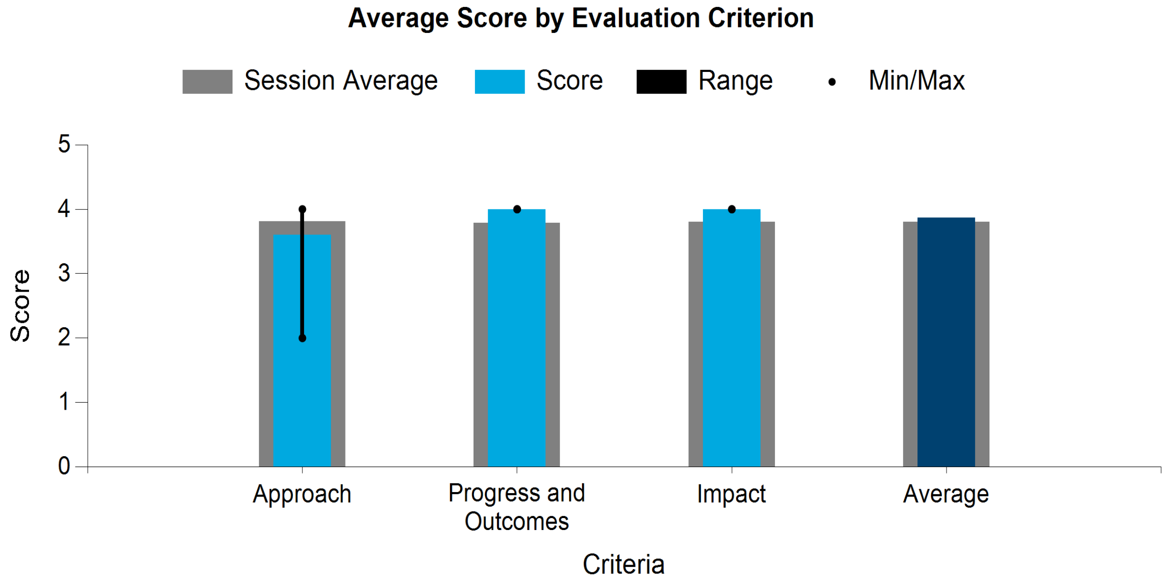
PROJECT DESCRIPTION

WBS:	3.5.2.405
Presenter(s):	Ryan Zebroski
Project Start Date:	01/15/2017
Planned Project End Date:	02/01/2023
Total Funding:	$9,341,328

The Advanced Biofuels and Bioproducts With American Value-Added Pulping (AVAP) project involves upscaling the patented AVAP pretreatment technology, coupled with innovative sugar fermentation to mixed alcohols, which are then converted to full-replacement liquid hydrocarbon biofuels at AVAPCO's existing biorefinery site in Thomaston, Georgia. The targeted scale is 100 dry TPD of woody biomass from neighboring sawmill residues and harvesting operations and 1.2 million gallons/year SAF and renewable diesel. The coproducts include the Nanocellulose Dispersion Composite (NDC) rubber masterbatch for commercial sale to the tire industry and cellulosic sugars for conversion to a biochemical by a confidential global chemical industry partner.

In the AVAP fractionation, the process starts with wood chips fed into a continuous digester. The chips are impregnated with sulfur dioxide-ethanol-water liquor and cooked. These conditions dissolve nearly all lignin and hemicellulose without creating unwanted side products. The chemicals are recovered via washing and stripping, and they are recycled to the digester, resulting in a hemicellulose sugar stream and a high-purity cellulose stream. Part of the clean cellulose is directed to produce nanocellulose, followed by the NDC rubber masterbatch. The rest of the cellulose is enzymatically saccharified at a low enzyme dose for hydrolysis to C6 sugars for off-site conversion.

The remaining cellulosic and hemicellulosic sugars are fermented to produce ethanol. The remaining lignin and fermentation residuals are burned for process energy. In the hydrocarbon plant, these alcohols are first converted to ethylene by Petron Scientech and then converted to full-replacement liquid hydrocarbons using a catalytic synthesis process that produces petroleum distillate equivalents with overall LCA reduction greater than 90% at the commercial scale. Jet fuel from the pilot plant has undergone advanced U.S. Air Force testing for JP-5 and JP-8 grades with the unique ability to vary aromatic content. Byogy was a finalist as one of 4 companies of 90 under the Federal Aviation Administration's Continuous Lower Energy, Emissions, and Noise (CLEEN) program, where rigorous engine testing was performed by Rolls Royce that demonstrated Byogy's fuel characteristics provide a premium full-replacement renewable aviation fuel.



COMMENTS

- I do not see a clear business case in the presentation. It is a combination of multiple components without a clear strategy. I do not see any economics or studies to show the competitiveness of the solution. No yields either. It seems that nanocellulose composite is the main product, and SAF is a byproduct, when it should be all the way around. It is unclear why the company does not maximize ethanol production, as an SAF precursor, fermenting both cellulose and hemicellulose. The pretreatment uses SO_2; has the company studied the effect of sulfur in fermentation and ethanol-to-ethylene conversion? It is very common to see sulfur as an irreversible poisoning agent of the catalysts. I cannot determine whether the company has produced any SAF yet in the previous stages of the project. The company is seeking $80 million in grants from DOE. That means that the project cost will be at least $160 million for 1.2 million gallons/year of SAF. It seems to be very intensive in capital needs for such a small output.

- AVAPCO and its partners seem to have taken a sound approach to trialing, optimizing, and piloting its process and is now scaling up to the demonstration scale. High-value bio-based coproducts enable the production of low-value commodity liquid fuels. What are the technical scale-up challenges for the demonstration plant? For the next scale-up plant? The presentation indicated the usage of 340,000 dry TPD of biomass for a 100-million-gallon/year SAF plant. Is the roundwood required to obtain this amount of feedstock within an economic draw radius?

- This project uses the well-proven pretreatment process for wood used in making pulp for paper, with the noncellulosic portion normally being diverted to black liquor and burned for fuel value. The separation and fractionation of cellulosic feedstocks into component streams that are clean enough to use as intended may be the biggest challenge for this project. Handling diverse and variable feedstock compositions and producing consistent quality intermediates has been a difficult challenge in past integrated biorefineries. Making clean nanocellulose is critical to the overall economics of this process, along with large-scale demand. Similarly, making cellulosic glucose with the same fermentability (lack of inhibitors) as dextrose seems challenging if the intent is to use GMOs, especially at near-neutral pH, to make high-value products other than ethanol. Once the path to ethanol is demonstrated, ethanol-to-olefins and advanced biofuels seems straightforward. Need to see the TEAs and IRRs of the integrated process to understand if the impact suggested is likely.

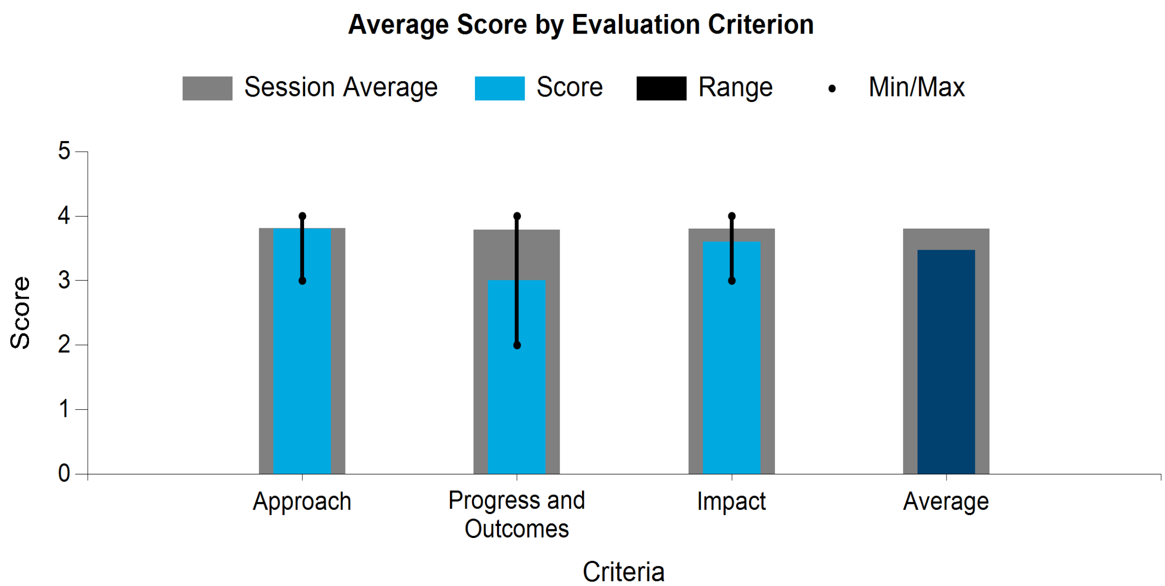
- It is critical to ensure that this project meets the requirement of converting at least 50% of biogenic carbon to fuels as the cellulose portion of the feedstock is being converted to C6 sugars and NDC; therefore, it is crucial to establish a mechanism for monitoring this conversion rate. Regarding the replication and scaling of the current design, the team needs to develop a clear plan that outlines the necessary steps for upgrading the current model from the demonstration scale. As the project approaches its end, it would be beneficial to present a comprehensive table outlining the final cost, environmental impact, and reduction of GHG achieved. Additionally, I recommend including a section that details the lessons learned and how unanticipated changes were effectively addressed during the project's execution. Finally, a risk register should be integrated into the project deliverables to ensure that all completed projects include an assessment of potential risks that might adversely affect the project's goals and objectives.

- The project approach seems to align with the BETO Multi-Year Program Plan for the production of fuels and high-value coproducts; however, the production of the coproducts seems to be the main target, whereas SAF and renewable diesel production seems to be a very minor component. It would also be useful to clarify whether the further scale-up is expected to integrate the ethanol-to-ethylene and the SAF production components with the AVAPCO component (even though it is not part of this project). It is not clear whether the hemicellulose and cellulose fractions, produced after digestion, contain significant contaminants and inhibitors that may impact the fermentation and other downstream processes, and this should be clarified because it could have a significant impact on ethanol production and yield. No specific strategy or approach indicates how this will be addressed. Information should be provided on the proposed source of enzymes for the hydrolysis of the cellulose, and information should be provided on the fermentation organism. According to the presentation, SimaPro was used to calculate the LCA, but GREET is the model used specifically for fuel production, and it should be assessed. For purposes of the Inflation Reduction Act, the CORSIA model must be used for SAF, and this could have a significant impact on the outcome because energy allocation is used. In the case of nonfuel coproducts, energy allocation will likely change the carbon intensity of the SAF fraction.

RIALTO ADVANCED PYROLYSIS INTEGRATED BIOREFINERY

Rialto

WBS:	3.5.2.601
Presenter(s):	Andrew Dale
Project Start Date:	04/01/2017
Planned Project End Date:	12/31/2023
Total Funding:	$6,391,391



COMMENTS

- The project has completely changed its initial objective of producing pyrolysis oils from biosolids to enhance biogas production in an anaerobic digestor to destroy PFAS in biochar to allow land application. The new PFAS regulations that the EPA published in 2021 prevented the use of Anaergia pyrolysis oils in biogas production because they contained PFAS exceeding the allowed limits. Now the company has focused on ways to remove PFAS from biochar and obtain a permit for its land application. Although PFAS have been almost entirely removed by thermal oxidation at 650°C, the presence of concentrated metals in the biochar may restrict its applicability as a fertilizer. The company has tried to get the best results, but there is still a big question mark regarding the usefulness of this technology for biochar treatment. It is certainly not a project focused on biofuels.

- As part of its commercialization plan, the team has taken the appropriate steps to investigate the potential to convert the biosolid waste stream into valuable products, which helps solve the biosolids disposal issue and increases the supply of low-carbon fuels. The project found that the condensable oils cannot be used for fuel production due to the PFAS content. Although the project could not achieve its original objectives, it is useful to elucidate where PFAS ends up in the pyrolysis process. In response to the new EPA rules regarding PFAS, the project shifted the objectives to PFAS removal from the biochar product for land application uses and PFAS destruction. The team was able remove the PFAS from the biochar and make the biochar usable for land application. This seems like a very reasonable pivot. The biochar market is still a nascent market, and the economic feasibility would need to be shown by a TEA.

- High-temperature pyrolysis of municipal waste sludge to eliminate PFAS, then granulating with fertilizer to produce a safe and valuable product seems like a reasonable plan, provided there are low enough levels of heavy metals in the biochar to not cause problems with absorption by plants. That risk needs to be addressed as part of the plan. Halogens from PFAS destruction will be captured by scrubbing gases with caustic. Heat integration will be critical, along with good TEA and IRR results. The project will need to show that the material and energy balances are economic and sustainable in terms of safety and GHG impact (farm to farm).

- Please provide information on the starting and ending TRLs for this project? Have there been any studies conducted on the market acceptance of biochar produced from this project? In addition, we are curious about how the metal content in biochar is being managed for land application. Are there any measures in place to prevent metals from being absorbed by plants? To make a proper assessment, it would be beneficial to have access to additional information, such as specific operating data, LCA, GHG, and economic analyses.

- This project was initially intended to produce pyrolysis bio-oil to be added to the anaerobic digester operated by the company to increase yields of RNG from the facility. The bio-oil was found to contain PFAS, and the project was changed to achieve the destruction of the PFAS through thermal oxidation of the volatilized compounds. Temperatures of 650°C were required to remove the PFAS from the biochar, allowing the biochar to be used as a fertilizer. The additional equipment and conditions for the thermal oxidation and the subsequent fate of the fluorides were not presented and should be added. The application of the blended biochar as a fertilizer is undergoing field trials, and initial studies show promising results, although trial experimental design was not clear. Why is nutrient uptake in the leaves tested as opposed to different metrics, such as fruit production, etc.? Was the biochar blended product fully formulated as equivalent to other types of fertilizers? Analytical results should be added. How does the cost of the biochar fertilizer compare with commercial fertilizers? Has a TEA been carried out? How does the biochar product compare with other biochars available on the market (cost and composition)?

NOVEL ELECTRIC REFORMER FOR DROP-IN FUELS FROM BIOGAS OR WASTE CO_2

Gas Technology Institute

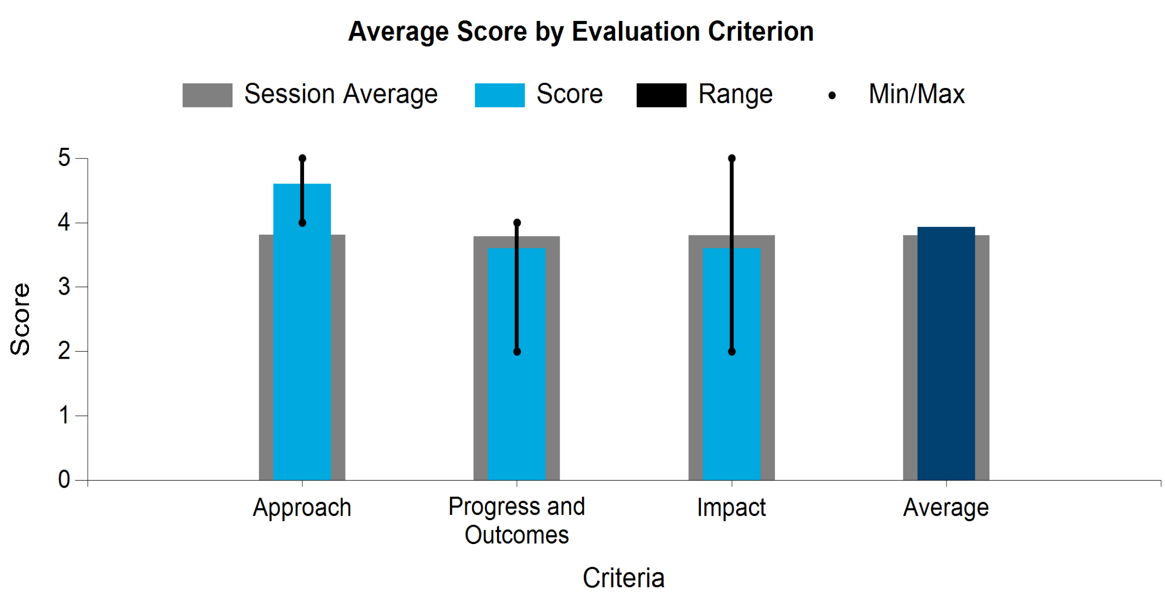
PROJECT DESCRIPTION

WBS:	3.5.2.701
Presenter(s):	Terry Marker
Project Start Date:	10/01/2021
Planned Project End Date:	03/31/2024
Total Funding:	$5,008,195

The goal of this project is to significantly reduce biogas-to-liquid costs by scaling up an electric reformer/reverse water gas shift reactor for the conversion of waste carbon dioxide from ethanol plants or biogas from digestors to synthesis gas. The synthesis gas from the reformer will be used to make drop-in fuels using the Cool GTL technology or will be used in other GTL processes. The ultimate objective is to produce biofuels from biogas or waste CO_2 from bioprocesses for less than $2.75/GGE with greater than 70% reduction in GHG emissions. In this project, the electric reformer/reverse water gas shift reactor will be modeled, designed, constructed, and tested for more than 500 continuous hours for two cases covering biogas conversion to liquids (Case 1) and waste CO_2 utilization (Case 2). This project will scale up GTI's electric reformer design, which has been tested at a smaller scale, as the first stage of the Cool GTL process (this produces 1–2 gallons/day) to a larger scale.

A key goal is to ensure that the model correctly predicts the internal heat transfer and that the reactors ultimately produce the desired synthesis gas composition of 2.2–2.5/1 H_2 to CO at expected temperatures. To achieve this, the project includes extensive mechanical, structural, and electrical design, reactor performance parametric studies based on an anchored model, and the preparation of engineering design drawings and procurement specifications for a commercial electric reformer. Also, this study will accurately determine the capital cost, techno-economics, and life cycle advantages of a large commercial electric reformer as the basis of renewable fuels production.

The major benefit is to greatly reduce the reformer or reverse water gas shift reactor's capital cost, size, and waste carbon dioxide production.



COMMENTS

- The electrical reformer is an interesting concept for CO_2 or biogas conversion to syngas in relatively small applications where an industrial-size reformer is unsuitable. In other words, this concept could apply to distributed production; however, the design of electrically heated equipment has limitations that must be addressed when working with hydrogen. According to ATEX regulations, the maximum superficial temperature for hydrogen is 450°C. This means that the heating element in the presence of hydrogen cannot surpass that temperature if there is a risk of having oxygen in contact with hydrogen because it autoignites at 550°C. Electrical heating of hydrogen is very cumbersome, and I strongly recommend that GTI thoroughly investigate safety issues and ATEX limitations immediately. I also have big concerns about the maximum size of this type of equipment. Heating elements with large power demand are not in the market today. Although GTI is working with Siemens, this issue should not be disregarded. GTI has not presented any TEA to allow me to check their $2.75/GGE cost of production. This is the first of a set of projects on the Cool GTL technology.

- This project takes a sound technical approach to developing an electric reformer that provides the advantages of a smaller footprint, reduced cost, and eliminates air emissions impacts. Clean renewable electricity is used in place of natural gas. With a smaller footprint and lower cost, the electric reformer has the potential to make smaller, distributed biorefineries economically feasible as well as larger refineries. The preliminary TEA projects a jet fuel production cost of $2.75/GGE. What size plant was this TEA performed for? It would be interesting to see the range of scales for which the electric reformer would be economically feasible.

- Conceptually, substituting new large-scale reformers with smaller electric reformers could allow for the use of that unit operation in smaller and more decentralized applications as well as significantly increase the feedstock-to-fuels yields. Critical to prove out is the robustness of the reformer design and performance in producing syngas with the right composition, especially with scale-up. The project would benefit from more of a market analysis to determine the size and number of units that ultimately might be deployed, if the design and materials of construction prove to be economic. A comparison to current reformer technology should include both energy utilization and CapEx. To a great extent, this project assumes that renewable energy from solar and wind will be available, so that question should be addressed in the implementation plan. Siemens seems like a good partner for this development.

- This project is interesting because it employs a technically robust approach. I'm very curious about the scale of the experimental electrical reformer system in the lab and how the mathematical model accounts for wall and end effects and their influence on scale-up. It is very critical to ensure that the operability and robustness of the electrical reformer are ascertained for the actual feedstock as opposed to mock components and compositions mimicking the actual feedstock. Economic comparisons for the proposed electrical reformer should be with the current reformer system before embarking on the path of electrical reformer technology. It is crucial to adhere to safety standards (see slide 14) with proper personal protection equipment for all personnel involved in this project. To gain a better understanding of GTI's various projects, it would be helpful to have illustrations that highlight similarities and differences between them. Additionally, it would be beneficial to learn about how project team members from different projects collaborate during the execution phase and share learnings from various projects.

- This project has significant potential for developing small GTL technology based on biogas and steam or CO_2 and hydrogen. The Cool electric reformer is novel and has a much smaller footprint than a traditional natural gas reformer. The TEA and LCA to be carried out will be important to assess the viability of this technology. The carbon intensity of fuels will be impacted by the source of the electricity, and perhaps different electricity sources can be compared in the LCA. Although the FTS is not part of this project, it would be advisable to check whether the catalyst formulation in the Fischer-Tropsch reactor will comply with ASTM D7566 Annex 1.

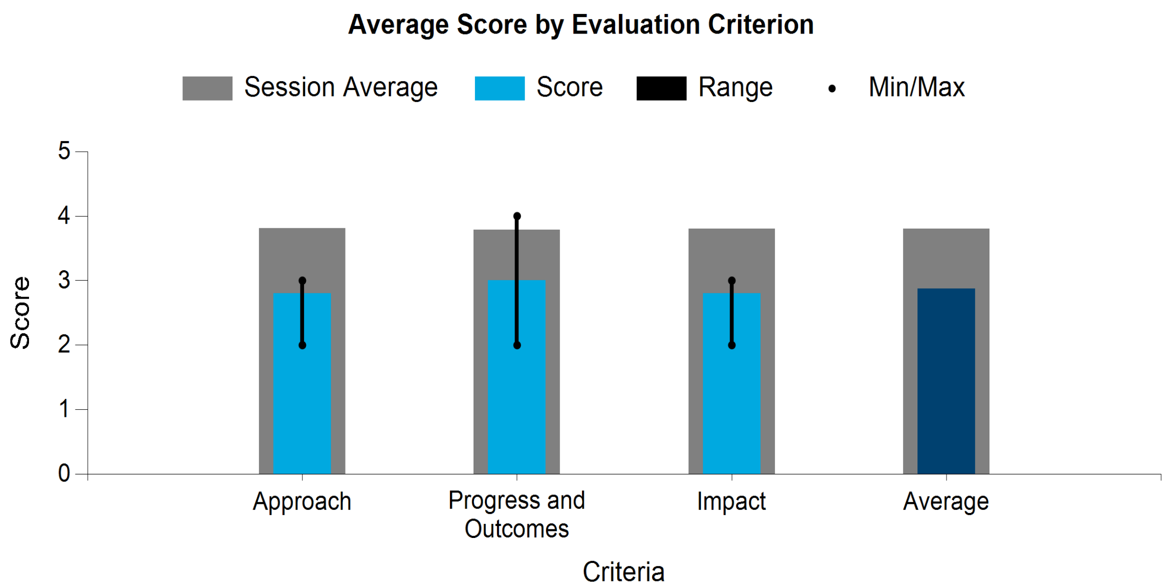
PI RESPONSE TO REVIEWER COMMENTS

- Most hydrogen and synthesis gas is produced from steam methane reforming of natural gas. This reaction is done at 850°C–900°C, well above 450°C, which is the autoignition temperature of hydrogen. The ATEX regulation the reviewers mention do not really apply to the temperature of hydrogen inside a steam methane reforming reactor. In general, there is little or no oxygen present in a steam methane reformer. GTI is aware of all the safety regulations around the use and production of hydrogen and does indeed carefully review all designs to ensure they are safe.

DIRECT AIR CAPTURE ALGAE CULTIVATION

Global Algae Innovations

WBS:	3.5.2.702
Presenter(s):	David Hazlebeck
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2023
Total Funding:	$5,000,000



COMMENTS

- The presenter has not described any work done regarding the direct air capture of CO_2. The company seems to have been doing preliminary work for the pilot plant in California but nothing related to CO_2 capture. I cannot find if the scope of work is to build a pilot plant or is something different, especially considering that the company has another project to construct the pilot plant. The company needs to clarify the scope of work of the three awarded projects and the final outcome of this DOE investment.

- The presentation did not provide any description on the direct air capture technology and the capital cost; thus, and evaluation is not possible. For this funding opportunity, Global Algae Innovations is planning to scale up the project to 2 acres of raceways. What is the scale-up factor from the pilot plant in Kaui? The California project will incorporate many newly developed technologies. This may pose a challenge to integrate and deploy many new technologies at the same time.

- The project has proceeded with the selected strains in locations where piloting facilities were established. It is not yet clear where future commercial scale-up will occur, and the algal productivity of 15 gm/m^2/day was not translated into number of ponds needed for a specific oil and coproducts production target. The approach to avoid contamination in open ponds was not fully disclosed, nor how that approach compared to closed systems fed by concentrated CO_2 sources in terms of productivity and capital use. Water use also was not fully addressed. The TEA of this technology would be more helpful if it looked at the relative performance of this approach versus other biomass-to-fuels pathways.

- Evaluating the use of direct air capture for algal cultivation involves several factors, including the current concentration of CO2 in the air, which stands at around 410 ppm. Although direct air capture technology holds great potential for reducing CO_2 levels in the long term, current efforts are still in the research phase. In the near term, concentrated sources of CO_2 may prove more economically viable for the development of processes to produce biofuels and bioproducts from algae; however, the cost of producing biofuels from algal biorefineries remains prohibitively high, which hinders their widespread adoption and impact. To gain a better understanding of the various projects undertaken by Global Algae Innovations, it would be helpful to have an illustration that highlights their similarities and differences. Moreover, it is important to understand how team members from different projects collaborate during project execution to ensure their success. By improving transparency and communication, stakeholders can better assess the potential impact of these initiatives.

- According to the presentation, the facility in Hawaii was supplied with CO_2 via slipstream from an adjacent power plant stack. In this project, the source of CO_2 is direct air capture; however, there are no details on what "direct air capture" means, and this needs to be clarified for project evaluation. Is CO_2 concentrated from air similar to carbon capture technologies (which is very expensive)? How does this compare with the economics and life cycle of using CO_2 from a power stack? How is the CO_2 supplied to the algal ponds? Algal cultivation for biofuels production has not been successful in the past, and companies shifted to the production of higher-value coproducts rather than extracting lipids for biofuels production. Although biofuel is a target of this project, shifting all the lipids to other high-value products will likely improve financial viability. The location of the facility in a water-scarce area is problematic and may impact sustainability certification. Water consumption compared with various crops should be shown (not just alfalfa). The cost per GGE is given for cultivation at a 5,000-acre scale. What is the cost per GGE for the proposed 160-acre scale?

R-GAS ADVANCED GASIFICATION PRE-PILOT DEMONSTRATION FOR BIOFUELS (BIOR-GAS)

Gas Technology Institute

PROJECT DESCRIPTION

WBS:	3.5.3.101
Presenter(s):	Zach El Zahab
Project Start Date:	10/01/2021
Planned Project End Date:	03/31/2024
Total Funding:	$4,999,898

Objectives: The R-GAS Advanced Gasification Pre-Pilot Demonstration for Biofuels (BioR-GAS) project will demonstrate that aviation fuel, diesel, or marine fuel can be produced at the commercial scale from biomass and sorted MSW for less than $2.75/GGE and with a reduction in GHG emissions of greater than 70% over the petroleum-derived equivalent. The proposed pathway is R-GAS entrained flow gasification followed by FTS of fuels from the resulting syngas. The project will demonstrate the feed and gasification units of this entrained flow gasification pathway at a scale of 6 TPD.

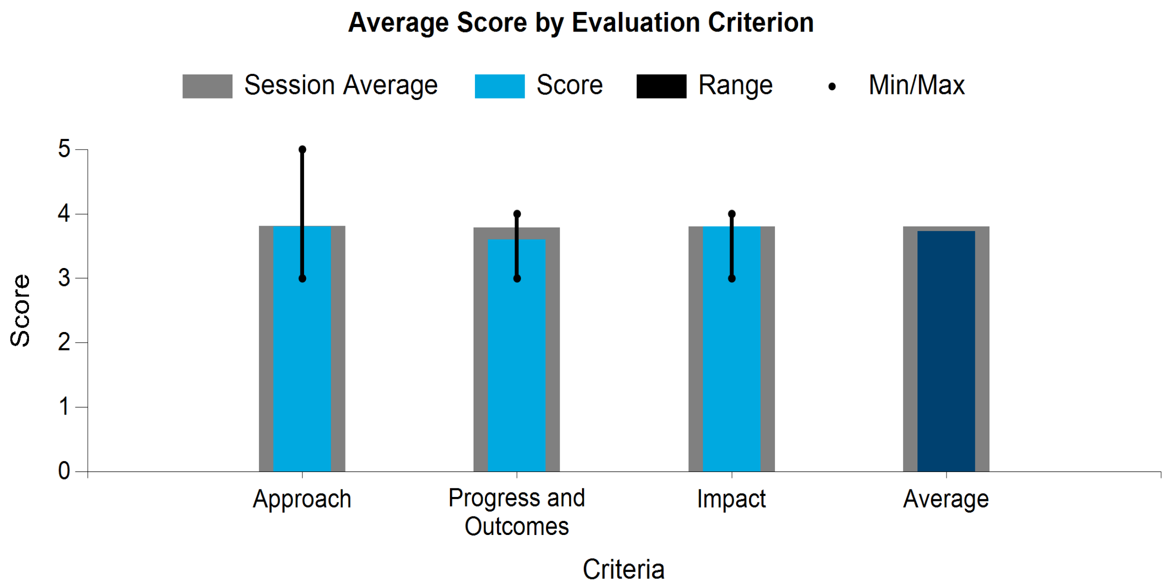
The objective of Budget Period 1 is to independently verify the proposed technical and programmatic baseline plans to successfully meet the topic area metrics. The objective of Budget Period 2 is to select a maximum of three types of biomass and/or sorted MSW, with associated preprocessing, for integrated feed system/gasification demonstration testing in Budget Period 3, from up to eight candidate feedstock/preprocessing combinations and evaluation in our flow system. The final Budget Period 3 objective is to complete a cumulative total of at least 500 hours of gasifier operation, with at least one 100-hour continuous run, and satisfy the overall project objectives by completing a commercial-scale TEA and LCA.

Methods to be employed: GTI has selected a low-risk work plan that involves an informed decision process on the economic and viable feedstock selection and preparation technologies. GTI has in-house tools, including economic models, Aspen Plus process modeling with capital cost estimation, and internal capital cost databases and GREET LCA software to perform the analysis required to make these decisions. The biomass and sorted MSW processing methods to be evaluated are torrefaction, steam explosion, and nonthermal drying and pulverization.

GTI has pilot-scale, ultra-dense phase pneumatic conveying equipment, gasification hardware, and all necessary utilities and auxiliary equipment to process and dispose of the syngas that will be leveraged for the proposed flow evaluation and gasification testing. Data acquired during these tests will be used for scale-up modeling and a detailed TEA and LCA on a commercial plant.

Benefits and outcomes: The primary benefit is the development of technology that will enable low-cost sustainable and low-environmental-impact biofuels production. Our plant cost-benefits include reduction in equipment sizing, eliminating the refractory lining, and eliminating the requirement for tar reformers because the high reactor temperatures do not allow tar formation. Our diversity and inclusion plan has identified the benefits of the program to include developing technology that will be developed and deployed in rural areas with high poverty rates, bringing well-paying jobs and clean technology to these underrepresented communities.

Major participants (collaborative projects): GTI, Ekamore, and INL.



COMMENTS

- The project has partially accomplished the objectives of Budget Period 2, which is the testing of corn stover preprocessing using three different methods: torrefaction, steam explosion, and nonthermal drying. The company still needs to characterize MSW and conduct the same testing. The company has selected torrefaction as its preferred pretreatment process for corn stover, with an energy requirement of 128 kWh/ton-out. Most of the energy (76%) goes to pelletization before torrefaction. And the pellet is ground using an additional 9.5 kWh/ton-out. My question is, why is it necessary to pelletize the corn stover? Could it just be torrefied once deconstructed? The nonthermal drying also presents a good opportunity, posing the same question again. Why is it necessary to pelletize? I hope GTI continues the research of nonthermal drying, the most promising alternative in terms of cost, and concludes the same research for MSW.

- This project has taken a sound approach to developing the R-GAS gasifier for commercial deployment by giving due attention to feedstock preprocessing, flowability, and feeding into a pressurized reactor, which has often been overlooked in past projects but is critical for ensuring reliable and consistent operations at the commercial scale. Additionally, techno-economic data were collected to inform the selection of the feedstock preparation method; however, corn stover collection, handling, contaminant removal, and storage have been not addressed. The project overview on slide 3 indicates woody biomass as a feedstock of interest, but the presentation provided information only on corn stover. Will woody biomass also be investigated? Has the team been able to modify the system/design to solve the plugging issues in the ultra-dense phase line? Because the project goal is to demonstrate the technical and economic feasibility of the R-GAS gasifier for biofuels production, TEA and LCA will be key activities for the remaining project work.

- This project is a feedstock preparation method competition for corn stover input to a flow gasification step, which generates syngas for downstream processing. The main criteria are energy input, suitability for conveying to gasification, and capital cost. A significant future criteria should also be the overall cost of producing advanced biofuels from syngas. TEA and IRR will follow in future work. The project should also consider the composition and quality of corn stover as well as other feedstocks to feed to a gasifier. Concerns about feedstock stability and variability also need to be assessed.

- This project builds on the insights gained from a previous endeavor that focused on the torrefaction of woody biomass feedstock. It is not obvious whether the current focus in this project will be woody biomass feedstock (see slide 3) or also involves corn stover (see slide 4) in addition to sorted MSW. Further, we are interested in understanding how the handling of solids, which posed a challenge in the previous project, has been addressed in this one. On slide 13, the carbon utilization is reported as approximately 37%—what does this mean? Is it the total carbon in the biomass or the carbon fraction in the biomass after torrefaction? A mass balance diagram would be useful to understand the reported utilization value. To gain a more comprehensive understanding of GTI's diverse range of projects, it would be useful to have illustrations that highlight similarities and differences between them. Additionally, it would be beneficial to learn about how project team members from various backgrounds collaborate during the execution phase and share knowledge from different projects.

- Gasification technology will play an important role in the production of biofuels from feedstocks such as MSW and lignocellulosic biomass. One critical challenge for the gasification of biomass is the production of tars and the subsequent syngas cleanup and the cost of cleanup. Using an entrained flow gasifier can overcome some challenges, but it requires very small and low-moisture particles to be effective. This project examined three methods for size reduction, measured particle size and energy requirements, and identified torrefaction and nonthermal drying as promising feedstock preparation methods. Whether these methods will scale up to a commercial level and provide similar performance will be a challenge. In real-life situations where feedstock moisture content may vary, the nonthermal drying method may not be effective. Testing in the gasification reactor will be critical in the next stage to determine if the particle size obtained is adequate. The subsequent TEA and LCA will also inform the financial viability of this project and its commercialization potential.

PI RESPONSE TO REVIEWER COMMENTS

- Response to Comment 1: Palletization is necessary because it will enable the pulverization process to result in improved particle size distribution. The nonthermal drying corn stover feeding tests to the gasifier were not reliable compared to the feeding of the torrefied corn stover. When analyzing the powder rheology results, it was found that the cohesive coefficient of the nonthermal drying corn stover is notably higher than the cohesive coefficient of the torrefied corn stover. Response to Comment 2: Within the context of the presentation, corn stover is meant to be a category of woody biomass. Yes, the team was able to implement a larger ultra-dense phase line, which resolved the feedstock plugging issues. Response to Comment 3: Within the context of the current project, the project team plans to assess the flowability of torrefied MSW in addition to torrefied corn stover. Response to Comment 4: Within the context of the presentation, corn stover is meant to be a category of woody biomass. Feeding torrefied sorted MSW will be part of this project. The 37% represents the utilization of the biomass carbon in the final biofuel product. Response to Comment 5: Agreed.

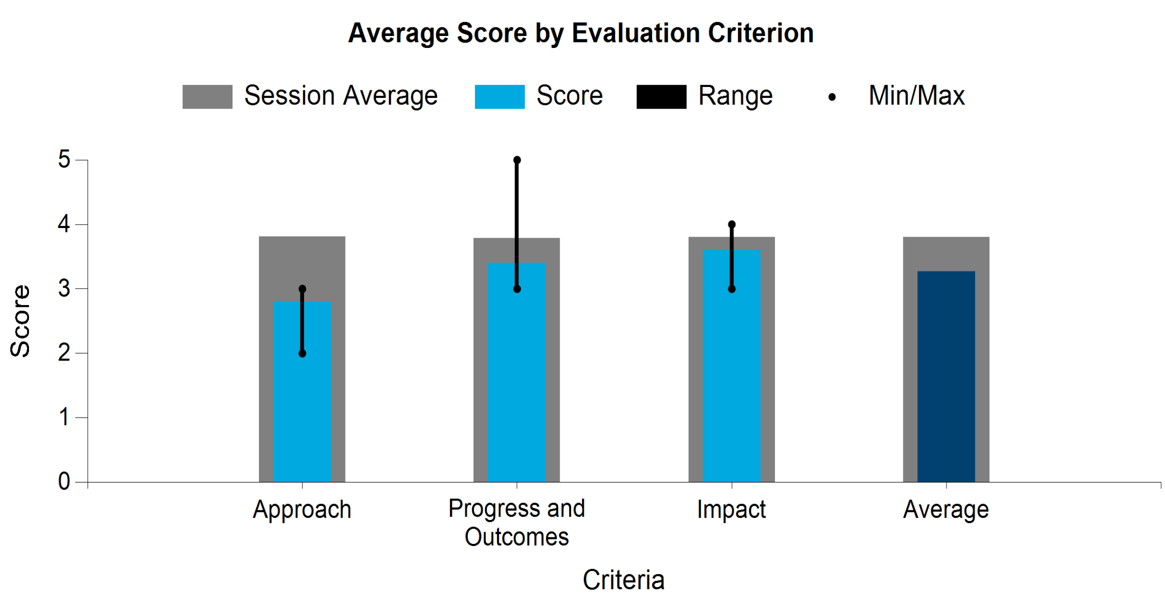
PRODUCTION OF SUSTAINABLE AVIATION FUELS FROM CORN STOVER VIA NREL'S DEACETYLATION AND MECHANICAL REFINING TECHNOLOGY (SAFFIRE)

D3MAX LLC

PROJECT DESCRIPTION

WBS:	3.5.3.103
Presenter(s):	Mark Yancey
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2022
Total Funding:	$999,976

Project SAFFiRE will demonstrate the reliable, low-GHG production of ethanol from corn stover in a fully integrated, 10-TPD pilot facility; the ethanol will be upgraded to SAF by LanzaJet at their commercial ATJ facility in Soperton, Georgia. The global aviation industry seeks to achieve net-zero GHG emissions by 2050. This will require 35 billion gallons/year of low-carbon SAF in the United States and 200 billion gallons/year globally. Multiple sources of SAF will be required to meet the U.S. and global demand for SAF. If successful, project SAFFiRE will: (1) significantly reduce the cost of SAF, allowing for wider use of SAF; (2) enable the production of billions of gallons of SAF from cellulosic ethanol; and (3) help the airline industry to decarbonize by producing SAF with >70% GHG reduction compared to Jet A. Our primary challenge is to design a pilot plant that will operate reliably, at the design rate of corn stover use, and obtain the design yield of ethanol from the stover. We are currently in Phase 1 of this two-phase project. We have completed Task 1: Verification of Application Data; passed the CD-1: Review Verification Outcome (Approve Budget Period 2); and completed Milestone M2.1.1: Design Basis Documents Complete and Milestone M2.1.2: Process Flow Diagrams Complete. We plan to complete Phase 1, Budget Period 2 by Aug. 31, 2023.



COMMENTS

- The project seems to have significant delays. No test has been done that will back up the PI's claims. Although the fermentation time is pretty good, the cellulosic ethanol cost of production required to get to $2.76/gallon seems to be a real stretch. No quantitative data, only qualitative. The project is based on

NREL's DMR technology. The presenter has not indicated if DMR has been proven at scale and has not commented on any plan for changing it from batch to continuous. The pretreatment does not produce sugars, just separates the three portions of biomass. How the company plans to prepare the corn stover for DMR treatment is unclear. How will the company handle dirt and ashes that have always been a problem? The presenter said it had been solved, but no information was given on this very important topic. I see big risks in the project. The presenter has not addressed them (bale handling, corn stover cleaning and shredding, DMR from batch to continuous, stream separations, inhibitors handling in fermentation, and impurities management).

- The project team is taking the right approach to ensure successful scale-up by piloting the conversion of a proven batch process to a continuous process; however, details on the strategies for conversion from a batch to a continuous process would be helpful to the reviewers. The integration of processes from one step to the next has often been the key challenge and risk to scaling up a project. What are the main integration challenges to be investigated for this project?

  The project team has taken lessons learned from past projects and appropriately identified reliable corn stover handling and processing as a key risk; however, the presentation did not provide a list of feedstock challenges to be investigated in this project. For example, will the project investigate the main contaminants of concern and determine how these contaminants will be detected and removed? What about long-term storage and degradation of corn stover?

  For the pilot plant, the team's mitigation strategy for wet corn stover is to identify dry sources of corn stover and arrange for the use of a bale dryer only if needed. What is the strategy for ensuring dry corn stover for a commercial plant? Will the TEA be performed for the commercial plant scenario or for the pilot plant?

- This project appears to depend on the utilization of excess infrastructure and ethanol refining capability at Generation 1 facilities to produce more ethanol, otherwise it would seem to be a substitute of corn grain feedstock for cellulosic feedstock. The opportunity to expand overall ethanol production is otherwise not elucidated. It also requires proving out at scale a biomass-to-sugar process suitable for fermentation, which so far does not appear to have been successful at a large scale. Both issues need to be addressed to ensure the economic expansion of bioethanol so that utilization by ethanol to advanced biofuels is achievable. Key learnings from unsuccessful corn stover demonstration plants to date need to be clearly incorporated into the design, and demonstration plans for piloting the front end of this process should consider those past learnings. Of particular concern is the ability to safely store biomass for long periods of time and the stability of the biomass during storage.

- Is there evidence to support the claim that the failure of past commercial cellulosic ethanol plants was largely due to their scale-ups exceeding 100:1? Although this may have been a factor, it is important to note that much of the failure was mainly attributed to issues with feedstock handling and processing as well as the degradation of feedstock that had been stored for extended periods of time. As such, any risks and mitigation approach taken by this project should include potential long-term storage risks of corn stover, such as decomposition and decay. Have appropriate measures been identified to mitigate these risks? This project aims to expand production without overburdening regional feedstock supplies and intends to use wheat straw and switchgrass as alternate feedstocks. It is vital that a comprehensive characterization be conducted to assess similarities and differences between these feedstocks and ensure their suitability for large-scale production. Additionally, it remains unclear what plans are considered for this project to move from batch operations to continuous operations of DMR as well as the integration of DMR with the D3MAX technology. Finally, the successful execution of this project will require the implementation of a variety of strategies to achieve commercial volumes of SAF, which would greatly impact and improve the industry.

- Meeting the goals of the SAF Grand Challenge will require the development of commercial cellulosic ethanol for conversion into low-carbon-intensity SAF. The lack of success of the previous commercialization of cellulosic ethanol has spurred the development of the new DMR approach by NREL (to be used in this project as a first demonstration of the integrated process). The DMR process has significant potential, and demonstration of the integrated process will be critical for future scale-up to the commercial level; however, one of the most important causes of the failure of previous cellulosic ethanol facilities is not adequately addressed here—namely, the feedstock supply and logistics. The DMR process has been demonstrated with clean feedstock of consistent quality, but this ideal situation will not be encountered in this project. It is well documented that feedstock harvesting, storage, handling, high contaminants, and inconsistent quality caused some of the most important challenges to commercialization. This project should include a clear strategy and approach to address this, particularly with a view to future scale-up where these problems will be amplified. A further aspect of this project is the lignin valorization and the potential value of this lignin ($350/ton shown in the presentation). Lignin recovery and its valorization into high-value applications have not been resolved, and it is not a foregone conclusion that this will be achieved. The specific strategy for lignin valorization is not addressed.

PI RESPONSE TO REVIEWER COMMENTS

- The SAFFiRE team thanks the reviewers for their time and thoughtful comments. Two things before we address specific reviewer comments: The DOE Project Peer Review is a public event, and our presentation, and this response to the reviewer comments, do not contain any confidential information, per DOE instructions. Many of the comments were directed at the lack of quantitative data and detailed information about our pilot project. The design of our pilot plant is confidential, including how we intend to process bales of stover and convert DMR to a continuous process. The second issue is that DOE specifically instructed us to address Phase 1 of our pilot project in our presentation, not commercial SAFFiRE plant issues. Many of the comments related to commercial operation are dead on, but, in general, we did not address commercial issues in our presentation. We will address many of those issues in this response.

  The reviewers correctly identified corn stover with high levels of sand, dirt, and ash as a key issue for our project. We plan to use a two-pass corn stover harvesting method, so we will have sand and dirt associated with the stover (external ash) as well as internal or structural ash. When we process the corn stover bales in the pilot, we will have a dirt/grit removal step as well as rock and debris removal. We have designs for both a wet and dry dirt/grit removal process. We have engaged experts at INL to assist in the design and equipment selection for our bale processing system, including the removal of external ash. Our goal is to remove 80% of the external ash to prevent excessive equipment wear. We also have a proprietary method to remove the remaining external and internal ash in the corn stover pretreatment process. This ash ends up in the DMR lignin coproduct stream. Our bale processing and pretreatment process will produce a relatively ash-free biomass for conversion to ethanol. We will harvest about 800 bales of corn stover this fall (2023) so that we can measure corn stover internal and external ash and evaluate stover degradation with various storage and bale tarping and storage methods. This stover will be stored for more than a year. Corn stover degradation in storage is caused by high moisture in the stover bales. High moisture (above 20%) and warm temperatures cause microbial growth in the stover and loss of carbohydrates. This leads to lower ethanol yields per ton of stover. The problem is that dry stover bales can absorb moisture unless the bales are stored in a covered enclosure, which currently is too expensive. Tarps can cause condensation under the tarp, and if exposed to rain, the sides of stover stacks can get wet. In Phase 2, we will conduct a cost-benefit analysis of storage costs versus stover degradation. Some degradation is inevitable. We will adjust our feedstock supply plan as necessary based on the results of our initial stover harvest and storage study. We will also explore the impacts of processing wet stover (moisture >20%) when we operate the pilot plant.

We are laser focused on feedstock supply and stover bale processing at both the pilot and commercial scales. Our project includes a subcontract with the stover supply consultant that designed the successful, but short-lived, feedstock supply system for the DuPont cellulosic ethanol plant in Nevada, Iowa. This plant was shut down by DuPont during startup when DuPont exited the cellulosic ethanol business. More than 50,000 tons of stover were collected for the DuPont project. We have also extensively studied the final technical report for POET-DSM's Project Liberty in Emmetsburg, Iowa (www.osti.gov/servlets/purl/1866610). In 2014, Project Liberty collected nearly 200,000 bone dry tons (BDT) of corn stover bales prior to the start of operations. Corn stover collection was one of Project Liberty's success stories: "Despite a concern for feasibility of biomass collection, POET-DSM proved that the large-scale commercial corn stover collection is possible and farmers are willing to participate in the process. The IBR in association with POET Bioprocessing - Emmetsburg enjoyed strong relations with surrounding corn growers. The trust and positive relations, together with new ideas for biomass collection such as POET EZ Bale and the right choice of baling equipment, contributed to the development of an efficient supply chain" (*Project Liberty Final Technical Report*, page 93) With the experience gained from DuPont's cellulosic ethanol project and Project Liberty, we are confident that we can design and implement a successful corn stover supply chain for both the SAFFiRE pilot plant (10 TPD) and planned commercial plants. Key concepts that we will implement include:

- We will capitalize on the relationships Generation 1 ethanol plants have with local corn producers to help develop our relationships with these producers that will provide corn stover for our pilot project and future commercial plants.
- We will fully compensate every party in the feedstock supply chain, including compensating corn growers for their stover. This includes nutrient replacement and profit in addition to harvesting and baling costs.
- We will provide options for corn growers: Corn growers can harvest the stover themselves or SAFFiRE will provide a custom harvester to harvest the stover.
- We will work with growers and the U.S. Department of Agriculture to establish sustainable stover harvest levels by developing guidelines to prevent wind- and water-induced soil erosion, maintain proper soil organic carbon, and sustain or improve chemical and physical properties associated with "soil growth."

Feedstock logistics for our pilot project are actually low risk because we will only process one corn stover bale per hour. If we ran the pilot 24/7 for one year, we would need only 8,000 bales of stover. A SAFFiRE plant that produces 20 million gallons/year of ethanol would require half a million bales/year. Our pilot project will demonstrate how we will harvest and transport corn stover to the pilot plant while mitigating stover degradation while in storage. Moreover, our feedstock supply chain must be scalable to very large SAFFiRE plants (i.e., to at least 20 million gallons/year of ethanol production or approximately 750 BDT/day of stover).

The major risks related to the use of corn stover to produce ethanol and our mitigation plans are summarized here:

- Corn stover moisture: High moisture in bales can lead to degradation in storage and yield loss. We will optimize storage costs to prevent high moisture versus yield loss. High-moisture bales can also cause plugging and reduced throughput in the bale processing system. We will develop storage techniques that minimize moisture migration into stored bales.
- Corn stover ash: Internal and external ash (dirt) is abrasive and can cause excessive equipment wear. We will remove external ash during bale processing. Additional external ash and internal ash

will be removed by our modifications to the DMR process. Our ash removal designs are confidential.

- Through our pilot design and pilot testing, we will develop a reliable bale processing system. Our commercial plants, however, will have redundant bale processing trains to increase plant reliability. This cost is in our CapEx estimate for commercial plants.
- Alkaline DMR pretreatment solves the issues created by dilute acid pretreatment. This issue was addressed in slide 4 of our presentation. Our Phase 1 verification test demonstrated that DMR produces a clean sugar stream with no significant fermentation inhibition. NREL has published several peer-reviewed papers on DMR that demonstrate greater than 90% sugar yield from corn stover with very low enzyme loading (approximately 10 mg of enzyme formulation per gram of biomass glucan content). These papers are based on pilot-scale DMR tests conducted by NREL and Andritz (for disc refining of the deacetylated corn stover). Our DMR, saccharification, and fermentation designs are confidential. Our Phase 1 designs will result in several patent applications, so protection of confidential information is very important until nonprovisional patent applications are filed.
- Lignin valorization: We agree with the reviewer who asked about our lignin valorization plans. We recognize that this is a risk for commercial SAFFiRE plants. We are exploring multiple near-term and potentially large markets for the SAFFiRE lignin coproduct. These plans are confidential and could not be presented at the Project Peer Review. There are small markets for lignin today, with prices significantly higher than our $350/ton in our financial proforma. We expect to have multiple letters of intent to test our lignin streams in industrial formulations by the end of Phase 1.

One reviewer commented, “This project appears to depend on the utilization of excess infrastructure and ethanol refining capability at Generation 1 facilities to produce more ethanol, otherwise it would seem to be a substitute of corn grain feedstock for cellulosic feedstock.” On the contrary, we believe that both Generation 1 and Generation 2 ethanol (along with many other sources of SAF) will be required to meet the projected U.S. demand for SAF of 35 billion gallons by 2050. We do not see Generation 2 ethanol replacing Generation 1 ethanol. Our colocation strategy takes advantage of a developed ethanol production site to reduce CapEx and OpEx costs for the Generation 2 ethanol. Expanding the utilities, if necessary, for an existing site is much cheaper than building a greenfield Generation 2 project. Staffing a Generation 2 ethanol plant at an existing ethanol plant also results in significantly fewer new employees than a greenfield project. For example, a 100 million gallons/year Generation 1 ethanol plant will have approximately 60 employees. Adding a 20-million gallons/year Generation 2 plant at that site will require approximately 20 new employees versus 80 employees for a greenfield Generation 2 plant.

There are no special integration steps required for the DMR sugars to be processed by the D3MAX technology for saccharification, fermentation, and distillation. D3MAX has commercialized these process steps at the commercial D3MAX plant at Ace Ethanol in Stanley, Wisconsin, which produces cellulosic ethanol from corn fiber. If I implied or stated that scale-ups exceeding 100:1 are largely responsible for past Generation 2 failures, I misspoke. Large scale-up ratios for past Generation 2 projects strained the ability to efficiently collect, transport, and store corn stover. All the reviewers stated this was an issue for past Generation 2 projects and an issue for our project. The past Generation 2 projects went from no or very little stover collection experience to 750 TPD or more. I think it is obvious that this is not a good strategy and did contribute to some project failures. POET-DSM’s Project Liberty seems to be the exception, with the equivalent of approximately 550 TPD of stover collected in 2014 when the Project Liberty plant began startup. POET began conducting stover harvesting trials in 2008, and this certainly contributed to their success in stover collection in 2014. SAFFiRE will begin stover collection trials in 2023. With our first commercial plant scheduled to be operational in 2028, this gives us 5 years to perfect our feedstock supply chain, just as POET did. In addition to low D3 RIN prices, Project Liberty's downfall was primarily due to the dilute acid pretreatment system. Even after a complete replacement, the pretreatment system did not operate reliably. Our TEA for Phase 1 will be done for commercial SAFFiRE plants; most likely our 200-BDT/day demonstration plant (5.6 million gallons/year of ethanol) and our target scaled plant of 750 BDT/day (20 million gallons/year of ethanol). The TEA in our proposal was done by NREL and demonstrated the potential to achieve the $2.75/GGE MFSP target for SAF based on valorizing lignin at $300/dry ton. Our project experienced a significant delay when our original cost-share partner left the project. We replaced that partner with Southwest Airlines, but finding the right partner and negotiations with Southwest resulted in a five-month delay in the project. Since the lifting of the conditional status of our award on July 21, 2022, allowing us to proceed with Budget Period 1, we are on schedule to complete Phase 1 by Aug. 31, 2023.

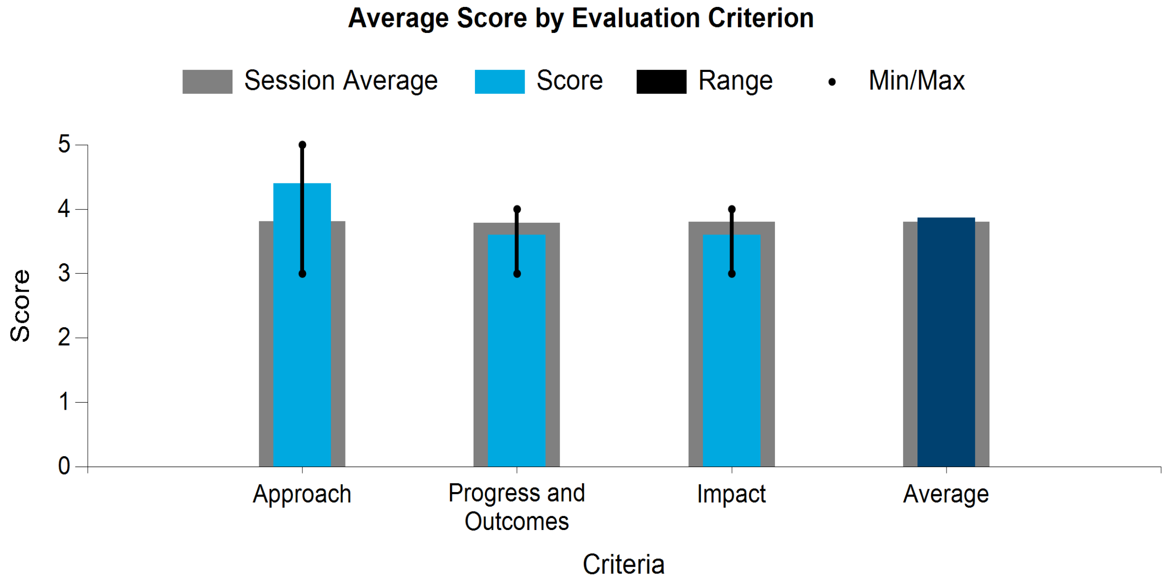
DEMONSTRATION SCALE-UP: TRIFTS BIOGAS TO RENEWABLE FUEL

T2C-Energy LLC

PROJECT DESCRIPTION

WBS:	3.5.3.105
Presenter(s):	Devin Walker
Project Start Date:	10/01/2021
Planned Project End Date:	09/30/2026
Total Funding:	$1,067,238

T2C-Energy developed and patented a proprietary process, we have trademarked TRIFTS, by which to convert biogas (or landfill gas) to liquid transportation fuels. This project seeks to scale the TRIFTS technology to enable the design and construction of a demonstration plant achieving a TRL of 7 by the end of the project. The TRIFTS process has been thoroughly tested at the pilot scale (during the past 2 years) processing a 9–24-scfm slipstream of raw biogas into drop-in renewable transport fuel. The process is capable of using both the carbon dioxide (CO_2) and methane portions of biogas and incorporates the biogenic carbon from them into the hydrocarbon backbone of the final fuel product of the process. In doing so, the technology essentially uses 100% of the biogas as a feedstock. The use of carbon dioxide is a critical cost reduction step because it represents 40%–50% of the total makeup of biogas, effectively doubling the utilizable carbon compared to technologies that remove CO_2 using expensive pretreatment processes. T2C-Energy and its project partners will implement a 1,400-scfm biogas capacity plant and produce more than 1,000,000 gallons/year of renewable cellulosic diesel. This renewable source of diesel resembles its petroleum counterpart both physically and chemically, passing ASTM D975 specifications, and it can be used in current-day engines with no engine modifications. The demonstration plant final fuel product is tunable with the ability to produce renewable fuels for the heavy trucking, aviation, and marine industries by varying process conditions within the FTS reactor with no equipment modifications required. By avoiding wax formation, we eliminate the necessity for expensive hydrotreatment, hydrocracking, and high-temperature distillation post-treatments of the FTS product. Proven performance at the demonstration scale makes future projects more financeable because technology risk is removed. Many of the inherent restrictions of waste-to-energy facilities in the United States will be solved by this project, including high capital costs, subsidy reliance, additional infrastructure costs, vehicle modifications, carbon capture, substandard financial performance, limited or specific feedstock, low fuel output, and scalability.



COMMENTS

- Same comments as in the previous project. This is a good presentation. There is a lot of good data. It has credible information and is a good business concept. It can survive with no subsidies. Well done. I have concerns about the catalyst life. The presenter said it would last at least 6 months, but no proof was provided. There is very little information about the type of catalyst, cost, and regeneration procedures. It is not clear how the company is going to deploy the technology. Will it be in large biomass-producing sites, building large facilities, or installing mobile units and running campaigns?

- Same comments as the other T2C-Energy project: This project presents an investigation of a new catalytic process that removes five unit processes and thereby simplifies the GTL process platform while also using the CO_2 to maximize production. The capture and use of waste heat and FTS water helps to create a self-sufficient process, is a best practice for sustainability, and may be key in making this process economically feasible at the commercial scale. The project seems to replicate actual commercial operation conditions by using raw biogas as a feedstock and using the FTS water in the process (with results showing a lack of impact on the process and products).

  Slide 8 shows that the TRIFTS system produces the jet fraction. A distillation system, which is a well-proven technology, would be needed. The project team has chosen to produce only renewable diesel to minimize the number of unit processes and associated costs and to keep the number of products down to one.

  The presentation indicated an independent engineer-validated MFSP of $2.91/GGE without subsidies or credits, which is commendable. At what scale was the MFSP of $2.91/GGE calculated? It would be helpful to see at what scale this process is economically feasible, given that FTS is generally economic at large scales.

  Can the catalysts (for tri-reforming and FTS) be regenerated, and if so, how many times? How long does it take to regenerate? Would the catalyst be regenerated in place, or would it be removed from the reactors and regenerated off-site? What does the waste industry scale translate to in terms of range of production volumes of the renewable diesel (in gallons or barrels)?

Additional questions for this project: Does the process water contain any toxic or hazardous components that are a concern for disposal? What treatment, if any, is required for proper disposal? What integration and scale-up challenges will the project team focus on for the demonstration project?

- In addition to the concerns previously stated about the availability and aggregation of biogas, this process depends on reformer performance, including mitigating any sensitivity to contaminants, proving catalyst life, and understanding the impact of corrosion on capital cost for installations. The Fischer-Tropsch reactor also has to perform well, and it may not be too capital intensive. The TEA is promising, but the project needs to look at the net present cost of the fuels produced, which would include the capital cost impact and comparison to other routes to advanced biofuels. Reliance on capturing RINs and other incentives may not be sustainable for the long term.

- To enhance the understanding of the project's progress, providing information on the project's execution would greatly benefit the reviewers. It would enable them to understand the various milestones achieved, the challenges encountered, and the overall progress made toward achieving the project's goals. On slide 20 displaying the impact, it is evident that the numbers used are from another project (WBS 3.5.1.201). To ensure accuracy, it is suggested to update the figures to align with the current information and performance of the project. Additionally, slide 17 depicts operators without safety glasses, hard hats, or cut-resistant gloves, which is not meeting the safety requirements. Providing safety training and mandating the use of safety gear should be implemented to avoid such instances in future. These comments are in addition to the ones provided for another project (WBS 3.5.1.201).

- This is an exciting project, and the approach is comprehensive with substantial merit. It has a clear management plan, and risks have been identified with appropriate strategies in place. The long-term impact of the technology and the project approach can be significant, but they will depend on the scale-up potential. The technology was demonstrated at a small scale and a modular approach, and it is not entirely clear how this will translate into larger-scale production. This demonstration project is therefore important, but it would be good to have a clear idea of the future potential for scale-up and the potential capacity of facilities using this technology. The future impact of the technology will rely on achieving large-scale production of renewable fuel. Although extensive industry engagement has taken place in the development and demonstration of the technology, commercialization and scale-up will need industry partners that can take it to the next level. Although the current focus is on renewable diesel, the potential production of SAF should be further explored for larger-scale facilities. It will be useful to separate and analyze the jet fraction against ASTM specifications. Note that a bifunctional catalyst will likely not meet current ASTM D7566 Annex 1 specifications for SAF.

PI RESPONSE TO REVIEWER COMMENTS

- Catalyst and process longevity studies were done during a seven-month continuous pilot study on-site at the Citrus County central landfill using the raw biogas produced at this MSW landfill. During this pilot demonstration, the plant consistently achieved methane conversions of 88%–92%, at times approaching the theoretical maximum conversions of 99%. CO_2 conversions were consistently between 30%–40%, at times reaching 50%–60% conversions. Conversion efficiencies during the long-term pilot demonstration aligned with bench-scale results as we proved the ability to maintain high conversions throughout the entirety of the demonstration. During the entirety of the demonstration, the reformer was able to produce the ideal syngas composition with an H_2:CO ratio of 1.7–2.2. This is one of the unique aspects of our tri-reforming capabilities to tune the syngas H_2:CO ratio as needed throughout the demonstration. During this pilot demonstration, the plant consistently achieved CO conversions of 50%–70%. During the pilot demonstration, we intentionally limited the CO conversion to 60%–70% because it is known that higher conversions can lead to high partial pressures of H_2O and deactivate the FTS catalyst; however, there were little to no signs of FTS catalyst deactivation throughout the entirety of the demonstration, and, in fact, we achieved our greatest conversions toward the last few weeks of the demonstration.

Typical industrial gas to liquids have lifetimes of approximately 4–5 years, based on the long-term pilot data at Citrus. We believe the catalyst used in this project would meet or exceed industrial catalyst lifetimes. The reformer and FTS catalyst used in this project were produced in-house using the T2C-Energy patented catalyst. Currently, T2C-Energy manufactures the reforming and FTS catalyst at \$20.44/kg and \$85.59/kg, respectively. Current manufacturing capabilities allow us to produce approximately 10 kg/hour of catalyst. During the pilot demonstration, regenerative studies were performed using two techniques. The first technique involved regenerating the reforming and FTS catalyst while remaining online (*in situ* regeneration). Higher steam flows are fed to the reformer to oxidize carbon deposits on the catalyst surface. This increases the H_2:CO ratio of the syngas product while also removing carbon in the form of methane. The elevated H_2:CO ratios feeding the FTS facilitate carbon removal and shift the FTS products to a lighter boiling point fraction, allowing for continuous operations as the FTS catalyst bed is regenerated. This regeneration cycle typically takes approximately 2–4 hours to complete and return to steady-state conditions. The second regeneration technique requires the feed to both reactors to be removed and replaced with a steam/air feed, effectively oxidizing coke deposits on the catalyst surface. This is done over a 1-hour period, followed by a reduction gas mix of hydrogen and nitrogen to reduce the active metal of the catalysts. This second regeneration cycle takes approximately 24–30 hours to complete and return to steady state. The second regeneration technique is more rigorous and done approximately every 2,000 hours of run time or if the catalyst activity drops 10% below the desired conversion efficiencies. Both regeneration methods are performed within the respective reactors for reforming and FTS. Spent catalyst are disposed of according to EPA solid waste regulations (K171). This includes utilization to produce new catalysts and other useful materials, recycling through recovery of metals, and treatment of the spent catalyst for safe landfill disposal.

The full-scale TRIFTS modular system is designed to accommodate biogas production facilities generating 123–1,750 scfm. This is T2C-Energy's short-term serviceable available market because most commercial technologies struggle to remain profitable within this range. Larger centralized facilities with traditional construction methodologies will be deployed once confidence within the waste-to-energy sector is gained through proven full-scale operational data at the 123–1,750-scfm biogas range. The average biogas flow rates of an anaerobic digester facility and landfill in the United States are 210 scfm and 1,380 scfm, respectively. At these biogas flow rates, using the TRIFTS process, the average size anaerobic digester would produce 230,000 gallons of renewable fuel annually, and an average size landfill would produce 1,470,000 gallons of renewable diesel fuel annually. The independent engineer-validation MFSP of \$2.91 was calculated based on a biogas feed rate of 1,500 scfm and excludes environmental attribute revenues. T2C-Energy has specifically targeted landfills producing >300 scfm of landfill gas, farm-based anaerobic digesters producing >123 scfm of biogas, and wastewater anaerobic digesters producing >275 scfm of biogas. Sites flaring the majority of their biogas and sites producing electricity from biogas with expiring electrical power purchase agreements meeting these biogas flow rate capacities are T2C-Energy's short-term market focus. "Stranded" facilities where the natural gas pipeline infrastructure does not exist are of particular interest for TRIFTS biogas-to-diesel projects. T2C-Energy has gained interest from these stranded facilities and also from developers wanting to avoid the costly gas connection/distribution fees of natural gas pipeline owners. Liquid fuel production simplifies logistics in that it can be stored and transported under ambient conditions; therefore, current freight and rail distribution channels are used, and project location becomes less relevant than RNG types of projects. TRIFTS landfill projects generate a carbon intensity score of -36 gCO_2e/MJ fuel, and, therefore, for the project to break even, the flow rate of landfill gas needed is 300 scfm. Whereas TRIFTS farm-based anaerobic digester projects have carbon intensity scores of less than -500 gCO_2e/MJ, and, therefore, for the project to break even, the flow rate of biogas needed is 123 scfm. Carbon intensity scores are based on the ANL GREET module that was completed under this project for the TRIFTS fuel production pathway.

The process water generated in the process contains 1% water soluble hydrocarbons, such as lower chain alcohols. Process water is recycled back to the process in the form of steam to the reformer, where the hydrocarbons are converted into the desired syngas product. Regarding water usage, approximately 10–30 gallons/minute of water are needed within the cooling tower unit due to evaporative losses.

Scale-up challenges addressed during this demonstration project are related to the integration of waste heat streams associated with the reformer furnace to produce green electricity, continuous quality control of diesel and jet fractions, unsteady-state startup conditions and regeneration cycles, proving an annual on-stream factor of >93%, reduction of OpEx costs, optimizing preventative maintenance cycles, long-term removal of contaminants, prevention of contaminant accumulation, producing long-term operational data at full scale, effective operational management at full scale, and proving the ability to produce more than 1 MM gallons/year of renewable diesel meeting an MFSP of <$2.50/GGE.

In general, the project execution strategy will follow this framework: DOE award notification; planning and mobilization; formal kickoff meeting with DOE, engineering contractor, and applicable third parties; global document orientation and review; process optimization studies; update material and energy balance; long-lead identification/sizing/sourcing; hazard and operability study; basic engineering reviews; issue for design (completion of engineering); initial 3D modeling/isometrics/physical design; development model reviews; vendor identification and initial procurement activities; final 3D modeling/physical design (inside battery limits and outside battery limits); development model reviews; vendor data reviews; detailed engineering reviews; drawing production/physical plans; model freeze; preconstruction and commissioning reviews; issue for construction; fabrication and factory acceptance testing; installation and commissioning; and plant handover and operations.

T2C-Energy will review expectations, global documents, design criteria, budget, schedule status, limitations, design standards, templates, specifications, lessons learned, project history, deliverables, and specific responsibilities of the team members of each organization. At the outset of the project, the primary focus of the execution team will be full definition of all global documents for the demonstration project. These documents define the engineering decisions that will be reflected in the procured materials and physical design. Any changes to these documents later in the project will directly impact the quality, cost, and schedule of the overall effort. These documents include but are not limited to: design basis, process flow diagrams, general arrangements/plot plans, piping and instrumentation diagrams, one-line diagrams, and communication block diagrams/control architecture. Internal and external reviews will be conducted by T2C-Energy, the engineering contractor, and appropriate project stakeholders. Initial efforts are focused on ensuring that all engineering definitions, input, and decisions are properly captured and vetted up front with all project team members and stakeholders. This will ensure that the procurement and physical design can effectively proceed with the issued for design (IFD) milestone. Safety reviews, the hazard and operability study, and process hazard analyses will create action items that will be incorporated/addressed in updated designs. Additional reviews on global documents will include construction representatives of T2C-Energy, the engineering contractor, vendors, and other project stakeholders. The main objective of these additional reviews is to have all required personnel contribute to the design up front, such that decisions on paper at the IFD milestone represent a thorough, vetted, accurate consensus from the project team. This will minimize and effectively manage the impact of design changes downstream, during procurement and physical design. The global documents will undergo a complete yellow-line check prior to IFD. Although not expected to be true construction quality at the IFD milestone, these deliverables are expected to contain all required information for procurement and physical design to proceed through project completion without any further development. Any gaps found on the global documents that would prevent procurement or the physical design from proceeding will be addressed or approved to be placed on hold due to circumstances outside the direct control of the project team. A master document register will be generated capturing all tasks, documents, drawings, and activities associated with the statement of project objectives. The master document register will be used to support the earned value productivity tracking at the deliverable level throughout the life of the project. The work breakdown structure is the basis for the schedule and is used to link the task timelines and key milestones to ensure that the target delivery dates are achieved with the allocated resources. The Gannt chart will assist in planning the resource allocation and tracking the work progress. The project schedule is managed via conventional critical path method. Project reviews are scheduled to ensure efficient execution of the project deliverables. Internal and external stakeholder reviews will ensure that all input is captured and a set of frozen IFD deliverables are released. The IFD documents serve as the basis for the specification and procurement of components and the physical design. Internal and external reviews conducted on 3D models, isometrics, and structures ensure that all input necessary to obtain a static, stable design is in hand prior to the issue for construction deliverables. All drawings and models are reviewed to ensure regulatory compliance and to meet expectations defined in the initial project reviews prior to the release of a construction-quality bid package.

T2C-Energy's management philosophy is to provide an experienced, quality team with management procedures and systems emphasizing an efficient team concept. The establishment of strong, internal coordination of efforts is key to success. Generally, this coordination is accomplished through clear project organization, where responsibilities are defined and understood. Direction is provided through internal meetings and control lists, with action items assigned with due dates, defined procedures/criteria for engineering and drafting reviews, performance assessment systems, checklist verifications, and project audits. This type of personnel management highlights potential problems before they occur, ensures adequate interaction between disciplines, and provides the key personnel with a basic knowledge of all facets of the project. T2C-Energy involves all levels of project personnel in work discussions to establish specific actions, set delivery dates, and challenge/motivate people to do a quality job, which instills a positive team spirit. T2C-Energy will initially staff this project with current employees and obtain third-party contract support for engineering. T2C-Energy has highly skilled engineers; project control specialists; environment, health, and safety specialists; operations and maintenance staff; and administrative personnel ready to mobilize for this effort. Work performed by the assigned resources is coordinated by the project manager and project engineer, with additional supervision of resources by their respective supervisors. The overall management of a project is the direct responsibility of the project manager (PI). The project manager is ultimately responsible for the successful coordination and execution of the overall project. To help ensure that the project manager has all the necessary support from the organization to achieve this goal, T2C-Energy will assemble the following project leadership team to assist the project manager throughout the duration of the project effort. The project leadership team functionally reports to the project manager. The project engineer; process engineering lead; environment, health, and safety lead; project controller; operations manager, and additional support personnel and specialists will be added to the team as required through the life of the project. The project manager is responsible for the following: overall coordination and project work scope; overall management of engineering, procurement, and construction and third-party contractors; management of stakeholder relationships; on-schedule submission of deliverables; regulatory compliance; design compliance; technical accuracy and standards compliance; compliance with T2C-Energy standards and procedures; overall project quality; resource planning; project execution plans; change management (supported by project leads); status reports; interface management; project reviews and audits; recordkeeping of all documents and drawings (support from projects); day-to-day coordination (inter- and intra-discipline checks); and quality control. The project engineer and engineering lead is responsible for: discipline-specific scope, budget, and schedule; compliance, technical design criteria, and internal standards; defining work scope interfaces across inside battery limits and outside battery limits; coordination with engineering contractor and project stakeholders; deliverable production; quality control checks and signoffs; interface management with other disciplines; technical accuracy and standard compliance on deliverables; inter- and intra-discipline checks; resource forecasting and planning; vendor management and data collection; scheduling internal model reviews; drawing reviews, checks, and signoffs; and compliance with design criteria. The environment, health, and safety lead is responsible for: environmental compliance; federal, state, and local regulatory compliance; construction and operation permit approval and compliance; compliance with internal and external environment, health, and safety policies; safe execution of the project; LCA reviews and development; and renewable fuel regulatory compliance. The project controller is responsible for: recordkeeping of all documents and drawings; project budgeting and accounting; resource allocation; quality control; coordination with the engineering contractor and project stakeholders; and administrative management. The operations manager is responsible for: day-to-day operations; supervision of all operations and maintenance staff; coordination with contractors; participating in project reviews; plant layout development; supervising the T2C-Energy commissioning team; vendor coordination; maintenance planning and scheduling; and meeting plant performance metrics. T2C-Energy uses project planning and control systems to assist in planning, monitoring, and managing all execution activities. Focus is placed on defining the cost and time frame for completion of the statement of objectives. The deliverables listed in the statement of project objectives detail all the documents, drawings, tasks, activities, etc., required to complete the work scope. Earned value productivity is established by developing a master document register and standard rules of credit during the initial efforts. Man-hours and costs are established at the deliverable level. Standard rules of credit provide objective, quantifiable means of measuring completion status per deliverable as the project progresses. Using project management software, the entire project is planned and tracked. Critical path analysis, planned versus earned graphs, cost curves, schedule performance index, cost performance index, variance reports, completion forecasts, and resource-leveled schedules are provided as required to effectively monitor and manage the work being performed.

LANDFILL OFF-GAS TO ULTRA-LOW-CARBON-INTENSITY SAF (LOTUS)

SkyNRG Americas Inc.

PROJECT DESCRIPTION

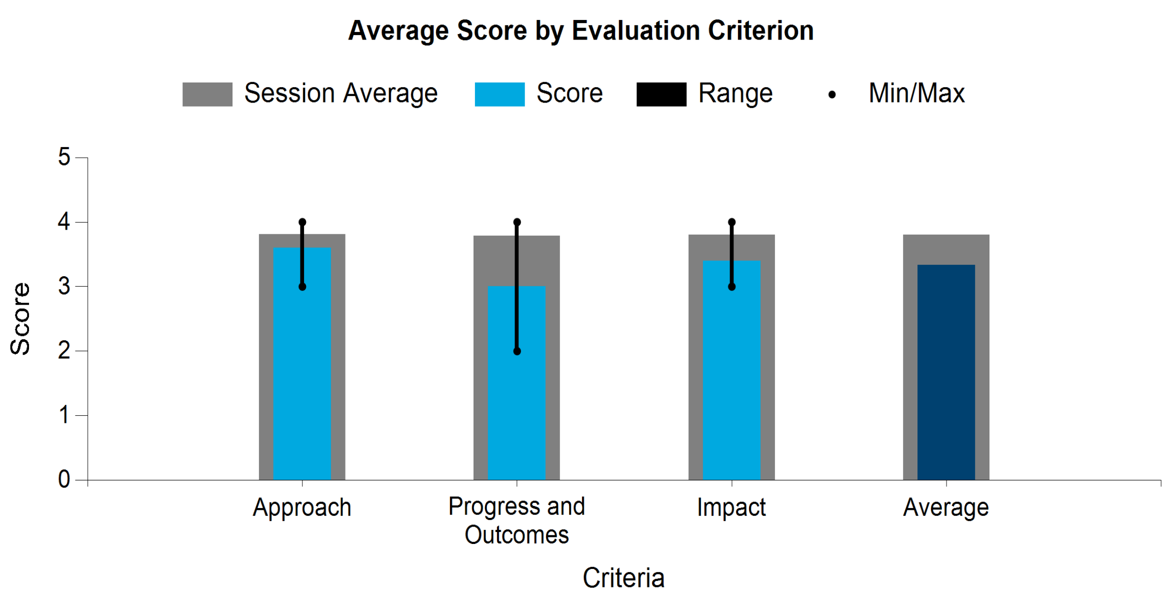
WBS:	3.5.3.107
Presenter(s):	Brian James
Project Start Date:	10/01/2021
Planned Project End Date:	03/31/2023
Total Funding:	$2,000,000

Major partners: SkyNRG Americas, LanzaTech, Linde, LanzaJet, Energy Vision, PNNL, and ANL.

Project objectives: Construction and operation of the first RNG-to-SAF commercial demonstration facility.

Project description: SkyNRG Americas, the project developer, and its commercialization partner, LanzaTech, will design, engineer, build, and operate a unique demonstration-scale facility that will convert RNG into SAF. In Phase 1, the team will verify the TRL and complete a −15/+30 cost estimate. In Phase 2, the team will continue engineering and site construction, leading to a 5-million-gallon/year nameplate capacity demonstration site for RNG to SAF.

Project impacts: The aviation sector is challenged by commitments to reduce GHG emissions in the face of continued dramatic growth. The goals can only be met by SAF. The United States uses 26 billion gallons of jet fuel but produces less than 4 million gallons of SAF. Project LOTUS will provide a new supply chain for producing SAF while reducing methane emissions and improving air quality that is applicable to the entire nation due to the wide distribution of RNG production facilities across the United States. The resultant fuel is high quality, low soot forming, and sustainably derived, reducing GHG emissions by up to 110%. DOE funding will accelerate the commercial rollout of SAF production from RNG by reducing the technical and financial risks for future integrated commercial plants.



COMMENTS

- The project sponsor was flexible in changing the feedstock to allow for better project economics. The technology components were independently tested before the project started. The project has demonstrated the production of ethanol, not SAF.

The economics of the project are based on heavy subsidies. I do not think that this is the right long-term business model. RNG is a very expensive feedstock. Although the presenter said that RNG would be cheaper in the future, he can get long-term purchase contracts at much lower prices than today. This is to be seen. It is very unlikely that the project will be economically feasible. The presenter says that the conversion of ethanol to SAF is not part of the project. I think that the project needs to prove that with the ethanol produced, it is possible to produce SAF. It is not enough to produce ethanol.

The cost of a first-of-a-kind plant producing 30 million gallons/year of SAF is estimated at $500–$700 million. This level of investment is very unlikely to be assumed by any private investor. I think it is difficult to justify a sustainable financial return on this project.

- Technically, the project presents a well-planned approach for the scale-up of the process technology platform and pathway from RNG to SAF and renewable diesel, with a high selectivity (90%) for SAF.

  The presentation indicates that the Linde hot oxygen burner partial oxidation reformer can "easily tolerate variation in feedstock composition and flow rate." Can the hot oxygen burner respond in real time to variations to feedstock composition?

  The economics seems challenging using RNG as a feedstock. Currently, RNG enjoys high incentives when sold as a transportation fuel. As such, procurement of RNG as a feedstock for SAF would be expensive and currently seems uneconomic. SkyNRG indicates that RNG will become more affordable as incentives decline and more RNG production facilities come online. What is SkyNRG's forecast for when RNG will become an economic feedstock for the LOTUS ATJ process platform?

  Will the results of the BETO scale-up project provide sufficient demonstration to reduce the technical risk for landfill owners? If not, what else is needed for landfill owners to accept the LOTUS process platform?

- This project depends on a number of critical factors for large-scale impact, two of which are the availability of RNG at large enough centralized locations to reach economy of scale and continuing RINs to offset costs. The overall project also depends on multiple not yet fully proven steps, so an assessment of the variability of the RNG amount and composition and that effect on each subsequent step to liquid fuel production would be advisable to understand the potential for large-scale impact and economic success. In addition, it might be useful to compare the value creation with this approach to the alternative uses of RNG in the current routes to market. The value of RINs long term seems uncertain, and, in addition, understanding the costs as they relate to project location (oxygen availability, for example) and the energy integration opportunity is critical. CapEx and OpEx for a fully integrated facility at scale are a concern, and their effect on IRR should be evaluated. Overall, the concept appears worthy of development—at least to the point of prove out at a semicommercial scale.

- To ensure the success of this project, it is imperative to include an assessment of the availability of the required quantities of RNG. Additionally, the impact of using RNG in the form of compressed natural gas for heavy-duty vehicles must be carefully evaluated. When selecting feedstock sources, it is essential to consider the physical and chemical characteristics of RNG from various sources as well as the requirements for purification. Further, the potential for competing uses of RNG, such as replacing natural gas for electricity generation, must be considered when estimating the costs of RNG within the TEA. Ultimately, the successful outcome of this project will greatly contribute to the increased commercial availability of SAF, and thus it is vital to carefully consider these key factors throughout the process.

- This project proposes to produce SAF through multiple steps using RNG to make syngas to be fermented into ethanol using LanzaTech's technology, after which the ethanol will be used to produce SAF through the ATJ process. The production of syngas through partial oxidation is fully commercial, whereas the syngas fermentation technology has been operating at a commercial scale but using industrial off-gases. The scope of the project was changed from using biogas to using RNG because the production of fuels using CO_2 is not currently EPA-approved, and therefore RINs could not be generated. This seems to be an inefficient approach because biogas must first be upgraded into RNG, with carbon lost in the process. RNG has multiple other efficient applications, and competition with these applications may impact the availability and price of RNG. The syngas fermentation step and yields of ethanol should be provided. The solubility of CO and H_2 and gas transfer limitations will impact yield in this step and will impact the overall commercial viability of the process. TEA and LCA will be carried out in the next phase, and results will be critical.

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