

## Office of ENERGY EFFICIENCY & RENEWABLE ENERGY



# 2019 PROJECT PEER REVIEW

U.S. DEPARTMENT OF ENERGY BIOENERGY TECHNOLOGIES OFFICE



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## INTRODUCTORY LETTER

Dear Colleagues,

In the spring and summer of 2019, the U.S. Department of Energy's (DOE's) Office of Energy Efficiency and Renewable Energy's (EERE's) Bioenergy Technologies Office (BETO) continued its long-standing commitment to transparency by implementing the ninth biennial external review since 2005 of its research, development, and demonstration portfolio. Conducted in accordance with EERE peer review guidelines, the review was designed to provide an external assessment of the projects in BETO's portfolio and collect external stakeholder recommendations on BETO's overall scope, focus, and strategic direction. Results from the peer review process are used to inform programmatic decision-making; enhance active project management; and modify, expand, or discontinue existing projects.

This review process is critical to the success of our mission: to develop technologies that convert domestic biomass and waste resources into fuels, products, and power; to enable economic growth and innovation in affordable energy and chemicals production; and to support the growth of the domestic bioeconomy. The 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 an advanced bioeconomy.

The 2019 Peer Review comprised three levels of review: (1) individual projects were scored on the basis of technical approach, relevance, progress, and future direction; (2) each technology area portfolio was evaluated for overall potential impact, innovation, synergies, focus, appropriate level in technology development pipeline, and recommendations; and (3) the structure and overall strategic direction of BETO was reviewed by an external steering committee. This report contains the results of each level of review and the inputs of approximately 400 participants in the peer review process, including principal investigators, reviewers, steering committee members, and BETO's staff and contractors.

BETO thanks all the reviewers and members of the steering committee who participated in this review, as well as the nearly 600 attendees of the Project Peer Review in March 2019. BETO appreciates the valuable insights and contributions provided throughout the peer review process. 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 and a sustainable bioeconomy.

Tonton L. Male

Jonathan L. Male Director, Bioenergy Technologies Office Office of Energy Efficiency and Renewable Energy U.S. Department of Energy

## **EXECUTIVE SUMMARY**

BETO manages a diverse portfolio of technologies covering the full spectrum of bioenergy production, from the feedstock source to end use, as illustrated in Figure 1. BETO systematically prioritizes research and development (R&D) into technology opportunities across a range of emerging scientific breakthroughs and technology-readiness levels. This approach supports a diverse R&D portfolio while developing the most promising and widely applicable technologies, testing technologies as integrated processes, and verifying integrated processes at the engineering scale. These technologies will use a broad variety of currently underused domestic biomass and waste resources to produce increasing volumes of biofuels, bioproducts, and biopower.



#### Figure 1. Biomass-to-bioenergy supply chain.

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. BETO completed these reviews in 2019. This report includes the results of both the Project Peer Review meeting held in March 2019 and the Program Management Review meeting held in July 2019.

## ACRONYMS AND ABBREVIATIONS

| A&S             | Analysis and Sustainability                                  |
|-----------------|--|
| AAS             | Advanced Algal Systems                                       |
| ABBA            | Advanced Biofuels and Bioproducts with AVAP                  |
| ABPDU           | Advanced Biofuels and Bioproducts Process Development Unit   |
| ACED            | Atmospheric CO <sub>2</sub> Enrichment and Delivery          |
| ACN             | acrylonitrile  |
| ACSC            | Advanced Catalyst Synthesis and Characterization             |
| AD              | anerobic digestion   |
| ADC             | (TRI) Advanced Development Center                            |
| ADO             | Advanced Development and Optimization                        |
| AGNPS           | Agricultural Non-Point Source Pollution Model                |
| ANL             | Argonne National Laboratory                                  |
| AOP             | annual operating plan  |
| ARS             | Agricultural Research Service                                |
| ASEC            | Affordable and Sustainable Energy Crops                      |
| AST             | Allegheny Science & Technology                               |
| ATEC            | Algae Technology Educational Consortium                      |
| ATJ             | alcohol-to-jet   |
| ATM             | Assessment of Likely Technology Maturation                   |
| ATP3            | Algae Test Bed Public-Private Partnership                    |
| ATS             | algal turf scrubber  |
| AVAP            | American Value-Added Pulping                                 |
| AWARE-US        | Available Water Remaining for the United States              |
| AzCATI          | Arizona Center for Algae Technology and Innovation           |
| BAT             | Biomass Assessment Tool                                      |
| BDO             | butanediol   |
| BECCS           | bioenergy with carbon capture and sequestration              |
| BETO            | Bioenergy Technologies Office                                |
| BFI             | biofuel intermediate   |
| BFL             | Bioenergy Feedstock Library                                  |
| BFNUF           | Biomass Feedstock National User Facility                     |
| BIC             | Biofuels Information Center                                  |
| Bio-BDO         | bio-based 1,4-butanediol                                     |
| BioSep          | Bioprocessing Separations Consortium                         |
| BioSTAR         | Bioenergy Sustainability Tradeoffs Assessment Resource       |
| BIP             | Biofuels Infrastructure Partnership                          |
| BMP             | best management practice                                     |
| BODIPY          | boron-dipyrromethene   |
| BR&D            | Biomass Research and Development Board                       |
| BSCR            | biomass supply chain risk                                    |
| BSI             | boosted spark-ignition                                       |
| BSM             | Biomass Scenario Model                                       |
| BTD             | Bioproduct Transition Dynamics                               |
|                 |  |
| BTS<br>Cal Daly | biomass-to-syngas<br>California Palutaalmia Stata University |
| Cal Poly        | California Polytechnic State University                      |
| CAP             | combined algal processing                                    |
| CapEx           | capital expenditure  |
| Cas             | CRISPR-associated  |
| CCPC            | Consortium for Computational Physics and Chemistry           |
| CFD             | computational fluid dynamics                                 |
| CFP             | catalytic fast pyrolysis                                     |

| ChemCatBio      | Chemical Catalysis for Bioenergy Consortium                                  |
|-----------------|--|
| CO <sub>2</sub> | carbon dioxide   |
| CORSIA          | Carbon Offsetting and Reduction Scheme for International Aviation            |
| CRADA           | cooperative research-and-development agreement                               |
| CRISPR          | Clustered Regularly Interspaced Short Palindromic Repeats                    |
| CTT             | cubical triaxial tester  |
| DBTL            | Design-Build-Test-Learn  |
| DEM             | discrete element method  |
| DFA             | directed funding award   |
| DFO             | directed funding opportunity   |
| DHSVM           | Distributed Hydrology Soil Vegetation Model                                  |
| DIC             | dissolved inorganic carbon   |
| DISCOVR         | Development of Integrated Screening, Cultivar Optimization, and Verification |
| DISCOVIC        | Research   |
| DMR             | deacetylation and mechanical refining  |
| DOD             | U.S. Department of Defense   |
| DOE             | U.S. Department of Energy  |
| DOM             | dissolved organic matter   |
| EERE            | Office of Energy Efficiency and Renewable Energy                             |
| EISA            | Energy Independence and Security Act of 2007                                 |
| EMDS            | Ecosystem Management Decision Support  |
| EOS             | engineering of catalyst scale-up   |
| EPA             |  |
| EV              | U.S. Environmental Protection Agency<br>electric vehicle                     |
| FCC             |  |
| FCIC            | fluid catalytic cracking<br>Feedstock-Conversion Interface Consortium        |
| FCTO            |  |
|                 | Fuel Cell Technologies Office<br>finite element method                       |
| FEM<br>FOA      |  |
| FOG             | funding opportunity announcement   |
| FPEAM           | fats, oils, grease<br>Feedstock Production Emissions to Air Model            |
|                 |  |
| FSL             | Feedstock Supply and Logistics   |
| FY              | Fiscal Year  |
| GAI             | Global Algae Innovations, Inc.   |
| GARDN           | Green Aviation Research and Development Network                              |
| GBEP            | Global Bioenergy Partnership   |
| GCAM            | Global Change Assessment Model   |
| GDP             | gross domestic produce   |
| GGE             | gallons gasoline equivalent  |
| GHG             | greenhouse gas   |
| GMO             | genetically modified organism  |
| GREET           | Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation      |
| H <sub>2</sub>  | hydrogen   |
| HiSCI           | High-throughput Screening of Cell-to-cell Interactions                       |
| HPF             | high-performance fuel  |
| HTL             | hydrothermal liquefaction  |
| HTP             | hydrothermal processing  |
| HVO             | heavy fuel oil   |
| HYPOWERS        | Hydrothermal Processing of WastewatER Solids                                 |
| IAB             | industry advisory board  |
| IBR             | integrated biorefinery   |
| IDL             | indirect liquefaction  |
| IEA             | International Energy Agency  |

| ILM           | Integrated Landscape Management                         |
|---------------|---|
| ILUC          | indirect land-use change                                |
| INL           | Idaho National Laboratory                               |
| IP            | intellectual property                                   |
| IPCC          | Intergovernmental Panel on Climate Change               |
| JEDI          | Jobs and Economic Development Impact                    |
| JudO          | Jet fUels blenD Optimizer                               |
| KDF           | Knowledge Discovery Framework                           |
| LAP           | laboratory analytical procedures                        |
| LBNL          | Lawrence Berkeley National Laboratory                   |
| LCA           | life cycle assessment                                   |
| LEAF          | Landscape Environmental Assessment Framework            |
|               |   |
| LEAPS         | Laboratory Environmental Algae Pond Simulator           |
| LLNL          | Lawrence Livermore National Laboratory                  |
| LUC           | land-use change   |
| MAGIC         | Marine Algae Industrialization Consortium               |
| MBE           | MicroBio Engineering Inc                                |
| MBSP          | minimum biomass selling price                           |
| MCCI          | mixing-controlled compression ignition                  |
| MFSP          | minimum fuel selling price                              |
| MIBR          | multi-stream integrated biorefinery                     |
| MMSI          | multi-mode spark ignition                               |
| MOOC          | Massive Open Online Courses                             |
| MSW           | municipal solid waste                                   |
| MW            | megawatt  |
| MYP           | Multi-Year Plan   |
| NAABB         | National Alliance for Advanced Biofuels and Bioproducts |
| NEPA          | National Environmental Policy Act                       |
| NIR           | near-infrared   |
| NREL          | National Renewable Energy Laboratory                    |
| OEM           | original equipment manufacturer                         |
| OpEx          | operating expenditures                                  |
| ORNL          | Oak Ridge National Laboratory                           |
| OSU           | The Ohio State University                               |
| P5CS          | <i>Pyrroline-5-carboxylate synthase</i>                 |
| PABP          | performance-advantaged bioproducts                      |
| PACE          | Producing Algae for Coproducts and Energy               |
| PBR           | photobioreactor   |
| PCR           | polymerase chain reaction                               |
| PDU           | Process Development Unit                                |
| PI            | principal investigator                                  |
| PNNL          | Pacific Northwest National Laboratory                   |
| R&D           | research and development                                |
|               | •   |
| RACER<br>RAFT | Rewiring Algal Carbon Energetics                        |
|               | Regional Algal Feedstock Testbed                        |
| RCFP          | reactive catalytic fast pyrolysis                       |
| RFS           | renewable fuels standard                                |
| RRB           | Red Rock Biofuels                                       |
| RUSLE2        | Revised Universal Soil Loss Equation 2                  |
| SAF           | sustainable aviation fuel                               |
| SCP           | single-cell protein                                     |
| SI            | spark-ignition  |
| SNF           | sucrose nonfermenting                                   |
|               |   |

| SNRKsucrose nonfermenting-related kinaseSOFASTStreamlined Optimization of Filamentous Arthrospira/Spirulina TraitsSOPOstatement of project objectivesSOTstate of technologySRWCshort-rotation woody cropSTEMStochastic Techno-Economic ModelSWATSoil and Water Assessment ToolTABBTargeted Algal Biofuels and BioproductsTCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown StructureWDLWhite Dog Labs Inc. | SNL    | Sandia National Laboratories   |
|--|--------|--|
| SOPOstatement of project objectivesSOTstate of technologySRWCshort-rotation woody cropSTEMStochastic Techno-Economic ModelSWATSoil and Water Assessment ToolTABBTargeted Algal Biofuels and BioproductsTCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | SNRK   | sucrose nonfermenting-related kinase                                 |
| SOTstate of technologySRWCshort-rotation woody cropSTEMStochastic Techno-Economic ModelSWATSoil and Water Assessment ToolTABBTargeted Algal Biofuels and BioproductsTCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | SOFAST | Streamlined Optimization of Filamentous Arthrospira/Spirulina Traits |
| SRWCshort-rotation woody cropSTEMStochastic Techno-Economic ModelSWATSoil and Water Assessment ToolTABBTargeted Algal Biofuels and BioproductsTCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | SOPO   | statement of project objectives                                      |
| STEMStochastic Techno-Economic ModelSWATSoil and Water Assessment ToolTABBTargeted Algal Biofuels and BioproductsTCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | SOT    | state of technology  |
| SWATSoil and Water Assessment ToolTABBTargeted Algal Biofuels and BioproductsTCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | SRWC   | short-rotation woody crop  |
| TABBTargeted Algal Biofuels and BioproductsTCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | STEM   | Stochastic Techno-Economic Model                                     |
| TCPDUThermal and Catalytic Process Development UnitTEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | SWAT   | Soil and Water Assessment Tool                                       |
| TEAtechno-economic analysisTEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | TABB   | Targeted Algal Biofuels and Bioproducts                              |
| TEGthermoelectric generatorTERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | TCPDU  | Thermal and Catalytic Process Development Unit                       |
| TERAToxic Substance Control Act Environmenmental Release ApplicationTRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | TEA    | techno-economic analysis   |
| TRIThermoChem Recovery International, Inc.TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | TEG    | thermoelectric generator   |
| TRLtechnology readiness levelTSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | TERA   | Toxic Substance Control Act Environmenmental Release Application     |
| TSFthree-stone fireUAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | TRI    | ThermoChem Recovery International, Inc.                              |
| UAVunmanned aerial vehicleUSDAU.S. Department of AgricultureUSEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | TRL    | technology readiness level   |
| USDAU.S. Department of AgricultureUSEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | TSF    | three-stone fire   |
| USEEIOU.S. Environmentally Extended Input-OutputUSFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | UAV    | unmanned aerial vehicle  |
| USFSU.S. Forest ServiceUSVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | USDA   | U.S. Department of Agriculture                                       |
| USVunmanned service vehicleVFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | USEEIO | U.S. Environmentally Extended Input-Output                           |
| VFAvolatile fatty acidsWATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure  | USFS   | U.S. Forest Service  |
| WATERWater Analysis Tool for Energy ResourcesWBSWork Breakdown Structure   | USV    | unmanned service vehicle   |
| WBS Work Breakdown Structure   | VFA    | volatile fatty acids   |
|  | WATER  | Water Analysis Tool for Energy Resources                             |
| WDL White Dog Labs Inc.  | WBS    | Work Breakdown Structure   |
|  | WDL    | White Dog Labs Inc.  |

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## **INTRODUCTION**

BETO research strategy is captured in two documents: the *Strategic Plan for a Thriving and Sustainable Bioeconomy* (Strategic Plan) and the BETO *Multi-Year Plan* (MYP). The Strategic Plan was released in 2016. The MYP was last published in 2016; it was recently updated and will be released again soon. Both documents can be found on the BETO website and are referenced throughout this report. The following section summarizes the Strategic Plan and MYP and introduces the vision, mission, goals, and structure of BETO. This is followed by an overview of the peer review process and format of this report.

#### STRATEGIC PLAN OVERVIEW

In 2016, BETO published the Strategic Plan reflecting the transformation and the advancements made in the bioenergy industry since the 1990s. This plan expanded BETO's mission beyond the cellulosic ethanol market to include renewable drop-in fuels (including diesel and jet fuels), bio-based chemicals, and bioproducts. The new strategy also emphasized the need to address environmental concerns associated with increased agricultural demand, including water and soil quality. The Strategic Plan was intended as an operational guide for managing and coordinating activities among technology areas. The Strategic Plan is BETO's blueprint to tackling the challenges and opportunities associated with building a sustainable U.S. bioeconomy. Although the BETO vision is set for 2040, it is important that processes are in place to verify progress, understand competing technologies, and periodically revisit the strategy.

BETO's Strategic Plan encompasses programmatic-level guidance and sets the foundation as the driver for the MYPs, annual operating plans (AOPs), and technology road maps. The MYP identifies R&D pathways and performance goals for the next 5 years and outlines how BETO plans to meet its mission and vision. AOPs are prepared and reviewed annually prior to each fiscal year for all programs within DOE's EERE. National laboratory AOPs and the project management plans from competitive funding opportunity announcements (FOAs) describe implementation plans to achieve strategic and performance goals.

The main components of BETO's Strategic Plan include key opportunity areas, a strategic goal for each key opportunity area, and strategies for accomplishing each strategic goal. These components are intended as crosscutting programmatic-level guidance and should be used to determine how to adapt and align BETO activities and project portfolios to best meet its objectives and carry out its mission in a continually changing environment.

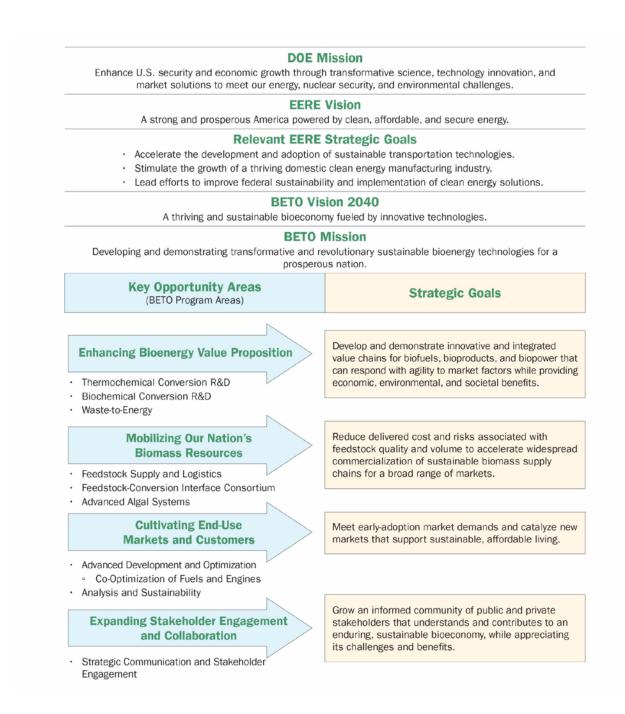
Figure 2 summarizes BETO's Strategic Plan. Key opportunities reflect the best paths available to support BETO's mission, and each opportunity is aligned with a strategic goal that will be achieved by implementing a range of strategies. Progress on these activities will be measured against success indicators or milestones.

BETO conducts early-stage R&D and experimental development activities through an integrated supply chain approach addressing supply (feedstocks), conversion, distribution, and end use. Several activities underscore the R&D conducted by BETO—such as sustainability and strategic analysis—that enable the development and dissemination of knowledge and tools related to the economic, environmental, and social dimensions of advanced bioenergy.

Although cellulosic biofuel production is the primary focus, BETO supports the production of chemical intermediates that are traditionally petroleum-derived but can be coproduced from biomass. These intermediates are converted into high-value bioproducts, including bioplastics, bio-based chemicals, lubricants, solvents, cosmetics, and food ingredients, such as algal oil—all of which have places in future commercial markets. These also seek to maximize the value of fuels and coproducts produced within an integrated biorefinery based on this successful model in petroleum refineries.

BETO's Strategic Plan is aligned with the goals of the Biomass Research and Development (BR&D) Board's Bioeconomy Initiative. In March 2019, the BR&D Board released *The Bioeconomy Initiative: Implementation* 

*Framework*, which lays out the key technical challenges that the BR&D Board member agencies will work to address to unlock the full potential of the U.S. bioeconomy.





#### MULTI-YEAR PLAN OVERVIEW

The MYP, which is updated periodically, sets forth the goals and structure of BETO and identifies the R&D, process development, and crosscutting goals and activities that BETO will focus on through the year 2030. The

MYP describes how these activities will contribute to U.S. energy supplies, create domestic jobs to support the growth of the domestic bioeconomy, secure the nation's global leadership in bioenergy and clean energy technologies, and enhance U.S. energy security. The MYP is intended as an operational guide to help BETO manage and coordinate its activities as well as a resource to communicate its mission, goals, plans, and priorities to stakeholders and the public.

BETO manages a diverse portfolio of technologies covering the full spectrum of bioenergy production, from the feedstock source to end use. The MYP identifies technical, process, and scale-up challenges, barriers, and uncertainties to be addressed for each program area as well as those that cross the entire supply chain. BETO R&D activities focus on high-impact technologies that are applicable across multiple technology pathways and products.

Figure 3 shows how BETO's program areas align with supply chain elements, with major emphases on feedstock supply, the conversion of biomass- and waste-derived feedstocks, and how crosscutting programs support all areas. Key components of the portfolio include:

- R&D of feedstock supply systems that can reliably deliver industrially relevant quantities of quality feedstocks
- R&D of high-productivity advanced algal systems
- R&D of conversion technologies able to efficiently process diverse and variable feedstocks into biofuels (e.g., gasoline, diesel, jet, and marine fuels), bioproducts, and biopower
- Development of integrated processes, tested and verified at the engineering scale, to reduce technology uncertainties and enable industry deployment
- Codevelopment of high-performance fuels with advanced engine designs
- Crosscutting sustainability and strategic analysis of economic, social, and environmental effects to inform decisions, identify emerging opportunities, and assess technology progress.

#### RESEARCH AND DEVELOPMENT

FEEDSTOCK SUPPLY AND LOGISTICS Develop and supply high-quality, energy-dense, and sustainable conversion-ready feedstocks.



#### ADVANCED ALGAL SYSTEMS

Increase algal productivity, while maximizing the yield of fuels, products, and chemicals.



Optimize conversion efficiency while maximizing value of fuels, products, and chemicals.

PROCESS INTEGRATION, SCALE-UP, AND END USES

#### ADVANCED DEVELOPMENT AND OPTIMIZATION

Develop, test, and verify integrated processes for industry to demonstrate and deploy. Develop high-performance fuels for advanced engine design.



## Ģ

#### STRATEGIC ANALYSIS AND CROSSCUTTING SUSTAINABILITY

Understand and enhance the environmental, economic, and social benefits of advanced bioenergy and bioproducts and reduce potential negative impacts.

#### Figure 3. BETO program area alignment with biomass-to-bioenergy supply chain.

Note: Conversion includes Biochemical Conversion, Catalytic Upgrading, Performance-Advantaged Bioproducts and Separations, Waste-to-Energy, Lignin Utilization, Agile BioFoundry, and Carbon Dioxide Utilization. Advanced Development and Optimization includes Process Integration and Scale-up, Analysis and Modeling, and Co-Optimization of Fuels & Engines.

#### **BETO 2019 PEER REVIEW OVERVIEW**

The Project Peer Review meeting took place on March 4–7, 2019, in Denver, Colorado. During the event, 447 projects in BETO's research portfolio were presented in 14 simultaneous review sessions and two poster sessions. Projects were systematically reviewed by 57 external subject matter experts from industry, academia, and federal agencies. The 14 review sessions included presentations of projects grouped within the following technology areas, some of which are subcategories of the primary program areas, as indicated:

#### FEEDSTOCK SUPPLY AND LOGISTICS

#### FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

#### ADVANCED ALGAL SYSTEMS

#### CONVERSION RESEARCH AND DEVELOPMENT

Agile BioFoundry Consortium Biochemical Conversion Carbon Dioxide Utilization Catalytic Upgrading Lignin Utilization Performance-Advantaged Bioproducts and Separations Waste-to-Energy

#### ANALYSIS AND SUSTAINABILITY

#### ADVANCED DEVELOPMENT AND OPTIMIZATION

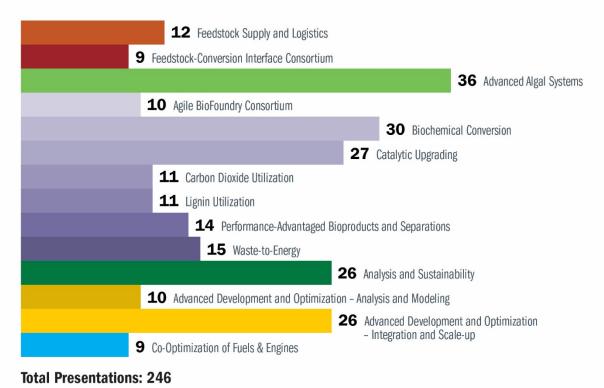
Analysis and Modeling

Process Integration and Scale-Up

#### **CO-OPTIMIZATION OF FUELS & ENGINES**

The Program Management Review meeting took place on July 17, 2019, in Golden, Colorado, and provided an office-level assessment of strategic planning and programmatic initiatives. The 246 presentations reviewed, representing 447 projects, represent approximately 94% of BETO's portfolio and a total DOE investment during the period covered by this peer review (FY 2016–FY 2019) is nearly \$860 million. Each review panel developed overall recommendations regarding the focus, management, and impact of the projects in each technology area. In addition, an external steering committee developed overall recommendations for BETO based on the summary reports from each review panel. Results of the 2019 Peer Review have been, and will 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 peer review brought together reviewers, BETO staff, principal investigators (PIs), and other stakeholders along the entire bioenergy supply chain. Converging stakeholders in this way creates synergy across technology areas and enables the cross-fertilization of ideas and expertise while providing a more comprehensive review process. Figures 4 and 5 depict the number of presentations reviewed by technology area session and the associated funding allocation.



### Number of Presentations Per Program Area

Figure 4. Number of presentations by technology area session.

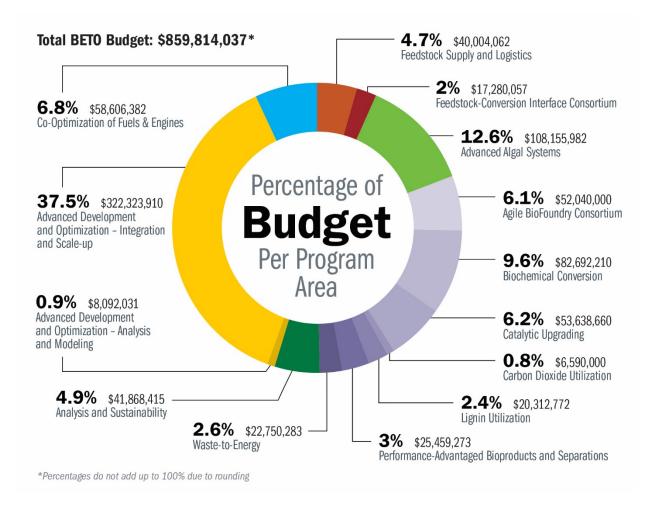


Figure 5. BETO presentation portfolio: total budget by technology area session.

#### Roles and Responsibilities

The BETO 2019 Peer Review was conducted by an internal planning committee, an external steering committee, 14 external review panels, and a selection of poster reviewers. Upon initiation of the review process, an internal BETO planning committee was designated with the responsibility for coordinating all aspects of the review process, from initiation through completion. This committee included a lead and support person for each of the 14 technology areas as well as a chair and overall coordination support. Support contractors from Allegheny Science & Technology (AST), BCS Incorporated, Redhorse Corporation, and The Building People, LLC provided planning support for each session and for the peer review overall. AST developed a reviewer evaluation system.

At the beginning of the process, the BETO planning committee identified and recruited an external steering committee to represent perspectives of academia, industry, the financial community, and nongovernmental organizations. The steering committee provided independent and impartial guidance on planning activities and the selection of external reviewers; participated in the review process; and developed crosscutting recommendations on BETO's overall focus, scope, and strategic direction.

Review panels for each technology area consisted of four to six external experts who were selected based on technical expertise and high-level qualifications in their designated technology area. Individual candidates

were proposed by the BETO technology area teams and submitted to the external steering committee for input. Efforts were made to ensure balance within each review panel by including a mix of reviewers from industry, academia, and federal agencies, with a range of expertise in the many subfocus areas within each technology area. Review panel members were required to sign legal agreements stipulating an absence of a conflict of interest with the projects they reviewed. Final decisions on reviewer selection were made by the internal planning committee and BETO's director. Each review panel was guided by a lead reviewer who in most cases had previous experience participating in a BETO Project Peer Review.

Table 1 and Table 2 list the members and affiliations of the peer review steering committee and the lead reviewers, respectively. Members of each technology area review panel are listed within each technology area session summary.

#### Table 1. Steering Committee Members

| Name           | Affiliation                               |
|----------------|---|
| Bill Crump*    | Leidos                                    |
| Suzanne Lantz  | DuPont                                    |
| Kelsey McNeely | ExxonMobil                                |
| John Sheehan   | Colorado State University                 |
| Stephen Costa  | U.S. Department of Transportation - Volpe |
| * Chairman     |   |

\* Chairman

#### Table 2. Lead Reviewers

| Name           | Affiliation             |
|----------------|-------------------------|
| Alissa Park*   | Columbia University     |
| Brandon Emme   | ICM, Inc.               |
| Charles Abbas  | iBiocat                 |
| Emma Master    | University of Toronto   |
| Glenn Farris   | AGCO                    |
| Joe Bozzell    | University of Tennessee |
| Kristin Lewis  | Volpe DOT               |
| Larry Bauer**  | LBJ Chemical Consulting |
| Luca Zullo     | VerdeNero, LLC.         |
| Raghubir Gupta | Susteon Inc             |
| Toby Ahrens    | Larta Institute         |

\* Report drafted by reviewer Jason Ren (Princeton University)

\*\* Report drafted by reviewer Jesse Bond (Syracuse University)

#### PROJECT CATEGORIES AND EVALUATION CRITERIA

Each project in the BETO portfolio was categorized based on its start and/or end date. To capture projects that have been active since the 2017 Project Peer Review, the three project categories included sunsetting (projects that ended prior to March 2019), ongoing (projects with end dates after February 2019 and start dates prior to October 2018), and new (projects with start dates after September 2018). Project scoring involved weighting the evaluation criteria based on a project's category. Table 3 lists the assignment of weighting for each project category and evaluation criteria.

|                              | Sunsetting<br>Projects<br>(Ended Prior to<br>March 1, 2019) | Ongoing Projects | New Projects<br>(Started After<br>October 1, 2018) | Directed Funding<br>Award (Lab Projects<br>with Industry Partners) |
|------------------------------|---|------------------|--|--|
| Approach                     | 25%   | 25%              | 25%  | 50%  |
| Accomplishments/<br>Progress | 50%   | 25%              | 0%   | 25%  |
| Relevance                    | 25%   | 25%              | 25%  | 0%   |
| Future Work                  | 0%  | 25%              | 50%  | 25%  |

#### Table 3. Project Evaluation Criteria Weighting

Review panel members were asked to evaluate each project on specific criteria including approach, accomplishments/progress, relevance, and future work. These evaluation criteria served as the standard template for the scores and comments provided to each project:

- **Overview:** Projects were evaluated on the degree to which the project performers communicated the project's history, the context in which the project fits into the portfolio, and its high-level objectives.
- Approach: Projects were evaluated on the degree to which:
  - The project performers implemented technically sound research, development, and deployment approaches and demonstrated the results needed to meet their targets.
  - The project performers identified a project management plan that includes well-defined milestones and adequate methods for addressing potential risks.
  - The project performers clearly described critical success factors that will define technical and commercial viability and explained and understand the challenges they must overcome to achieve success.
- Technical progress and accomplishments: Project were evaluated on the degree to which:
  - The project performers made progress toward reaching their objectives based on their project management plan. The project performers described their most important accomplishments in achieving milestones, reaching technical targets, and overcoming technical barriers.
  - The project performers clearly described the progress since the period of the last review.
- **Relevance:** Projects were evaluated on the degree to which:
  - The project performers described how the project contributes to meeting program/technology area goals and BETO objectives as cited in the MYP.
  - The project performers considered applications of their expected outputs.
  - The project performers presented the relevancy of the project and how successful completion of the project will advance the state of technology and impact the viability of commercial bioenergy applications.
- Future work: Projects were evaluated on the degree to which:

- The project performers outlined adequate plans for future work, including key milestones and gono-go decision points.
- The project performers communicated key planned milestones and addressed how they plan to deal with upcoming decision points and any remaining issues.

#### FORMAT OF THE REPORT

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

- 1. **BETO overview:** This section provides an overview of BETO's mission, vision, and goals as well as descriptions of BETO's approach to achieving technical goals and the challenges in doing so.
- 2. **Peer review report introduction:** This section contains overview information on the peer review process, roles and responsibilities, and project evaluation criteria.
- 3. **Technology area summaries:** This section contains 14 chapters that represent the comprehensive evaluation for each technology area reviewed. All technology area reports in this section were prepared independently by the review panel and the lead reviewer. Each chapter includes:
  - A. Introduction: An overview of the technology area's project portfolio, including total funding obligated for FY 2016–FY2019 and percentage of total BETO project portfolio.
  - B. **Program overview:** Background information about the BETO program that operates the given technology area, including the program scope, R&D activities, and important definitions. This component also includes context regarding the program approach for overcoming challenges as well as for supporting BETO strategic and performance goals.
  - C. **Review panel members:** A list of names and affiliations for each individual who provided project evaluations and contributed to the Review Panel Summary Report.
  - D. Technology area score results: This chart depicts the average weighted score for each project in each technology area.
  - E. **Review panel summary report:** This summary of project evaluations provides insight regarding the technology area's overall impact, level of innovation, leverage of synergies, appropriate focus, feasibility for commercialization, and top recommendations. This chapter was drafted by the lead reviewer for each technology area in consultation with the full review panel. Consensus among the reviewers was not required, and reviewers were asked to include differences of opinion and dissenting views within the report.
  - F. **Technology area programmatic response:** Represents the program's official response to the recommendations provided in the Review Panel Summary Report.
  - G. **Project evaluations:** The project reports constitute two- to three-page reports that summarize the results of each project evaluated during the review process, including the following elements:
    - i. **Project name and the work breakdown structure (WBS) number:** The full project name is listed as the heading with the identifying code below in parentheses. Project evaluations for each technology area are ordered by WBS# from lowest to highest.
    - ii. Weighted project score: Each project's average weighted score is stated numerically. A bar chart depicts the average scores for each evaluation criteria and whiskers illustrating the range of scores given to the project by the individuals within the review panel. The

average value for each evaluation criteria across all projects within the technology area is also indicated.

- iii. **Summary table:** Reference information about a project, which includes the recipient organization, PI name, project dates, project type, and funding values.
- iv. **Recipient:** Indicates the organization tasked with leading the project (might include multiple organizations in situations where the project has more than one recipient).
- v. **PI:** The PI is the individual affiliated with the recipient organization and assigned to lead the project.
- vi. Project category: Sunsetting, ongoing, or new, depending on start/end date.
- vii. **Project type:** There are many types of projects within the BETO portfolio, but this review focused primarily on two types of projects—AOPs, which are core R&D projects performed by DOE national laboratories; and projects awarded through a FOA, which are indicated in this table by listing the FOA name, number, and fiscal year.
- viii. **Funding:** The project budget allocated. Values for AOPs are available on a fiscal year basis, whereas competitively awarded project funding is available only as a total value.
- ix. **Project descriptions:** Compiled from the abstracts submitted by the PI for each project.
- x. Overall impressions: Verbatim comments made by the review panel, edited only for grammar and clarity. Each bulleted 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.
- xi. **PI response to reviewer comments:** The response to the reviewer comments provided by the PI. In some cases, PIs chose to respond to each bullet point of the comments made by the reviewers; in other cases, PIs provided only a summary response. Responding to reviewer comments was optional, and in some cases PIs chose not to respond.
- 4. **Programmatic evaluation:** The overall summary feedback and final recommendations of the external steering committee following the conclusion of the Program Management Review. This report was based on the participation of the steering committee in each component of the peer review process as well as closed-door, facilitated review sessions following the Project Peer Review and the Program Management Review meetings. Components of this report include identification of overall strengths and weaknesses, comments on the portfolio impact, assessment of BETO's strategic plan, and input regarding technologies and market trends that could affect BETO's ability to achieve its goals.
- 5. **BETO programmatic response:** The official, comprehensive response from BETO leadership on the feedback and recommendations provided by the steering committee evaluation.

# FEEDSTOCK SUPPLY AND LOGISTICS

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## INTRODUCTION

The Feedstock Supply and Logistics (FSL) Program is one of 14 related program areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place on March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 12 projects were reviewed in the FSL session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$40,004,062 (Fiscal Year [FY] 2016–FY 2019 obligations), which represents approximately 4.7% of the BETO portfolio reviewed during the 2019 Project Peer Review. During the Project Peer Review meeting, the principal investigator (PI) for each project was given 20 to 30 minutes (depending primarily on the funding level) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the Project Peer Review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the FSL Program, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. Mark Elless as the FSL review lead, with contractor support from Mr. Andrew Kobusch (Allegheny Science & Technology). In this capacity, Dr. Elless was responsible for all aspects of review planning and implementation.

## FEEDSTOCK SUPPLY AND LOGISTICS OVERVIEW

FSL research and development (R&D) focuses on technologies and processes that transform renewable carbon sources to biorefinery conversion-ready feedstocks. Terrestrial lignocellulosic biomass (i.e., plants and plant-based materials not used for food or feed) is an abundant, renewable, and sustainable resource for producing biofuels, bioproducts, and biopower. Biomass and other renewable carbon sources or reusable carbon sources commonly used for bioenergy applications include agricultural residues (e.g., corn stover), forestry residues (e.g., logging residues and forest thinning), dedicated energy crops (e.g., switchgrass, miscanthus, energy cane, sweet sorghum, high-biomass sorghum, hybrid poplars, and shrub willows), and waste streams and reusable carbon sources (e.g., the nonrecyclable organic portion of municipal solid waste [MSW], biosolids, sludges, waste food, plastics, carbon dioxide, and manure slurries).

#### FEEDSTOCK SUPPLY AND LOGISTICS SUPPORT OF OFFICE STRATEGIC GOALS

The strategic goal of the FSL Program is to reliably and efficiently deliver conversion-ready feedstock intermediates to meet BETO's 2022 and 2030 goals of \$3/gallons gasoline equivalent (GGE) and \$2.5/GGE, respectively. The focus will be on agricultural and forestry residues and energy crops in the near term and economically advantaged feedstocks (such as sorted MSW, biosolids, and industrial waste streams) in the midterm (5 to 12 years).

#### FEEDSTOCK SUPPLY AND LOGISTICS SUPPORT OF OFFICE PERFORMANCE GOALS

The FSL performance goals outlined in BETO's Multi-Year Plan (MYP) are to (1) identify the key feedstock quality and variability factors for corn stover and pine residues to meet a modeled operational reliability of 80% for advanced feedstock supply-logistics-conversion systems at a modeled delivery cost of \$86/dry ton and (2) to deliver corn stover and pine residues with the necessary specifications for 2022 verification in support of a minimum fuel selling price of \$3/GGE. In addition, by 2029, to identify the key feedstock quality and variability factors for conversion-ready feedstocks to meet a modeled delivered cost of \$73/dry ton.

#### FEEDSTOCK SUPPLY AND LOGISTICS APPROACH FOR OVERCOMING CHALLENGES

The key barriers addressed by the FSL Program are the quality, cost, and quantity of available renewable carbon sources that can be sustainably supplied and reliably converted into high-quality biofuels, bioproducts, and biopower. To meet requirements of conversion facilities, FSL R&D will need to improve feedstock quality from harvest and collection through delivery while meeting conversion performance and cost goals. The following critical areas will be emphasized within the FSL Program through early-stage R&D:

- Feedstock availability and cost
- Production
- Feedstock genetics and variety improvement
- Sustainable harvesting
- Feedstock quality
- Biomass storage systems
- Biomass physical state alteration
- Material handling and transportation
- Feedstock supply system integration and infrastructure
- Operational reliability.

The FSL Program overcomes these barriers by developing science-based strategies and technologies and defining requirements and specifications to reduce costs, improve quality, and increase the quantity of sustainable, renewable, and reusable carbon-based feedstocks. FSL activities include biomass production (in collaboration with the U.S. Department of Agriculture [USDA]), supply chain analysis, feedstock logistics R&D (including harvesting or collecting, storage, transportation, and preprocessing), and research into conversion-ready intermediates. FSL R&D focuses on improving the efficiency of feedstock logistics operations, developing a fundamental understanding of the interactions between feedstock properties and conversion performance, and identifying the key feedstock quality and performance factors affecting biorefineries. FSL collaborates with the Conversion Research and Development and Advanced Development and Optimization programs for testing and verification of feedstocks and the relevant conversion pathways at the engineering scale. FSL also works with the Analysis and Sustainability (A&S) Program to assess progress and identify and analyze sustainable practices. The FSL Program also works closely with the USDA and other federal agencies through the Biomass Research and Development Board.

This R&D work is performed by DOE national laboratories, universities, and industry partnerships, in addition to the Feedstock-Conversion Interface Consortium (FCIC). The FCIC project portfolio was also reviewed during the Project Peer Review. Please refer to the "Feedstock-Conversion Interface Consortium" section in this document for more information.

## FEEDSTOCK SUPPLY AND LOGISTICS REVIEW PANEL

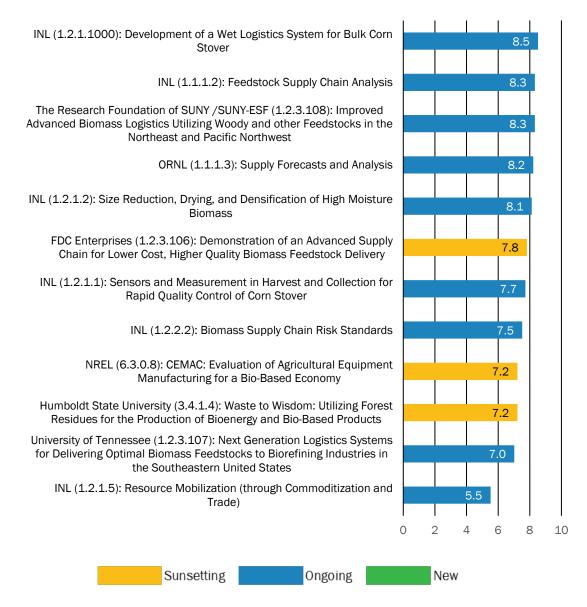
The following external experts served as reviewers for the FSL Program during the 2019 Project Peer Review.

| Affiliation                                   |
|---|
| AGCO Corporation                              |
| ICM, Inc.                                     |
| USDA Forest Service Southern Research Station |
| Michigan State University                     |
| WrightLink Consulting                         |
|   |

\* Lead reviewer

## TECHNOLOGY AREA SCORE RESULTS

#### Average Weighted Scores by Project



## FEEDSTOCK SUPPLY AND LOGISTICS REVIEW PANEL SUMMARY REPORT

#### Prepared by the Feedstock Supply and Logistics Review Panel

BETO recognizes that the availability of a sustainable, consistent, economic, and dependable supply of highquality feedstock is critical to a successful U.S. bioenergy industry. The FSL Program is central to the success of this mission.

The FSL Program projects reviewed encompass forest resources (short-rotation woody crops [SRWC] and forest residues), agricultural residues (corn stover), and dedicated energy crops. FSL projects address a range of topics, including sustainable economic feedstock production, feedstock resource assessments, supply logistics, supply scenarios, supply chain risks, and feedstock quality.

#### IMPACT

BETO's FSL project portfolio is particularly impactful for industry, and many of the projects will advance the state of technology (SOT) in the handling and logistics area. The government's investments here are particularly appropriate because they address industry problems that in many ways industry cannot address. The national laboratories on their own and sometimes with the involvement of university and industry partners have capabilities that companies alone do not have. This is currently seen in the cellulosic ethanol segment seeking to use agricultural waste, such as corn stover. Early industry projects seeking to convert corn stover into cellulosic biofuels are experiencing problems because of the variability of the material and its effects on downstream processes. This is particularly true when trying to control the moisture and ash content of corn stover.

Two FSL projects have significant direct and indirect consequences for the industry. Both are based on the handling of wet corn stover: Size Reduction, Drying, and Densification of High-Moisture Biomass and Development of a Wet Logistics System for Bulk Corn Stover. When used as a feedstock, large amounts of corn stover must be stored for long periods of time before use. During this time, it can experience significant degradation if wet, and managing moisture during baling operations is both challenging and expensive. Baling wet material, defined as greater than 20% moisture content, is sometimes required because of incoming weather events or farming activities required postharvest of corn grain.

The direct benefits are as follows: Being able to handle wet material and produce high-quality, economic feedstock for the conversion platform solves both the moisture and ash problem (microbial degradation) in the case of a wet logistics management system. For a densification system, intense drying of the material and production of fines in the pellets are the two most significant problems addressed by the project. Less intense drying will decrease the cost of densification, and the reduction of fines will increase efficiency in downstream operations.

Indirectly, the cost of baling material will reduce the cost of the baling operation by at least 10% in a typical three-pass baling system. Further, it would enable the use of the single-pass system, which would reduce baling operation costs by as much as 35%. This system has always been unable to address the storage problems of baling wet material because most baling occurring at or near the time of grain harvest involves wet corn stover. The single-pass system has the added benefit of limiting the ash of collected corn stover to the intrinsic ash of the material because the material is not subject to dirt picked up by being in contact with the ground or picked up by being subjected to dirt blown on it by wind.

The drying and densification and the wet logistics projects are not the only projects in the FSL portfolio that will prove impactful to the SOT as it exists today. Other high-impact projects include those that address inforest processing systems, advanced logistics supply systems, rapid quality control, and the development of

biomass risk standards. BETO's portfolio is robust, and the review panel encourages BETO to continue existing work as well as fund new work replacing sunsetting projects with new funding opportunities when appropriate.

#### **INNOVATION**

The BETO portfolio has several other innovative projects as well. One advanced the SOT for processing forest residues in the forest where they are created and most often left. The technology solutions reduce the moving and handling of the waste, improve forest health, and reduce greenhouse gas (GHG) emissions from the rotting of the residues. The project produced three products that are currently sold in the marketplace, which has the potential to be profitable, depending on local conditions.

Another innovation under development is the next-generation logistics systems in the form of a feedstock collection and processing depot using both woody and herbaceous materials. This concept can become a focal point to produce high-quality economic feedstocks that can then be delivered to any number of fuel, chemical, or power production facilities surrounding the depot. When combined with the wet logistics and wet densification technologies, this concept could be groundbreaking and move the industry toward the commodification of biomass feedstocks.

Sensors for rapid quality control and the development of biomass supply chain risk standards are two more innovative projects. One of the most interesting features of BETO's FSL project portfolio is that many projects use existing technologies in new and innovative ways, and in doing so they pave the way for realization toward the use of the vast biomass resources identified in the 2016 Billion-Ton Report: Towards Commercialization.

#### **SYNERGIES**

One strong point of the FSL Program is the many synergies among the projects. The national laboratory project on Feedstock Supply Chain Analysis includes an analysis of all FSL projects, primarily to support BETO program planning and project tracking needs. This greatly facilitates synergies among FSL projects. In addition, the project incorporates industry data, Supply Scenario Analysis, and other BETO national laboratory projects that include techno-economic analysis (TEA) and life cycle assessment (LCA). The tracking component of the analysis project allows BETO to see if the research projects are meeting their goals in support of BETO's MYP. This project extends well beyond analyzing the cost of feedstock.

Beyond cost, the project's approach integrates the availability of the resources based on supply scenario analysis, improvements in logistics, advancements in technology, and environmental performance. Costs and interdependencies, previously unaccounted for or unidentified, are captured through new and innovative methods and computational abilities to model supply systems. This project naturally creates synergies among FSL projects when it identifies interdependencies and provides a platform for the PIs of any FSL project to locate not only information that can be helpful when problem solving but also encourages communication between the FSL PIs. Such communication is especially encouraged when interdependencies and technical advancements are identified in one area but will benefit another.

To say the final results of the comprehensive data assembly and analysis of feedstock supply chains will become an invaluable industry resource is a severe understatement. It is also valuable for identifying new project funding needs and opportunities to advance BETO's MYP. Although this panel is not familiar with all BETO program areas, this project should serve as a model and be repeated in the other programs where appropriate.

#### FOCUS

The FSL project portfolio is squarely focused on many issues that will benefit the SOT as it exists today, help existing projects, and spur investment and growth in the advanced bioeconomy. Addressing biomass variability, quality control, borrowing costs, supply risks, and advanced logistics will encourage investment in and the development of new projects in the bioeconomy and help BETO meet its goals according to the MYP.

The FSL review panel has some suggestions, however, for adding and refocusing some project efforts that would strengthen the projects and the review process.

As long as the baling of corn stover, wheat straw, and other feedstocks will be used to supply feedstock to conversion projects, one area that must be addressed is the disposal of baling twine (in the case of large square bales) or bale wrap (in the case of round bales). The disposal of this material is often overlooked, and it will become an imminent problem unless it is addressed. For example, a project that uses 350,000 tons of material per year that is baled and delivered as large square bales will yield between 15,000 and 18,000 miles of baling twine on an annual basis. There are two issues with this: (1) currently, most twine is polypropylene, which is not a bio-based product, therefore affecting issues around sustainability; and (2) the twine needs to be brightly colored to make it easy to see in the field.

When baling corn stover using a large square baler, it is inevitable that the twine will break during the baling operation and be left on the farmer's field. This could cause significant problems for the farmer in succeeding field tasks, such as tilling or planting. If left in the field, the twine could wrap around equipment and cause significant maintenance and operating issues. For the baling team to see and collect the twine, it needs to be brightly colored. Thus, there is a need for a new project to develop a sustainable bio-based twine with the same characteristics as those in the polypropylene.

In addition, the project portfolio would benefit from an impact assessment on the overall effect that the successful completion of the project portfolio technologies will have on the marketplace. For example, ample analysis suggests which price targets advanced biofuels must meet for a gallon of gasoline equivalent to encourage industry development of projects. All the projects have a financial goal—e.g., reducing the gallons of gasoline equivalent by X amount or reducing the borrowing costs of a project by decreasing the credit risk and achieving an investment grade credit. There seems to be little thought (by individual research projects), however, around how many commercial startups would likely occur, when and if the research or demonstration project goals are met, or what other conditions must be met to encourage the development of industry projects. More effort needs to be spent studying the business case for the project products and technologies produced by BETO's FSL work. This would help BETO direct funding toward the most impactful projects.

In addition, many projects would benefit greatly by including field trials involving industry. One sunsetting project (Demonstration of an Advanced Supply Chain for Lower Cost, Higher Quality Feedstock Delivery) showed both the benefits of this approach and the difficulties. Nevertheless, expanded efforts of this nature would give some real-world experience for the products or technologies developed in the FSL portfolio. Field trials would greatly improve the adoption of the FSL work by industry and increase the return profile for BETO's investment. This would give industry a chance to see the work of the national laboratories and universities as well as establish relationships that could prove valuable to both parties in the future. These relationships could also provide new investment opportunities as industry assesses what it needs to address technological challenges.

#### TECHNOLOGY DEVELOPMENT PIPELINE

Most recent BETO FSL portfolio projects have focused on corn stover and SRWCs, such as willow. The review panel believes that it might be time to expand logistics R&D to other feedstocks that were previously the focus primarily of biomass yield improvement. This is not to say that other feedstocks are not part of any of the studies or projects or that the existing projects would not have any place with other technologies and feedstocks; however, it might be time to start devoting resources to other feedstocks or to the impact that existing projects will have on other feedstocks. The bioeconomy's success will be realized only with a diverse set of feedstock choices, including but not limited to crops such as miscanthus, switchgrass, energy cane, and all forest resources. Even though high-biomass-yield productivity has been demonstrated in the dedicated crops by past BETO and USDA research, and they are included in national feedstock supply scenarios, supply logistics impediments exist to their availability at competitive costs.

One project that should be revisited for additional verification work is the readiness of agricultural equipment original equipment manufacturers (OEMs) to support an aggressively growing advanced bioeconomy. The required amounts of equipment needed are in-line with reports and studies of which the review panel is aware; however, this review panel questions the conclusion that OEMs are ready to produce the required tractors and implements if an aggressive project development growth curve develops. For example, currently the annual market for high-horsepower tractors such as those used in baling operations is approximately 25,000 units. The project estimates that the units needed to pull implements in the short term is slightly less than 50,000 units and in the long term is approximately 55,000 units. If conversion project development takes place throughout several decades, then the ramp-up for OEMs could be managed and planned. Should OEMs need to deliver in a shorter time frame of 10–15 years, this panel is not sure that is possible. More work with OEMs based on a sensitivity analysis with various growth curves would reveal much-needed information about their ability to meet the necessary demand.

For BETO to orient their investments to technologies that would most benefit the developing bioeconomy, the panel believes that BETO would benefit from carrying out a standard business case analysis of the effects on the industry upon the successful completion of a project. This could also become part of the application process when a respondent submits a project for funding under a funding opportunity announcement. This would help separate projects based on business merit and help understand what would or would not be attractive to industry, thereby increasing the chances for rapid adoption by industry. This practice would also reveal whether BETO's investments are occurring at the optimal stage of technology development.

#### RECOMMENDATIONS

Although it might not be appropriate for all projects, more of a business planning approach to projects should become part of the process. Prior to making any investment, industry frequently if not always requires a business plan and analysis. Analyses on the strengths, weaknesses, opportunities, and threats (SWOT) are performed to indicate how the investment will fit into an existing business and what risks are present versus the benefits to the investment. The panel understands that BETO looks at these types of issues within a general and broad framework, but the panel believes that there would be great benefit to delving into detail in this area. The business plan might gauge the effects of the project and answer such questions as: How and why will the SOT be advanced with a successful project? How many projects will be built and/or how will this project improve existing projects? What will this mean for employment within the industry? This would help BETO create priority for projects and could reveal new opportunities for investment and improvement of existing programs.

The review panel believes that it would be extremely beneficial for each project partner to share with BETO, at a minimum, a report on findings that did not go well or according to plan and how those issues were resolved. This would be most beneficial if shared widely within all BETO program areas. Frequently, projects experience similar problems, and knowing how others solved a problem might save significant time and effort. This would also be useful information to share with industry.

It has come to the attention of the review panel that the national laboratories have within their structure marketing departments. Thus, the final recommendation is that BETO include a budget for marketing as a regular line item. It is not the recommendation that BETO or DOE form a marketing department but that funds be available for specific marketing duties and plans within the laboratories to promote the projects many of them are working on and that BETO is already funding. This would have several positive effects, not the least of which would be increasing the profile with industry of not only the work currently being performed at the national laboratories but also the national laboratory capabilities. This could lead to more future work and/or investment opportunities for BETO.

## FEEDSTOCK SUPPLY AND LOGISTICS PROGRAMMATIC RESPONSE

#### INTRODUCTION/OVERVIEW

The FSL team appreciates the Peer Review Panel statements affirming that FSL funding has enabled research productivity, innovative approaches, and significant advances along the SOT as well as excellent synergies among projects, with no notable gaps. FSL further acknowledges the recommendations that:

- Performing a SWOT analysis would be a potentially useful method for prioritizing projects and revealing new opportunities.
- Reporting on issues that did not go according to plan, and how these issues were resolved, to both the rest of BETO and possibly industry would allow everyone to learn from the "negative" results.
- BETO should use the marketing structures within the national laboratory complex to more effectively communicate the work that BETO funds within both the bioenergy community and the public at large.

#### Recommendation 1: Business Plan-Incorporate a business plan/SWOT into each project.

BETO recognizes the importance of a sound plan for directing future research that accounts for opportunities and risks. Currently, BETO project planning incorporates an evaluation of the risks associated with each project and the strengths that each project lends toward completing BETO's stated goals and advancing the current SOT in the industry. At this point, project management does not focus on identifying opportunity space. BETO will strongly consider adding an opportunity analysis to the project planning stage.

## Recommendation 2: Lessons Learned—Write/share lessons learned and how issues were resolved.

BETO fully agrees with the importance of open dialogue, along with the collection and communication of lessons learned, such that all results can be used. Currently, it is common practice to include a section on lessons learned in each quarterly report sent from project performers to BETO that includes a description of at least one challenge faced by a project and the path for resolving the challenge. BETO will consider a path for aggregating and disseminating this information while remaining sensitive to the protection of proprietary data and information that could be contained within the described challenge and solution.

## Recommendation 3: Marketing—Enhance focus on marketing. FSL program should set aside specific funding for marketing to be provided to the national laboratories for execution.

BETO currently works to make its impacts known through conferences, the DOE Office of Energy Efficiency and Renewable Energy website, and other platforms such as social media. We appreciate the review panel's suggestion to extend our outreach and marketing efforts through our national laboratory partners, and we acknowledge a great opportunity to take advantage of BETO's BioComms effort—a communications partnership of nine BETO-funded national laboratories. BETO will work with the laboratories to improve overall outreach and continue to increase the profile of the bioenergy industry writ large. This could be accomplished through ongoing efforts at the laboratories to publicize attendance more widely at conferences, by encouraging national laboratory researcher participation in professional society leadership roles, in addition to better advertising the capabilities of the various national laboratory process demonstration units such that partnerships with industry can be enhanced.

## FEEDSTOCK SUPPLY CHAIN ANALYSIS

#### Idaho National Laboratory

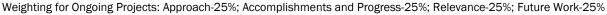
#### **PROJECT DESCRIPTION**

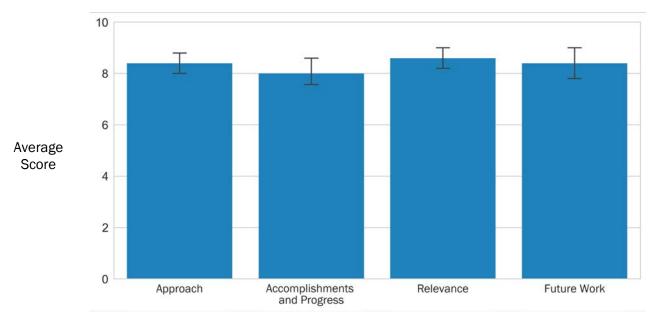
The billion tons of biomass potentially available for bioenergy comprises widely distributed, low bulk density, and widely spatially and temporally variable biomass types, moisture levels, and compositions. This creates a unique challenge to the development of reliable, costeffective biorefineries to provide low-cost, high-volume biofuels that can compete with petroleum-based fuels. Today's pioneer biorefinery industry lacks a consistent and reliable biomass supply, and thus it relies on vertical integration of its feedstock supply to minimize supply risk using conventional feedstock supply systems that were developed for industries that are less sensitive to feedstock composition characteristics. Without reducing feedstock

| WBS:                      | 1.1.1.2             |
|---------------------------|---------------------|
| CID:                      | NL0015591           |
| Principal Investigator:   | Dr. David Thompson  |
| Period of<br>Performance: | 10/1/2014-9/30/2020 |
| Total DOE Funding:        | \$3,779,968         |
| DOE Funding FY16:         | \$765,000           |
| DOE Funding FY17:         | \$900,000           |
| DOE Funding FY18:         | \$1,114,968         |
| DOE Funding FY19:         | \$1,000,000         |
| Project Status:           | Ongoing             |
|                           |                     |

costs and improving biomass consistency, it is difficult to see a viable pathway to both achieving the DOE/BETO 2030 goal of \$2.50/GGE (2016\$) using an industrially relevant feedstock and competing on a cost basis with oil selling at less than \$50 bbl. This project fulfills a critical role for DOE by developing supply system designs, delivered feedstock cost and volume targets, and forward-looking analyses to track R&D progress and guide the direction of R&D toward the highest-impact operations. The overarching goal of this project is to provide BETO with credible, objective analyses of feedstock supply systems and strategies to support their investment in a sustainable, economically viable, national-scale bioenergy industry. This project directly informs BETO through barriers Ft-A: Terrestrial Feedstock Availability and Cost and Ft-M: Overall

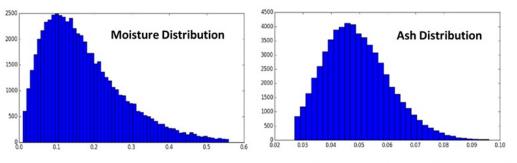
#### Weighted Project Score: 8.3





 $oldsymbol{I}$  One standard deviation of reviewers' scores

Integration and Scale-Up. This project develops and vets innovative strategies that meet cost, quantity, and quality specifications while minimizing environmental impacts and delivering robust data sets with flexible analysis tools to enable industry to implement a successful biofuel supply system. This project also tracks technology progress based on technology improvements identified and verified annually in R&D activities. Historically, we have investigated both conventional feedstock supply systems and a number of advanced (active quality management) feedstock supply system strategies, including blending and commoditizing biomass to meet modeled cost, quantity, and quality specifications required to meet long-term U.S. biofuel production goals. Complete field-to-reactor throat feedstock supply infrastructures and systems are analyzed, including, but not limited to, innovative harvest and collection equipment, advanced preprocessing technologies, biomass composition variability, and the interface between feedstock variability and conversion performance. This project leads the development of the pathway to the 2022 Multi-Year Plan (MYP) target for the 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 more than \$85.51/dry ton (2016\$), and contribute to meeting a delivered feedstock cost target of \$71.26/dry ton, in support of achieving the \$2.50/GGE minimal ethanol selling price target for 2030. Finally, this project develops new computational tools to advance the state of the art in feedstock supply and preprocessing modeling capabilities. Examples include continual updates to the Idaho National Laboratory (INL) Biomass Logistics Model, new analysis tools to enable dynamic simulation of throughput and operational performance, and feedstock supply and preprocessing system optimization tools that simultaneously consider multiple aspects of delivered biomass quality and supply.





Equipment Down Time – 1-year Discrete Event Simulation (DES)

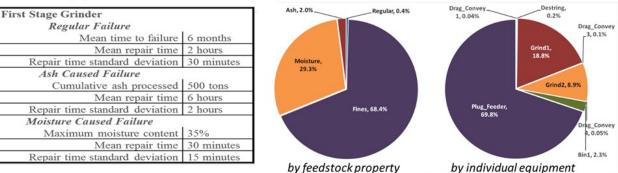


Photo courtesy of Idaho National Laboratory

#### OVERALL IMPRESSIONS

• In summary, managing the information in presentations such as this—where information comes from many diverse sources, programs, and in different formats—is a difficult task. As a reviewer, after the goals, sometimes I would like to see approach sections (both managerial and technical), then take one key goal/milestone and describe the process in great detail, including how mitigation were steps, if any; how gaps were identified and filled; and what the thought process was. Then state whether the other goals and milestones were met or not and where to find additional information should we wish to see it.

That way, I could make more informed decisions about the strengths and weaknesses of the project and presentation.

- TEA is key metric for all BETO research, and as such the importance of this project cannot be questioned. The project did a good job of incorporating new SOT concepts, such as depot and wet pelleting (as well as FCIC changes, such as inclusion of process variability). For future peer reviews, I suggest picking an example—good or bad—and showing how it goes through the project cycle, including touch points with different projects and team members. This would help reviewers understand the actual project approach.
- The project has met the demands of the FSL/FCIC project needs, and an evaluation of different control strategies has been executed (bale rejection, et al.); thus, the TEA is being used as more than only as a metric—it is being used to help define processing strategy. It was not completely clear from the presentation how these scenarios are brought into the analysis process. Consider whether more visibility and clarity here could bring more clever ideas from outside the project team members.
- This project has a long history of providing valuable analytic support to BETO for use in developing strategic MYPs. The proposed plans are very well in tune with analysis and planning needs identified by BETO. The individuals involved at several DOE labs have developed analysis expertise that can be called upon to provide quick responses to questions from Congress, industry, and the general public. This is a resource that should have value not only to BETO but also to other DOE offices and potentially to specific commercial project development activities.
- Modeling work such as this project helps identify missing information and guide new research.
- This feedstock quality and cost modeling project integrates the available modeling and SOT work to inform BETO and other users of progress toward goals and identify challenges to overcome.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We understand the reviewers' perspective. This project supplies system TEAs for all conversion technology platforms that use terrestrial feedstocks. This is in contrast to the majority of BETO's TEA projects, which typically focus on single conversion processes. This currently amounts to four different feedstock supply chains, which makes it difficult to cover any in detail in the allotted time and provide a good overall picture of the breadth and scope of the project's accomplishments and impacts. Unlike other TEA projects that use standard packages such as Aspen Plus and CHEMCAD to perform their analyses, we must continually develop and upgrade analysis tools to perform our analyses (progress on which is tracked by additional milestones). Developing these tools is an accomplishment in and of itself because the resulting ability to model something that was not heretofore possible to model has substantial impact on the ability of BETO to understand what must happen to successfully develop a robust bioeconomy. A good example of this is the throughput analysis approach and model developed by this project, which brought to the forefront the operational issues than can be attributed to feedstock quality variations.
- Design cases are developed approximately every 5 years that lay out the expected technology development pathways that are needed to achieve BETO program goals and targets during the next period. The design cases are developed with participation of the R&D project PIs, and then supply system analysis is used to model the impacts of technology improvements toward the technical targets. Annual SOT reports track R&D progress toward individual technology targets as well as the overall supply system targets.

## SUPPLY FORECASTS AND ANALYSIS

#### **Oak Ridge National Laboratory**

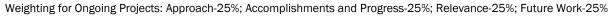
#### **PROJECT DESCRIPTION**

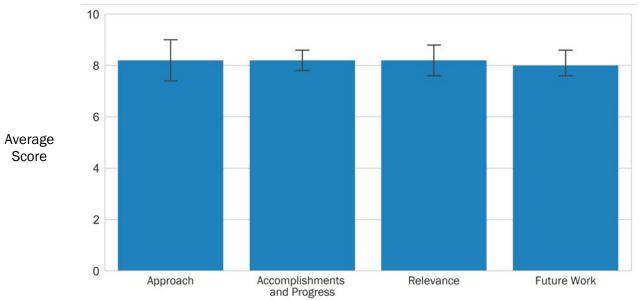
The goal of the project is to provide DOE and bioeconomy stakeholders with biomass feedstock data needed to develop strategies to derisk the biomass supply chain. These data include information regarding biomass feedstock quantity and cost as well as environmental effects associated with producing, harvesting, and transporting biomass. Because these data can vary by feedstock type and spatial distribution, they should be generated under assumptions that reflect specified bioindustry scenarios. For example, biomass feedstock data should reflect the scenario-specific feedstock demand characteristics regarding type, quantity, and spatial distribution of feedstock required. Economies of scale

| WBS:                      | 1.1.1.3             |
|---------------------------|---------------------|
| CID:                      | NL0015593           |
| Principal Investigator:   | Dr. Matt Langholtz  |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,875,180         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$1,375,180         |
| DOE Funding FY19:         | \$500,000           |
| Project Status:           | Ongoing             |
|                           |                     |

from the position of the biorefinery, as well as "Nth-plant" mature-industry feedstock use, run counter to potential diseconomies of scale in feedstock supply. This project applies feedstock supply analytics to account for these scenario-specific feedstock supply attributes. Further, understanding the environmental effects of marginal additions of biomass in the United States or in a region—as well as the intersection of cost and environmental effects—can help DOE and bioeconomy stakeholders identify feedstocks and regions that constitute the best opportunities to grow biomass. We are examining the relationship between potential county-level agricultural and forest biomass supply and environmental effects in 2040, based on 1% and 3% yield growth scenarios from the *2016 Billion-Ton Report*, using a novel environmental supply curve visualization.

#### Weighted Project Score: 8.2





 $\square$  One standard deviation of reviewers' scores

An additional objective is to examine trade-offs or synergies between price and environmental effects as biomass supply, especially energy crops and residues, increases across the United States. Water quality and quantity, GHG emissions, air quality, and biodiversity outcomes are considered. Preliminary analyses have shown some synergies between price and reduced adverse environmental effects. For example, GHG emissions intensities are low for low-price corn stover, especially after logistics are included in the cost and environmental effects. Moreover, we identified regions where particulate emissions were high, and costs of production were among the highest in the United States. We also identified trade-offs between price and environmental effects, as in water and nutrient losses from soil to streams that coincide with the least expensive forest biomass to harvest. For water quality, we worked with A&S Project 4.2.1.40 to internalize some environmental externalities into total cost curves, showing the clear economic benefits of the water quality loading reductions associated with energy crops. Data visualizations were developed in Tableau data visualization software.

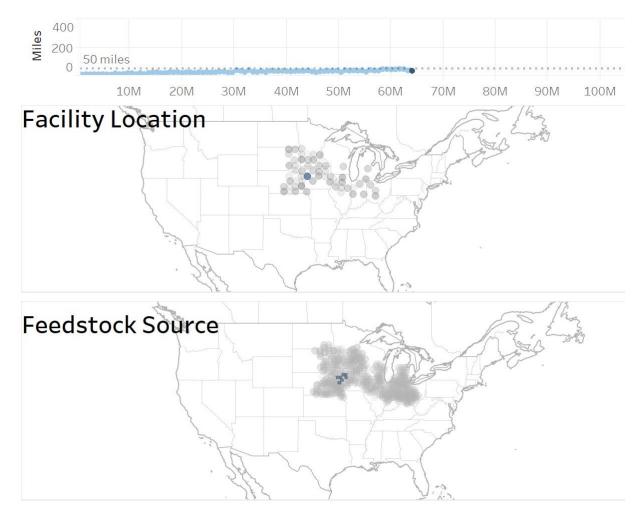


Photo courtesy of Oak Ridge National Laboratory

#### OVERALL IMPRESSIONS

• Although I am fully in favor of such studies, I am always suspect of the assumptions behind the conclusions reached in the study about the price of the commodities in question, whether corn stover, switchgrass, forest residue, or clean wood chips, to name a few. I am not trying to question the validity

of the conclusions or the assumptions; I do not find enough information in the presentation about their source to decide.

- This is important work to understand the potential of the industry. The model's current detail is very impressive, and the tools that have been developed to suggest likely biorefinery sites are interesting. From the presentation, it was difficult to understand the full granularity of the variables included in the model, although it was evident it was rather expansive. Some factors to consider including in future work might be municipal readiness (i.e., road access) because this will often be tied to the capital project by local government, as well as gradual impact of climate change because it relates to the rollout of the plants, from pioneer to the *n*<sup>th</sup>-plant, over some period of years.
- Despite what one might easily argue is the most comprehensive feedstock model short of oil exploration, the project specifically stopped short of saying the models should be used to site actual plants. The reviewer can appreciate liability impacts; regardless, either it will be used by industry or not, and if not, it might not be as valuable. Consider owning the accuracy of the model and the great work it is, and use it to actually go to some of the sites and understand how well your model captures what would be the actual logistics and local support of a plant located where the model predicts.
- The development of sophisticated analysis methodologies and the results published in the three previous *Billion-Ton* reports have made a very strong contribution to the development of MYPs and strategies by BETO. The recent focus on scenario and specific end use locations is a very valuable addition. Future work plans are well in tune with R&D needs identified by BETO. The goal of making the outputs of the work available to several other BETO projects has been clearly accomplished. The individuals involved—from several DOE labs and a university—have developed analysis expertise that can be called upon to provide quick responses to questions from Congress, industry, and the general public. Downloads of the data shared in public databases have been very high, but finding a way to also share the expertise developed by the analysts with project developer stakeholders would also be valuable.
- This project has a national scope and is foundational to biomass feedstock supplies and logistics.
- This spatially based feedstock quantity and cost modeling project is useful to biorefinery developers as well as policymakers. It will integrate well with other BETO modeling projects as well as growth and yield databases.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The reviewer's suspicions of reported prices are understandable given the limited detail provided during the peer review presentation. Technically, we do not consider cellulosic biomass resource commodities because quality specifications have not been widely accepted for commoditization; however, methods and assumptions of the economic modeling were reviewed by more than 30 external reviewers from industry, government, and research sectors. The assumptions and the review process are described in the 2016 Billion-Ton Report (http://energy.gov/eere/bioenergy/2016-billion-ton-report). Further, methods used in the report are applied in various peer-reviewed manuscripts. Acknowledging prices are impossible to predict with certainty because future macroeconomic and technical innovations are impossible to predict.
- We appreciate the reviewer's suggestions regarding municipal readiness, climate change, and explicitly characterizing accuracy.

# SENSORS AND MEASUREMENT IN HARVEST & COLLECTION FOR RAPID QUALITY CONTROL OF CORN STOVER

### Idaho National Laboratory

### **PROJECT DESCRIPTION**

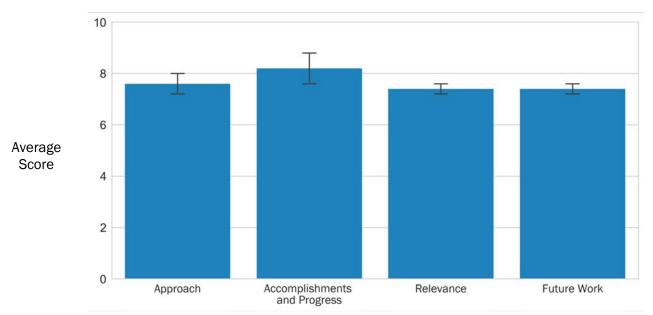
Results from pioneer integrated biorefineries and research at INL show negative impacts of moisture and soil content in baled biomass. Impacts include biological degradation, displacement of valuable biomass components by soil, and increased preprocessing and handling costs. Existing harvesting and storage practices have proven ineffective at reducing bale-to-bale variations in moisture and ash from soil content that occur in commercially harvested corn stover delivered throughout the year to a biorefinery. The project goal is to demonstrate the major components of an information-driven biomass supply design that has potential to reduce harvesting- and storage-related quality variations in delivered biomass between annual harvesting

| WBS:                      | 1.2.1.1             |
|---------------------------|---------------------|
| CID:                      | NL0015076           |
| Principal Investigator:   | Mr. Bill Smith      |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$5,021,373         |
| DOE Funding FY16:         | \$1,190,000         |
| DOE Funding FY17:         | \$1,190,000         |
| DOE Funding FY18:         | \$1,716,373         |
| DOE Funding FY19:         | \$925,000           |
| Project Status:           | Ongoing             |
|                           |                     |

operations. Components include: (1) in-field and in-storage characterization of moisture, carbohydrate, and ash using a novel near-infrared (NIR) spectroscopic bale probe, (2) storage stability prediction based on measurable biomass and environmental conditions, and (3) a logistics management algorithm incorporating yearlong storage performance that selects lots for periodic delivery based on user inputs such as target moisture and carbohydrate content. Storage performance—i.e., moisture migration and dry matter stability will be characterized based on physical and computational models of heat flow, multiphase moisture dynamics, and biological activity in storage. Research products include improved NIR spectroscopic analytic methods for

### Weighted Project Score: 7.7

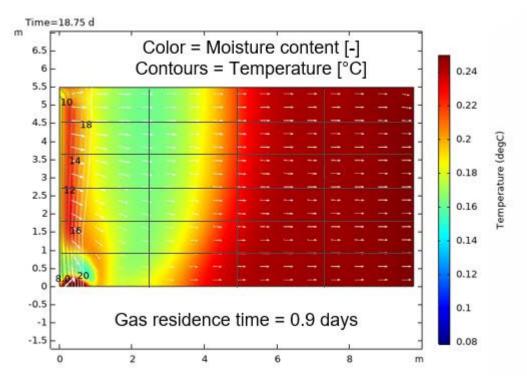
Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

total ash in baled corn stover using INL's bale probe; development of laboratory-proven "first-principles" models describing storage performance; and demonstration of a logistics system design that uses composition, storage performance projections, and climate data to reduce composition variations over time. Results to date show that changes in biomass composition over time can be anticipated and managed to reduce temporal variations in moisture, carbohydrate content, and ash as a result of carbohydrate loss using a simplistic model of storage performance; however, more complex models are needed to evaluate commercially relevant storage conditions in and outside of the U.S. Corn Belt. The complexities of commercial storage systems include variations in biomass composition anatomical fractionation resulting from harvesting operations, interactions between stacked bales and the ground surface storage pad, weather climate conditions, and potential storage improvements such as active and passive ventilation. Ongoing work aims to evaluate the physical, chemical, and biological phenomena driving biomass storage stability relative to moisture dynamics (wetting/drying) and biological activity (dry matter preservation); create computational models to test our understanding of these phenomena; and develop means to employ these principles to reduce temporal variations in delivered biomass quality during a year's storage period.





Photos courtesy of Idaho National Laboratory

### OVERALL IMPRESSIONS

- Overall, this is a well-executed project thus far, with promising results that should pay off in helping industry create better handling and preprocessing system designs. There are two areas I wish the presentation and project performers would have taken time to explore, however: (1) the current economic estimates of the economic effects of the work and (2) the early potential design characteristics that are developing or what problems the designs need to solve.
- This is a very impactful set of work to date that creates a lot of deeper understanding on how bale storage impacts quality parameters. NIR probe work has been very important and valuable to increasing the understanding of how bales store. That said, the reviewer is concerned that mitigation techniques are not clearly defined in the project scope. Ideally, outcome of the future work would educate on how to maximize storage stability (i.e., new storage practices) or illustrate a method for removing poor-quality portions from the bale or bale lot.
- It was not clear how the NIR probe testing would be scaled up, although that seemed to be one aim of the work. Consider how red-scale/infrared scans could be correlated with actual probe data such that drones or other noninvasive approaches could be used to grade bales/bale lots.
- This project involves a lot of fundamental research but promises to address and demonstrate very practical solutions to current problems in the types of herbaceous residue handling activities that are likely to be the most common in near-term commercial activities. This fundamental research project is also focused on the end goal of obtaining industry adoption of the fundamentals being researched (ash/moisture avoidance practices, analytic tools, and biomass storage management practices/tools). The close linkage between this fundamental research project and the FDC Enterprises field demonstrations of advanced supply chain practices is a great example of focused, goal-oriented R&D. The substantial amount of data presented shows that the project is progressing nicely, but actual progress toward the end of the project goal is difficult to assess at this time.

- Fast physical biomass characterization is important to suppliers when they are paid on a dry-ton basis.
- This project has succeeded in developing the tools and models to understand the moisture and dry matter dynamics of baled stover. This is helpful to inform the storage and use of this feedstock at biorefineries. Next steps should include expanding this work to include other baled feedstocks.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The project team thanks the review panel for their time and thoughtful comments. We have worked extensively throughout the project lifetime to understand the largest cost drivers in harvest, collection, and storage operations. Under best-case scenarios, storage costs as low as \$6.41/t have been reported within this task previously and are reflected in the analyses of INL's Feedstock Supply Chain Analysis task (WBS: 1.1.1.2). Best-case storage scenarios are not always a reality, however, and excess moisture in bales occurs for several reasons, including harvest timing, field conditions, and climate. The current research goals of this project focus on optimizing storage conditions to reduce the variability and improve downstream reliability as biomass enters preprocessing, which ties closely with the goals of the FCIC. To that end, this task has focused on two reported challenges: (1) variations in bale moisture content, especially at the upper end of moisture content; and (2) degradation that occurs as a result of high moisture content over time. Our supply system designs focus on enhancing bale drying rates in storage—early, before biodegradation occurs—through cost-effective means. These include using naturally occurring wind patterns through informed site selection and stack configuration, using microbial-generated heat to increase internal stack temperatures to enhance drying, using multiple storage methods to balance storage cost and storage performance, and using predictive models based on physical and biological properties to identify which lots should be delivered at what time to minimize compositional variations and maximize the value of the harvested biomass.
- Integral to this research effort is the NIR spectrometric probe, which was developed to overcome the challenges of within-bale variations in biomass composition and the need for rapid biomass analysis. This scope was transferred to this project from the BETO-funded Biomass Alliance for Logistics Efficiency and Specifications (BALES) High-Tonnage Logistics II project in FY 2019. We agree with the reviewer's comments regarding corn stover, and in FY 2020 we plan to expand the use of this tool to include baled switchgrass. Lessons learned in corn stover and switchgrass will be applied to expanding the number of commercially relevant baled and bulk biomass feedstocks beyond FY 2022. Although the current programmatic shift to more fundamental technical research might not permit INL to focus on the physical probe deployment and pilot-scale storage experiments, we will continue to work closely with external partners to develop robust and efficient means of probe application and confirmation of laboratory- and bench-scale results regarding storage stability and moisture migration in storage.
- We will continue to apply the tools that this project is developing, such as the NIR probe and the storage and queuing models, to anticipate and minimize variability such that high-quality biomass can be provided for preprocessing and conversion.

# DEVELOPMENT OF A WET LOGISTICS SYSTEM FOR BULK CORN STOVER

### Idaho National Laboratory

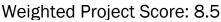
### **PROJECT DESCRIPTION**

The feedstock logistics supply chain relies on storage to supply conversion facilities year-round given that most biomass sources are only seasonally available. An estimated 60% of available corn stover is projected to be harvested at moisture contents that exceed 20% wet basis, making it susceptible to microbial degradation when stored aerobically. Likewise, corn stover bales are at risk of catastrophic loss by fire, as evidenced by bale yard fires at biorefineries. Active management approaches in the feedstock logistics supply chain, specifically the use of high-moisture storage, can protect feedstock from loss caused by fire or microbial degradation. Wet logistics systems using anaerobic storage to provide stable storage

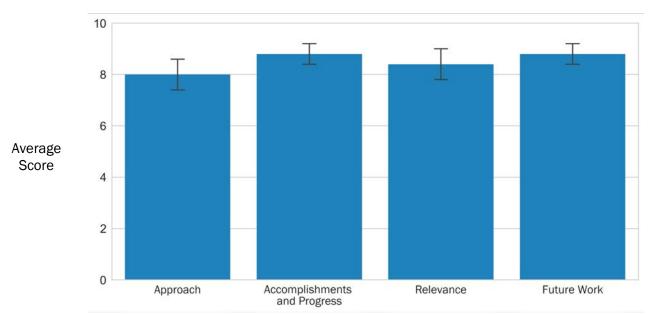
| WBS:                      | 1.2.1.1000          |
|---------------------------|---------------------|
| CID:                      | NL0028567           |
| Principal Investigator:   | Ms. Lynn Wendt      |
| Period of<br>Performance: | 10/1/2014-9/30/2020 |
| Total DOE Funding:        | \$1,938,454         |
| DOE Funding FY16:         | \$667,250           |
| DOE Funding FY17:         | \$385,000           |
| DOE Funding FY18:         | \$501,204           |
| DOE Funding FY19:         | \$385,000           |
| Project Status:           | Ongoing             |
|                           |                     |

and can be used to enable the nation's billion tons of biomass. Two barriers to large-scale storage operations include predicting storage performance at commercial scales and predicting the impact of wet storage biomass to biochemical conversion approaches. This project explores the possibility of storage add value by reducing biomass recalcitrance.

To understand the degradation potential in biomass stored under such conditions, we developed a numerical model that mathematically represents the gas and heat-transfer processes controlling dry matter loss and



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

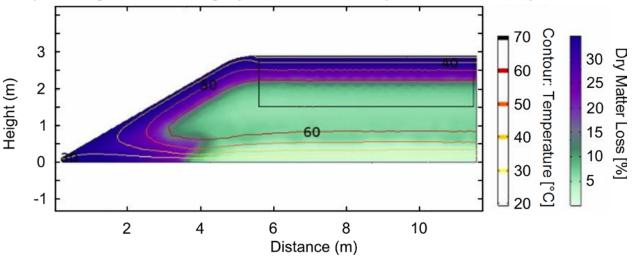


 $oldsymbol{I}$  One standard deviation of reviewers' scores

temperature in storage sites. This model was then tested against field data from a 500-t storage study using 40% moisture corn stover. With primary inputs based on laboratory-measured dry matter consumption rates, heat- and gas-transfer properties, and on local meteorological data, the model reproduces many primary observed trends in field data, specifically temperature and gas concentrations as well as dry matter loss over 6 months. The resulting model appears to provide an excellent means of testing how changes to storage conditions would likely affect storage performance. As storage bulk density decreases and porosity increases, for example, temperature and degradation increase. This effort demonstrates the impact that storage conditions could have on performance under commercially relevant settings.

Biochemical conversion approaches rely on pretreatment and enzymatic hydrolysis to create sugar monomers that can be fermented into biofuels. Aerobic and anaerobic storage methods were evaluated for wet corn stover in laboratory reactors as well as in the field. Assessment of sugar release as a result of dilute acid or dilute alkaline pretreatment and subsequent enzymatic hydrolysis suggested that when anaerobic conditions were maintained in storage, sugar release was either similar to or greater than as-harvested material depending on the pretreatment chemistry used.

The use of agricultural residues, which are harvested seasonally, necessitates storage to supply a biorefinery with a consistent feedstock supply year-round. The long residence time of storage offers an opportunity to perform low-severity treatments that can have benefits downstream. In-storage treatments can reduce costs and energy consumption of mechanical preprocessing and pelletization, chemical pretreatments, and enzymatic hydrolysis of complex carbohydrates. To accomplish this, we are using biological and chemical treatments that use the long residence of storage to begin to break down biomass components—including acetyl and hemicellulose as well as lignin—thus resulting in a feedstock that is less recalcitrant. Both fungal treatment and alkali treatment combined with a 1-month storage duration were shown to increase extractable compounds in the biomass and have promise to indirectly add value to the biomass in the storage operation. The overall product of this research will be performance data for a range of potential methods to add value in the supply chain. This research also addresses multiple MYP barriers and contributes to the \$2.50/gal goals.



In pile storage model showing dry matter loss and temperature after 200 days

Photo courtesy of Idaho National Laboratory

#### OVERALL IMPRESSIONS

• Wet storage of biomass is a great area for DOE/BETO to fully understand, most notably the cost implications as potential value addition is balanced against increased handling costs. An understanding of the current negative cost state suggests that some discussions of the cost development pathway

screening to accompany the characterization pathway need to occur with adjacent FSL projects in the portfolio, perhaps resulting in integration of some concepts to mitigate risks associated with each.

- Wet storage treatments have the potential to help normalize feedstocks/blends in support of creating fungible feedstock.
- This project is a valuable contribution to the BETO portfolio because it is developing economically viable methods to manage high-moisture feedstocks to produce biofuels and bioproducts. The approaches are well described, and the presentation shows that substantial new information has been generated that could be very useful to potential project development. Addressing the potential for using the storage period to partially pretreat the biomass is very positive with exciting impacts. Scaling up the research is a logical and valuable future work activity. The fact that an industrial partner is already working on demonstrating the value-added approach is a great success story at this stage in the value-added component of the project.
- Wet bulk storage systems could return to the forefront with new approaches to address dry matter loss and feedstock quality.
- This is one of the most relevant projects in the FSL portfolio. Success here will solve several of the most pressing problems around feedstock variability, at least regarding corn stover and other materials with similar qualities. In turn, this would encourage the investment in and building of projects to advance BETO objectives according to the MYP. There was a good explanation of the applications for the development of a full commercial-scale storage yard. I am not sure the PIs have thought through other indirect impacts that this work could have on other parts of the overall enterprise of a cellulosic biorefinery. With the ability to bale wet material, the current SOT in baling operation costs could be cut by 10% or more; and if advanced harvest and baling were used, by as much as 50%. Advanced baling methods would also reduce the ash content of corn stover and in turn solve another of the most pressing impacts caused by feedstock variability.
- This well-designed project has applied principles of ensiling to the storage of corn stover and succeeded in building a model for biorefineries to use when planning their storage systems. Significant progress has been made on using the wet storage of this material to the advantage of certain end-use processes.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The project team thanks the review panel for their time and thoughtful comments. We have worked extensively during the project lifetime to understand the largest cost drivers in harvest, collection, and storage operations. Under best-case scenarios, storage costs as low as \$6.41/t have been reported within this task previously and are reflected in the analyses of INL's Feedstock Supply Chain Analysis task (WBS: 1.1.1.2). Best-case storage scenarios are not always a reality, however, and excess moisture in bales occurs for several reasons including harvest timing, field conditions, and climate. The current research goals of this project focus on optimizing storage conditions to reduce the variability and improve downstream reliability as biomass enters preprocessing, which ties closely with the goals of the FCIC. To that end, this task has focused on two reported challenges: (1) variations in bale moisture content, especially at the upper end of moisture content; and (2) degradation that occurs as a result of high moisture contents over time. Our supply system designs focus on enhancing bale drying rates in storage—early, before biodegradation occurs—through cost-effective means. These include using naturally occurring wind patterns through informed site selection and stack configuration, using microbial-generated heat to increase internal stack temperatures to enhance drying, using multiple storage methods to balance storage cost and storage performance, and using predictive models based on physical and biological properties to identify which lots should be delivered at what time to minimize compositional variations and maximize the value of the harvested biomass.

- Integral to this research effort is the NIR spectrometric probe, which was developed to overcome the challenges of within-bale variations in biomass composition and the need for rapid biomass analysis. This scope was transferred to this project from the "BALES" High-Tonnage Logistics II project in FY 2019. We agree with the reviewer's comments regarding corn stover, and in FY 2020 we plan to expand the use of this tool to include baled switchgrass. Lessons learned in corn stover and switchgrass will be applied to an expanding number of commercially relevant baled and bulk biomass feedstocks beyond FY 2022. Although the current programmatic shift to more fundamental technical research might not permit INL to focus on physical probe deployment and pilot-scale storage experiments, we will continue to work closely with external partners to develop robust and efficient means of probe application and confirmation of laboratory- and bench-scale results regarding storage stability and moisture migration in storage.
- We will continue to apply the tools that this project is developing, such as the NIR probe and the storage and queuing models, to anticipate and minimize variability such that high-quality biomass can be provided for preprocessing and conversion.

# SIZE REDUCTION, DRYING, AND DENSIFICATION OF HIGH-MOISTURE BIOMASS

### Idaho National Laboratory

### **PROJECT DESCRIPTION**

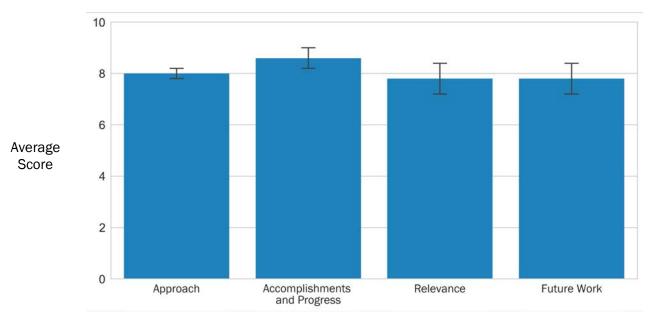
In FY 2017, the new processing technologies, fractional milling, high-moisture pelleting, and low-temperature drying were developed and demonstrated at the pilot scale using INL's process demonstration unit. TEA of the new technologies indicated that the corn stover pellet production cost was reduced by approximately 63% compared to a method that is currently followed by the pellet industry. High-quality pellets in terms of bulk density, 630–650 kg/m<sup>3</sup>, and durability, 98.4%, were produced by the new technologies. The studies also indicated that efficient moisture management, high-moisture pelleting, and going for 7/16-in. screen in the Stage 2 grinder had a significant impact on processing

| WBS:                      | 1.2.1.2             |
|---------------------------|---------------------|
| CID:                      | NL0026654           |
| Principal Investigator:   | Dr. Jaya Tumuluru   |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$4,856,804         |
| DOE Funding FY16:         | \$1,232,500         |
| DOE Funding FY17:         | \$1,232,500         |
| DOE Funding FY18:         | \$1,466,804         |
| DOE Funding FY19:         | \$925,000           |
| Project Status:           | Ongoing             |
|                           |                     |

cost. Several barriers still exist to deploying new pelleting technology to the biofuel and bioproduct markets. An INL National Renewable Energy Laboratory (NREL) annual operating plan project, FY 2017 2.2.1.102, and communications with industrial biofuel projects identified biomass particle attrition during preprocessing as a major issue for both biochemical and thermochemical conversion. Biomass particle attrition is the unintended size reduction that occurs during grinding and densification, resulting in the generation of increased fines. These fines are subsequently unrecovered in the downstream conversion processes. The INL NREL work showed an average mass loss of approximately 35% for corn stover pellets as a result of the generation of

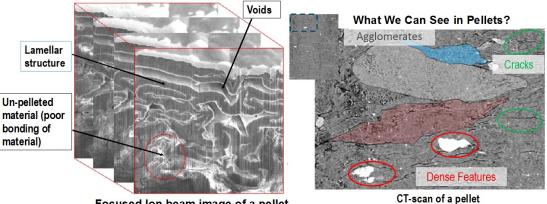
### Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

fines in the range of 400 microns-425 microns. During FY 2018-FY 2020, the project is extending the state of the art in biomass pelleting with science-based solutions to improve pelleting efficiencies and to meet the desired quality specifications. The major impact of this project is that it makes pelleting an economically viable solution to solve feed handling, quality, and cost issues. The overall objective of the project from FY 2018–FY 2020 is to solve the particle attrition of corn stover during preprocessing and enable pelleting as a viable option to produce conversion-ready cellulosic feedstocks. This is achieved by conducting fundamental research that allows proper matching of process variables with material properties to minimize biomass residence time in the pellet mill. Innovation will occur through an improved scientific understanding of biomass flow and compaction in a pellet mill, which will lead to technology improvements to produce optimized pelleted feedstocks. The end of the project goal is to reduce particle attrition during preprocessing of corn stover by 80%, i.e., less than 7% fines, of 425 microns, compared to the current value, 35% fines. In FY 2018, pelleting tests were conducted using a single pellet press to understand the impact of the pelleting process conditions, e.g., compressive force from 7 kN-11 kN; preheating temperature, 70°C-110°C; residence time, 45–150 s; corn stover properties moisture content, 10%–20%; wet basis; and screen size of the grind, 1 4-in. and 7 16-in. Results indicated that reduced moisture content of 10% increased the particle attrition, whereas increasing the moisture content to 15% wet basis (w.b.) and 20% w.b. decreased the fines in the pelleted material. Also, the study indicated that increased residence times of particles, 150 s, increased the fines in the pelleted product. At 10% w.b. moisture content and 150-s residence time, 26% fines were found in the pellets produced using a 6.35-mm grind, whereas increasing the grind size to 11.11 mm decreased the fines values to approximately 16%–17%. This study also indicated that the particle size distribution—mean particle size, D10, D50, and D90—in the corn stover pellets changes significantly with changes in the process variables. The optimized process conditions to minimize the fines in the pelleted corn stover to 12% were moisture content of approximately 20% w.b., 7 16-in. screen size of the grind, compressive force 9 kN, preheating temperature 90°C, and residence time of 45 s.



Focused lon beam image of a pellet



### OVERALL IMPRESSIONS

- Pelleting project relevance and success are notable, and the impact of process improvements is a key aspect of the biomass fungibility pathway. Congratulations. Great work by the project team.
- The reviewer would like to see some more diversity in the solution phase of the future work, especially regarding approaches to address the ash/fines issue. There are several industrial approaches to fines mitigation not presented that might be able to leverage even more added value to the process than the current state and future work plan.
- This very technical, narrowly focused project could be very useful to determining whether pellets can be an economically viable feedstock for bioenergy pathways. The research plan and implementation of the

plan has been excellent. The targets for the reduction of loss of biomass (particle attrition) were well defined, and clear progress has been made toward reaching those targets while providing valuable information about the feedstocks being studied and the composition of pellets. Future work on ash content removal is relevant. The presentation does not identify whether achievement of pellet technology improvement targets will result in making blended pellets economic at the total supply chain costs targeted by BETO.

- This project explores opportunities to reduce the cost of processing biomass while improving the quality.
- This is a very relevant project in the FSL portfolio. Success here will solve several of the most pressing problems around feedstock variability, at least regarding corn stover and other materials with similar qualities. Overall, I found the presentation to be informative about its goals, methodologies, and contribution to meeting BETO's goal of commoditizing high-quality biomass feedstock supplies; however, I find that the presentation is not detailed enough in its cost comparison because it compares only its cost to conventional pelleting processes. It should also consider avoided costs to current pretreatment methodologies at an integrated biorefinery research facility. In addition, I am not sure that the PIs have thought through other indirect impacts that this work could have on parts of the overall enterprise of a cellulosic biorefinery. If you could bale wet material, the current SOT in baling operation costs could be cut by 10%; if advanced harvest and baling were used, costs could be reduced by as much as 50%. The wide adoption of technology will occur only as we understand how it provides overall economic benefit to the industry it is addressing, which in this case is advanced cellulosic fuels and chemicals.
- This project is succeeding in demonstrating, at the pilot scale, how corn stover pelleting costs can be reduced and pellet quality can be improved through innovative drying, grinding, and compression methods.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- In FY 2020, we plan to collaborate with INL BETO projects that use chemical and microbial pretreatment methods for additional solutions to the fines issue during mechanical preprocessing. Mechanical methods such as fractionation and milling and mechanical separation techniques will be used to understand how various fractions, as well as the separation of fines in corn stover, impact the fines generation during grinding and pelleting. In FY 2020, we will explore chemical and microbial pretreatments methods tested in WBS 1.2.1.1000 (INL storage project), which can help remove most of the fines generating biomass components. We are working with the INL analysis team (WBS 1.1.1.2) to understand the technical and economic impact of using the fines that are generated during preprocessing for biochar production (which has a higher value as a soil amendment).
- The work focuses on improving the quality of the pellets for more reliable conversion performance. Even though pelleting enables many valuable logistics benefits that include storage, handling, and transportation, biomass particle attrition or fines in the product is a major impediment to the downstream conversion processes. INL reliability models also indicated that material properties such as bulk density, particle size distribution, and fines generated during preprocessing have a large impact on the feedstock supply cost to the biorefineries. The data generated in this project will be fed to the supply chain cost models developed in the project (WBS: 1.1.1.2). Also, we would like to clarify that in this project we are evaluating corn stover pellets, not blended pellets.
- Our INL analysis team analyzes the feedstock cost provided to a biorefinery by considering the feedstock supply, harvesting, storage, preprocessing, and transportation costs. The various projects in the FSL portfolio provide this information. We will work with our analysis team to consider in the SOT the impact of baling wet material and the impact of advanced harvesting and baling systems on the total cost of the feedstock provided to the biorefinery.

# RESOURCE MOBILIZATION (THROUGH COMMODITIZATION AND TRADE)

### Idaho National Laboratory

### **PROJECT DESCRIPTION**

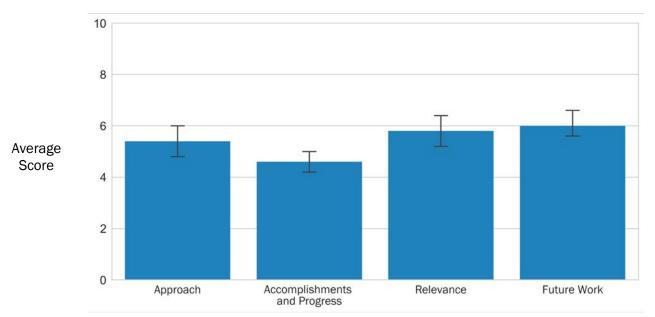
Key factors hampering the establishment of a national biorefining industry are the high costs and uncertainties of setting up the underlying supply chains, with one of the largest risks being access to a reliable and consistent supply of biomass feedstocks. Currently, access to feedstocks is exacerbated by the lack of producers willing to supply feedstock materials because of the immaturity of the industry and the personal risks involved in the production of biomass feedstocks. Although the benefits of establishing a biorefining industry include providing jobs and economic revenue, neither of the main actors—grower or biorefineries—have the perspective needed to solve the problem. Inherent in the problem is the conflict of interest

| WBS:                      | 1.2.1.5             |
|---------------------------|---------------------|
| CID:                      | NL0020844           |
| Principal Investigator:   | Dr. Damon Hartley   |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$1,086,340         |
| DOE Funding FY16:         | \$255,000           |
| DOE Funding FY17:         | \$255,000           |
| DOE Funding FY18:         | \$321,340           |
| DOE Funding FY19:         | \$255,000           |
| Project Status:           | Ongoing             |
|                           |                     |

between the parties involved: growers want to maximize their profits with limited supply chain buy-in, and the biorefinery needs to reduce supply costs with very limited bargaining power. The development of this industry is incumbent on increasing the value proposition to the grower through innovative supply chain and contracting structures. New feedstock companion markets that have the characteristics of commodity goods will ultimately reduce both cost and risk to the biorefinery. Companion markets would share new supply chain infrastructure, invest in new technologies, and contribute to the reduction of supply chain risk. Therefore, incorporating companion markets into the biomass mobilization strategy would increase recovery and use of

## Weighted Project Score: 5.5

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

all biomass fractions generated throughout the supply system and reduce supply costs to the biorefinery. Without the identification and development of mechanisms that drive the participation of growers into the development of feedstock supply chains, it will be nearly impossible to meet the BETO goal of fuel at \$2.50/GGE by the year 2030. This project directly supports this BETO goal by examining and identifying the opportunities that exist to increase value to the grower through comarkets and coproducts and supporting the mobilization of the billion-ton resource base. Specifically, this project addresses the barrier identified by BETO as Ft-A: Terrestrial Feedstock Availability and Cost. This project provides credible, objective analyses of feedstock supply systems and strategies to support BETO investments in the development of a sustainable, economically viable national-scale bioenergy industry. Additionally, this project (1) identifies drivers and barriers to participation for growers potentially supplying biomass, and (2) informs the development of advanced feedstock supply systems through the development of forward-looking analyses. As a result, this project helps BETO to guide R&D toward targets and gauge progress on feedstock supply system improvements across various research areas. Moreover, this project provides an opportunity to evaluate the feedstock supply system barriers faced by an expanding bioenergy industry in the United States.

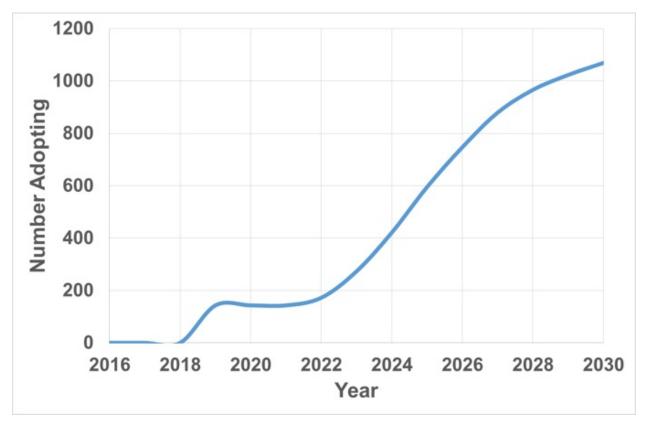


Photo courtesy of Idaho National Laboratory

### **OVERALL IMPRESSIONS**

- This project's goal is to identify and model socioeconomic behavior that will suggest strategies to increase farmer/producer participation in the biomass supply chain to support a growing bioeconomy. More work is needed not only on suggesting strategies but also on how to implement these strategies. Farmers are innovative but also slow to change from practices used for generations, and this will prove to be challenging.
- This is a very important project/effort.

- Deeper understanding of socioeconomic impacts on the adoption of biomass production is very much needed. Answering such questions at the necessary local (for accuracy) and regional/national (for policy) levels is extremely difficult. The project approach to build models and continue to add layers is reasonable; however, as noted by several members of the review panel, decision-making methodologies of farmers—when a lower price is the target—are very vast and fluid. The project needs to include more experience in this space, perhaps via more direct USDA partnership and relevant industry suppliers, to be able to have models that can be used to enable any short-term advance in feedstock availability.
- Fungibility of feedstocks via the depot concept is a parallel approach that would drive a different set of socioeconomic drivers, and based on the SOT analysis seems a reasonable way to focus the efforts as well as simplify the modeling to provide more clarity for policyholders.
- The reviewer would like to see some beta test cases applied in the future to validate models and to initiate "practice" policy models.
- The project has a worthy goal of trying to explain and model how socioeconomic factors affect grower decisions to produce new crops or modify existing crop production strategies to provide reliable supplies of bioenergy feedstocks; however, it is difficult to understand how the proposed management and technical approaches will achieve that goal. The project claims to be using "innovative" methods to evaluate barriers and opportunities for mobilizing resources; however, graphic results are shown without any explanation of which methods were used to derive them. The information on supply push developments that could result from reduced European demand for pellets is interesting, but the relationship to describing grower participation in providing feedstock supplies is not well explained. It is very unclear how the project will be able to meet the go-no-go goal of producing meaningful scenarios of strategies that are likely to increase grower adoption.
- Willingness for growers to participate in a bioeconomy is a complex socioeconomic problem.
- This socioeconomic analysis of feedstock growers' participation in the bioeconomy is a critical piece of modeling that needs to be closely integrated with other supply models. Progress here and plans to integrate this model with others being developed needs to be more fully explained.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree with the reviewer that the decision-making process employed by farmers is very heterogeneous and inconsistent depending on the scenario. We also agree that direct input from the producers and stakeholders is an invaluable resource when developing models like this. Throughout the project, we have been in contact with extension agents who work with the producers of bioenergy crops as well as businesses that are currently growing crops that could be used as bioenergy feedstocks. As the project continues, we plan to continue this dialog and hope to benefit from the knowledge gained through research projects such as the Sustainable Landscape Design (WBS 4.2.2.62), which is being led by the ANTARES Group and is collecting information about decision-making in terms of energy crops, directly from farmers.
- We are approaching the modeling in a stepwise approach in which behaviors and decision-making processes are being added to the model in a manner that allows for verification and validation. This type of modeling does not dictate the actions of the agent but rather institutes a set of rules that the agent must follow. Implementing the sets of behavioral rules in this stepwise manner allows us to ensure that the behavior that we have included in the model adheres to the specified rules and that the specification of the behavioral rules are manifesting behaviors that are reasonable.
- The presentation of this project represented two separate annual operating plan cycles, and between those cycles, the focus of the project morphed from a market analysis to a focus on the methods to affect

the adoption and implementation of bioenergy feedstocks. The information that was presented encapsulated two projects. Also, to represent all the work that had been completed, an overview of each was presented rather than a deep dive into a single topic.

• We agree that the impact of this project will be greater if the results are more fully integrated into the other modeling efforts; however the modeling that has occurred thus far has been different temporally. The modeling for the SOT projects is based on a mature industry, or  $n^{th}$ -plant scenario, and the feedstock supply analysis modeling is focused more on the potential that "could" realized given a set of future conditions and prices. The focus of this project is to try to understand the steps needed to attain the potential described by the feedstock supply analysis and ultimately reach the  $n^{th}$ -plant scenario described by the SOT analysis.

# **BIOMASS SUPPLY CHAIN RISK STANDARDS**

### Idaho National Laboratory

### **PROJECT DESCRIPTION**

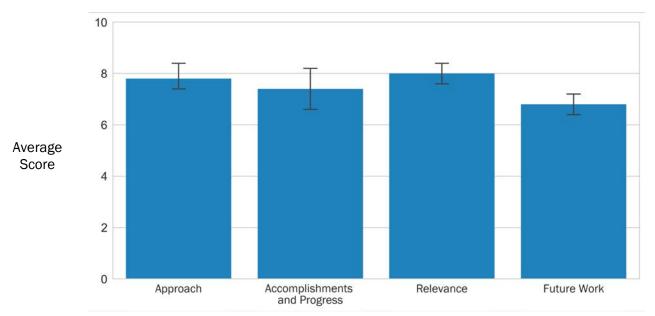
The Biomass Supply Chain Risk (BSCR) standards project was conceived to solve the problems of high costs of debt and slow takeoff of bioenergy projects in North America. Both issues are linked to poor understanding of the underlying supply chain risks, the inconsistent way the risks are evaluated by different stakeholders, and asymmetry of information on the risks. A three-phase approach was established to address the financial challenges of bioenergy projects. Phase I included the development of a BSCR standards framework database, housed at INL's Bioenergy Feedstock Library (BFL), to identify risk categories in the supply chain, various risk factors within each identified risk category, and various

| WBS:                      | 1.2.2.2             |
|---------------------------|---------------------|
| CID:                      | NL0019449           |
| Principal Investigator:   | Dr. Shyam Nair      |
| Period of<br>Performance: | 10/1/2014-9/30/2021 |
| Total DOE Funding:        | \$4,023,887         |
| DOE Funding FY16:         | \$752,250           |
| DOE Funding FY17:         | \$993,250           |
| DOE Funding FY18:         | \$1,267,089         |
| DOE Funding FY19:         | \$1,011,298         |
| Project Status:           | Ongoing             |
|                           |                     |

risk indicators within each identified risk factor. This is accomplished with inputs from a bioenergy industry stakeholders' group and an advisory board, together comprising more than 100 members, which were formed for this project. The current BSCR standards framework consists of six risk categories: supplier, competitor, supply chain, feedstock quality, feedstock scale-up, and internal organization. These risk categories represent more than 300 risk indicators categorized into the multiple risk factors identified for each risk category. The main focus in Phase II will be on developing a risk scoring and rating methodology that will be implemented using the database to allow consistent estimation of biomass supply chain risks for a bioenergy project as well as to demonstrate real-life reduction of the cost of debt coupled with a consistent understanding of risk,

### Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 ${f I}$  One standard deviation of reviewers' scores

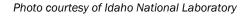
regardless of who conducts the assessment. In Phase III, the BSCR standards database, risk scoring, and rating methodologies will be verified across multiple bioenergy projects, and further efforts will be directed toward establishing an independent, industry-led standardization agency, a certification agency, and accreditation of the standards by ANSI.

Throughout all phases, a goal of this project is to provide state-of-the-science guidance for mitigating or assessing each risk indicator through identified resources, data, or knowledge built from existing data. The BFL houses not only the BSCR standards framework database but also a large amount of data on biomass and feedstocks across the United States, including analytic and metadata on more than 70,000 samples. For this project, publicly available BFL data will be formed into data sets, reports, and other tools to provide guidance on understanding and mitigating risk for relevant risk indicators. In addition, efforts are focused on creating a relevant data set and building a knowledge base for relationships between biomass variability in chemical characteristics and agronomic and environmental factors using historic data collected through the Regional Feedstock Partnership.

Using this three-phase approach, this project aims to demonstrate the utility of the BSCR to (1) more accurately quantify biomass feedstock supply chain risk and (2) verify the degree to which this standardized approach can decrease the debt costs of bioenergy projects based on real before/after investment data from actual bioenergy projects that require financing. The application of the developed potential BSCR standards and risk scoring and rating methodologies will be used with a case study to demonstrate a reduction in the project risk score of  $\geq 50\%$ .

|  | Rating   | Marks for Long-Te | rm Bonds Definitions  |
|--|----------|-------------------|---|
|  | High     | AAA               | Aost likely that debt obligations will be honored.  |
| <b>↑</b>   | <b>≜</b> |                   | High likelihood that debt obligations will be honored.  |
| Potential ratings increase with                          |          | <b>A</b> (+-)     | Reasonable likelihood that debt obligations will be honored.  |
| <b>Biomass Supply Chain Risk Sta</b>                     | ndards   | <b>BBB</b> (+-)   | There is a likelihood that debt obligations will be honored<br>but compared to the higher rating (A), there is the<br>possibility of a diminished likelihood of debt repayment. |
|  |          |                   | Repayment does not pose a problem at present<br>but may become problematic in the future.   |
| Typical bioenergy project ratings are in the junk region |          | <b>B</b> (+-)     | Probability of repayment is weak, with cause for concern  |
|  |          |                   | Repayment is uncertain and there is the danger<br>of default on debt obligations as a real possibility  |
|  |          | CC                | High likelihood of default on debt obligations  |
|  | +        |                   | Extremely high probability of default on<br>debt obligations.   |
|  | Low      | D                 | Defaulting on debt obligations.   |

Note: Credit ratings range from AAA to D, and are further subdivided into a total of 20 ratings (see chart) by the use of plus and minus signs for ratings AA to B.



#### OVERALL IMPRESSIONS

• This is interesting on a conceptual basis. Normally, one is reviewing the technical merits of a project that will hopefully solve a technical problem that is holding the biomass energy industry back. This is usually with a new conversion technology or some type of processing issue. This is extremely important work, however, because supply chain risk is one that the industry has never addressed in this manner. The rating agencies, i.e., Standard & Poor's, have never been able to assign ratings that take projects that are using conventional technologies or not out of junk financing status, which takes many projects out of

play because of the high borrowing cost. A successful outcome with this project will ensure the building of many projects.

- This project is a great effort in the direct response to feedback from earlier peer reviews. The TEA modeling (from other presentations) showed interest rates as the top cost sensitivity in the current *n*<sup>th</sup>-plant models; thus, the importance of success in this project should be a high focus for BETO (or else we will need to rely on the USDA to provide financing for some time).
- The approach and progress both seem sound. The reviewer understands there to be very good industry involvement but suggests vetting the list once more to ensure that the actual end user/stakeholders will endorse and use the rating as soon as the work is done.
- Often the result of looking deeper into factors and applying variation factors to *n*<sup>th</sup>-plant models is understanding that there is/are more risk(s) than originally perceived; thus, finalization of a feedstock supply risk reduction should be executed in tandem with variation control activities in other areas identified by the TEA team and presented together to avoid a swing in risk perception by investors.
- The need to better understand risk has been a major problem for research funded by DOE on all aspects of bioenergy development and demonstration since day one of DOE involvement (40 years ago). The creation of usable risk assessment tools could be a major assist to getting successful demonstration projects online and supporting the advancement of commercial enterprises. The extensive involvement of stakeholders in developing this risk evaluation tool is expected to contribute greatly to its usefulness. The need to balance detail and complexity with conciseness and ease of use will be ongoing. An aggressive effort to communicate the availability of this tool to a large array of potential users needs to be included in future plans.
- A supply chain risk tool can highlight areas that might otherwise be overlooked.
- Modeling feedstock supply risks will help credit sources understand aspects of the bioeconomy that they understand poorly now. This will help reduce capital costs if done accurately. Verifying the model developed here will be difficult because of the limited number of real case studies that exist.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The reviewer's comment that "a successful outcome with this project will ensure the building of many projects," is encouraging and confirms our belief.
- The project has vetted the FY 2018 BSCR standards with members of the advisory board and key industry stakeholders. This has resulted in a revision of the standards with primary focus on removing redundancies, consolidating risk indicators, and adding guidance to risk scoring to enable the actual end user/stakeholders to use the rating system effectively. The revised BSCR standards and the risk scoring and rating methodology with example application will be available for review at the end of FY 2019. The BSCR standards team is working in tandem with other TEA teams and other researchers at the national laboratories to ensure that results from this research are considered in the guidance for mitigating risks as well as for scoring and rating the risks. The BSCR standards database is designed to accept and review comments, store them in perpetuity, and accept changes to guidance for risk mitigation, scoring, and rating by team members in response to review comments or new research in the future directly from the advisory board and industry stakeholders' group. Additionally, the BSCR standards database is currently available online through the BFL (https://bioenergylibrary.inl.gov/Home/Home.aspx) and will made publicly available when the standards are finalized.
- The project recognizes the importance of disseminating the information on the risk scoring and rating tool to the stakeholders, and it has therefore submitted a separate proposal to BETO for technical

commercialization funding with matching interest from Canada with the sole purpose of accelerating the design and implementation of an outreach and communications plan. A key part of the effort is to get the BSCR standards accepted and accredited by Canadian and U.S. standards programs, such as the Standards Council of Canada and ANSI. Additionally, the BSCR standards database is currently hosted on the BFL (https://bioenergylibrary.inl.gov/Home/Home.aspx) and will made publicly available when the standards are finalized.

- This project has focused on gathering industry input from multiple facets of the supply chain to identify all the risk indicators that should be considered in the framework. This approach was intended to capture a large breath of risk and prevent "overlooking" aspects of risk that should be considered.
- The project understands the challenges posed in developing realistic case studies for the verification of the risk scoring and rating methodology. Ecostrat is a subcontractor for the BSCR standards project and a key member of the team with considerable experience in the biomass supply business. With the contribution from Ecostrat and other key stakeholders, we believe that we can design realistic case studies well in advance of the FY 2020 go-no-go decision on the project. Note that the case studies used throughout the project are intended to be reviewed and approved by the advisory board.

# DEMONSTRATION OF AN ADVANCED SUPPLY CHAIN FOR LOWER COST, HIGHER QUALITY BIOMASS FEEDSTOCK DELIVERY

### **FDC Enterprises**

### **PROJECT DESCRIPTION**

This project demonstrated an advanced biomass supply chain for high-impact, high-quality feedstocks from the field to the throat of a biorefinery. In doing so, the project addressed several key technical barriers identified by the BETO biomass feedstock supply platform. This project built on the earlier supply chain innovations of project team members to reduce feedstock costs. This work highlighted key gaps throughout the supply chain where

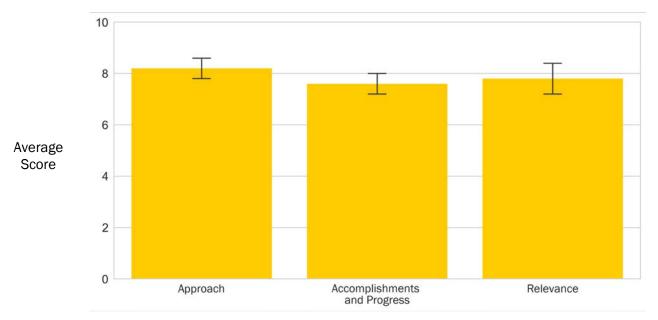
| 1.2.3.106           |
|---------------------|
| EE0006300           |
| Mr. Kevin Comer     |
| 9/30/2013-3/31/2018 |
| \$5,400,000         |
| Sunsetting          |
|                     |

biomass harvesting and preprocessing costs could be further decreased while maintaining the end user's feedstock quality specifications.

This effort included designing and deploying new systems associated with end-use processing (new milling equipment, advanced bale handling, NIR monitoring and sampling, etc.), further refinement of feedstock production equipment developed and demonstrated under prior efforts and testing by this and other project teams, and demonstration of new feedstock harvest and logistics equipment. Importantly, this included the development of equipment and processes to provide biorefiners and harvesters the flexibility to produce and use round and/or square bales more efficiently and cost-effectively than is possible using today's off-the-shelf conventional equipment. The project team designed, fabricated, and tested several new equipment innovations, conducted commercial-scale biomass harvest demonstrations, developed, and tested new methods for analyzing biomass feedstocks with NIR methods both in the field and in a process line, and addressed soil

## Weighted Project Score: 7.8

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

sustainability issues. Biomass preprocessing testing was also performed at pilot and commercial scales. The testing revealed new results that could better inform future equipment and system designs for preprocessing herbaceous biomass in a manner required to meet biorefinery specifications.



Photo courtesy of FDC Enterprises

### OVERALL IMPRESSIONS

- Great progress was made here developing prototype equipment for efficient bale-handling systems in the field, in transportation, and at the refinery. Manufacturers were engaged throughout the process, and systems were adequately demonstrated.
- This is a big project with a lot of moving parts (literally) that was able to develop and demonstrate several different front-end equipment systems. The project took considered needs along the entire system, including labor, soil health, and existing industry. The project developed several working systems, including one that has already been scaled up at POET-DSM Advanced Biofuels. The presenter did a good job of illustrating the design-build-test-learn (DBTL) cycles used to succeed.
- This project has a full complement of work in terms of feedstock supply and logistics from the in-field crop to the reactor throat. NIR analysis results, not yet available, will provide more information on the feedstock characteristics and potential end uses.

- This is a good project that achieved favorable results and will help BETO reach its goals in the MYP of providing terrestrial feedstock in the form of corn stover to a reactor at \$84/dry ton. That said, I believe that the results would be even better if these were compared to other similar operations, and cost comparisons were made. I think the project slips somewhat into a one-size-fits-all approach. For example, if you use a single-pass machine (combined with a baler attached) or a wind-rowing variable-rate corn head, you cannot separate the corn harvest from the stover harvest even though the stover might not be ripe for harvest simultaneously with the grain.
- This is an extremely comprehensive project aimed at increasing the probability of making the feedstock supply chains of corn stover and some herbaceous crops economically viable with boots-on-the-ground work. Much was accomplished in the 5-year time frame of the project. The project is a great example of what can be accomplished by a team of private-sector stakeholders working in collaboration with researchers and project developers.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# NEXT-GENERATION LOGISTICS SYSTEMS FOR DELIVERING OPTIMAL BIOMASS FEEDSTOCKS TO BIOREFINING INDUSTRIES IN THE SOUTHEASTERN UNITED STATES

### **University of Tennessee**

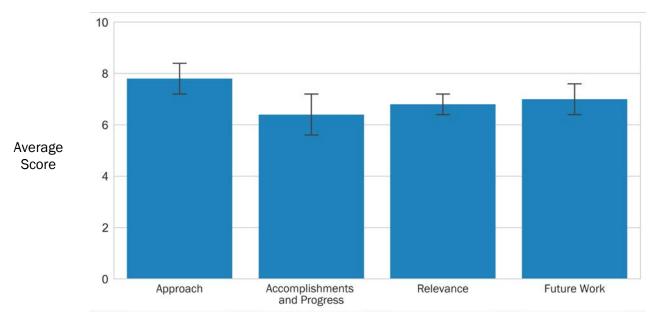
### **PROJECT DESCRIPTION**

The diverse portfolio of biomass sources that is available in the Southeastern United States, including a significant supply of pine "residue," represents a valuable strategic position for the region. Through blends formulated based on critical properties, this project will take full advantage of the range in biomass properties afforded by the portfolio to produce a consistent, high-performance feedstock for the industry while reducing cost. Key developments being

targeted to enable this potential include whole-tree transport to a state-of-the-art merchandising depot that will further access biomass from ongoing forest industry operations. The approach will more effectively use the tree and distribute cost while minimizing in-woods contamination of the woody biomass component. To implement this vision, information on the chemical composition and changes that are induced during multiple preprocessing steps (size reduction, moisture removal, densification, etc.) is needed. New NIR sensor technology will be developed for online monitoring of important biomass properties. The data will be incorporated into a statistical process control platform to improve process efficiency and meet required specifications. Advanced process models are being developed to inform the TEA and LCA of the program's impact. The new system will ultimately reduce operational risks from supply chain disruptions and allow for the operation of larger biorefineries.

### Weighted Project Score: 7.0

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores



Photo courtesy of University of Tennessee

### OVERALL IMPRESSIONS

- This project seeks to tap the woody and grassland resources of the Southeast in creative and synergistic ways. The novel idea here is to combine raw feedstocks in ways to meet quantity and quality requirements of a variety of bioproduct conversion processes. It remains to be seen how widely this technique will be adopted by a nascent bioeconomy, but the idea is intriguing.
- This is a key project in support of the SOT effort to reduce the cost of feedstock (depot concept).
- Despite some setbacks with regard to losing their site partner, the project has worked hard to prove out the concept and identify a new partner. The project will run over on time but not cost.
- The project contained all the needed components for feedstock supply chain system evaluation in the Southeast and pulled together an excellent team of collaborators. The evaluation of feedstock supply scenarios using depots and pelleting to assist in meeting storage and quality standards for biomass feedstock supplies is conceptually a valuable contribution to the BETO portfolio. There are hints that much good work has been accomplished; however, the presentation did not contain enough information to properly assess the progress or the likelihood of the project goals being accomplished.

- The project addressed a variety of identified FSL barriers. Methods explored for increasing pine biomass from the stump to the mill do not seem to require a large additional capital investment by traditional logging firms.
- I would have welcomed some detail about the relevance of past work and its relationship to this work in the presentation. The economics of operating an advanced merchandising depot were discussed, but I could not determine if the costs of getting raw biomass supplies to the depot was part of this work. If it was, it was not clear; and if it was not, I would have expected it to be included. Their reliance on switchgrass in this work and system makes for a better system, especially at large scales, but the barrier of access to potential large supplies necessary to operate this type of depot could seriously impair the development of this type of system.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# IMPROVED ADVANCED BIOMASS LOGISTICS UTILIZING WOODY AND OTHER FEEDSTOCKS IN THE NORTHEAST AND PACIFIC NORTHWEST

### The Research Foundation of The State University of New York College of Environmental Science and Forestry

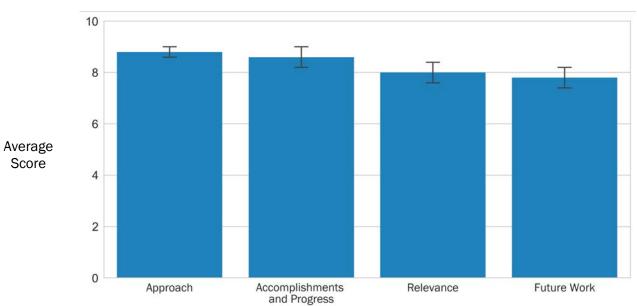
### **PROJECT DESCRIPTION**

The goal of this project is to reduce the delivered cost of hybrid poplar in the Pacific Northwest and willow woody crops in the Northeast to \$84/dry ton (\$92 dry Mg) by optimizing and demonstrating a supply system while maintaining the quality of the biomass. The project is divided into five task areas: (1) harvest and logistics, (2) transport and storage, (3) preprocessing, (4) feedstock characterization, and (5) logistic and economic modeling.

| WBS:                      | 1.2.3.108          |
|---------------------------|--------------------|
| CID:                      | EE0006638          |
| Principal Investigator:   | Dr. Tim Volk       |
| Period of<br>Performance: | 4/1/2016-6/30/2019 |
| Total DOE Funding:        | \$2,320,182        |
| Project Status:           | Ongoing            |

Tasks are integrated using an iterative process involving data collection from commercial harvests, provision of these data to modeling teams, and addressing data goals or application of suggested improvements in subsequent harvests. During this project, almost 800 wagon loads of willow and poplar chips were harvested and monitored in a wide range of field and crop conditions as part of Task 1 to assess the effect on machine performance and fill specific data gaps identified by the modeling task group. Studies of woody crop chips stored over time in Task 2 has provided valuable insights on how season, preprocessing, pile construction, and protection of piles affect dry matter loss, moisture, and other quality attributes. Some results raise questions about how quality is tied to biomass value and how growers are compensated for the material that is delivered. Field trials suggest that bulk density of willow chips is more variable in collection vehicles than has reported in the literature using standard methods on small containers. This has implications for cost and environmental

### Weighted Project Score: 8.3



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

 $oldsymbol{oldsymbol{oldsymbol{eta}}}$  One standard deviation of reviewers' scores

modeling of these systems. Task 3 process demonstration studies at INL suggest that high moisture densification and coarse grinding of willow and poplar reduce energy consumption by 20%–40% for densification. In addition, partners have identified the best choice of time and temperature to optimize the hot water extraction preprocessing technology and provided the necessary model inputs so hot water extraction can be included in the INL Biomass Logistics Model. In Task 4, wet chemistry data from 77 samples was used to develop NIR models, and spectra for more than 1,500 willow and poplar samples were collected. In Task 5, each of the three modeling efforts was impactful: Integrated Biomass Supply Analysis and Logistics modeling has shown that costs range from \$26 to \$45 per Mg and are lowest when silage trucks are collection vehicles. The West Virginia University model completed an optimized siting model identifying 15 potential locations for biorefineries in the northeastern United States and delivered biomass cost ranged from \$68 to \$87 dry Mg based on site and social factors.

#### OVERALL IMPRESSIONS

- This project addressed the highest cost aspects of SRWC production (harvesting and handling) and demonstrated ways to improve the state of the art and reduce costs. Progress was also made in exploring one option for feedstock upgrading using hot water extraction technology.
- This is a good project that created a lot of frontend data and laid groundwork for logistics needs for short-cycle woody biomass as well as compositional effects of storage. Effort changed the minds of several existing biomass operations with regard to taking willow into their operations, to the point where a competitor in Canada appeared. Finalizing the project will be important; it seems like there is a lot to do to finish runs at the Biomass Feedstock Process Development Unit.
- This project has a great team of collaborators with the correct expertise to develop information needed by BETO to meet national goals of developing sustainable technologies to provide a secure, reliable, and affordable woody feedstock supply for the U.S. bioenergy industry. This project has gone a long way toward catching up with the types of handling, storage, and processing information already known about corn stover and switchgrass so that SRWC have every possibility of being a feasible and desirable feedstock in regions where willows and poplars make the most sense as dedicated crops for bioenergy and bioproducts. The involvement of the private sector and state agencies in the project should accelerate the possibility that commercial entities will use the information. This integrated systems project appears to be progressing very well with all tasks; however, much work remains to pull all the information together for final reports and dissemination to stakeholders.
- This project provided a full complement of tasks for understanding the complexities of harvesting coppiced woody biomass.
- The project performers created a presentation that is clear, concise, and well executed. When completed, the project can have a solid effect on the bio-based economy by promoting the use of SRWC as a viable, high-quality, and sustainable source of feedstock. The only real weakness I see in the project and presentation, however, is that there was no attention in the future work on how to promote the use of these feedstocks and get our agriculture community to grow them.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# WASTE TO WISDOM: UTILIZING FOREST RESIDUES FOR THE PRODUCTION OF BIOENERGY AND BIOBASED PRODUCTS

### **Humboldt State University**

### **PROJECT DESCRIPTION**

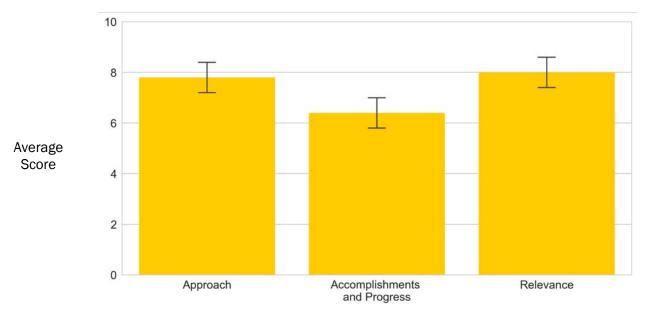
Overcoming the barriers to using low-value forest residues that are generated from forest management activities can be accomplished by employing biomass conversion technologies. At present, the greatest obstacle to increasing the use of these materials is the high transportation cost. Biomass conversion technologies can convert comminuted forest residues into biochar, torrefied pellets, and briquettes, thereby improving their market desirability,

| WBS:                      | 3.4.1.4              |
|---------------------------|----------------------|
| CID:                      | EE0006297            |
| Principal Investigator:   | Dr. Han-Sup Han      |
| Period of<br>Performance: | 9/30/2013-12/31/2017 |
| Total DOE Funding:        | \$5,881,974          |
| Project Status:           | Sunsetting           |
|                           |                      |

increasing their value, and increasing transportation efficiencies. The Waste to Wisdom project was part of the Biomass Research and Development Initiative, and funded by DOE (DE-EE0006297) at \$5.8 MM. Our interdisciplinary research team—comprising academics, business professionals, and land managers—worked together for approximately four years (September 2013 to December 2017) to (1) develop system logistics that improve the economics, accessibility, and production of high-quality feedstock; (2) evaluate and scale up stand-alone biomass conversion technologies that are operated at or near the forest for their commercialization; and (3) perform economic analyses and life cycle emissions analysis to enhance the sustainability of biomass use through improved knowledge of socioeconomic and environmental benefits. The Waste to Wisdom project found that the commercialization of biomass conversion technologies has the potential to improve the economics of forest management activities, improve forest health, reduce catastrophic wildfire, sequester carbon, and reduce GHG emissions. In addition, the project could create employment in the forest and energy sectors, support economic development in rural areas, and effectively reduce our nation's dependence on fossil

### Weighted Project Score: 7.2

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



L One standard deviation of reviewers' scores

fuels by incorporating renewable fuels into current bioenergy and coal-fired energy facilities. We encourage those who are interested to visit the project web site (http://wastetowisdom.com/) to learn more about the team's research on feedstock development, biomass conversion technologies, and the financial and environmental benefits of using forest residues for the production of bioenergy and bio-based products.

### **OVERALL IMPRESSIONS**

- This project explored ways to reduce the environmental and carbon impacts of current logging slash disposal practices in the Northwest while creating value-added products from this otherwise unavailable material. Unfortunately, the economics of this practice are still far from practical without allowing for the value of certain intangible benefits to the environment (e.g., air quality improvements, fire suppression).
- This is a good project result with no scaling factor to commercial scale as well as some reasonable window for commercial viability. The concept solves a real technical problem on how to handle forest thinnings in a practical way; however, the project did not seem to have a well laid out commercialization plan, and thus focus on the business case needs to be executed to validate the financial assumptions and define a commercialization partner/municipality.
- This project explored a wide variety of topics that add value to biomass prior to delivery to an end-user facility.
- Forest residue has long been looked at for use as a fuel or feedstock and is a significant resource according to the 2016 Billion-Ton Report; however, as most know, it is challenging from an economic standpoint to create a profitable enterprise. This project addresses that by bringing three different conversion technologies to the forest and then creating useful and profitable products at demonstration scale. A good marketing plan could help create some positive commercial activity around this concept and help elevate the work BETO is doing.
- The project achieved its stated goals of producing products from forest residues, developing three feedstock processing systems that could be performed near forestry operations sites, and evaluating the feasibility of the feedstock products for economic viability in bioenergy and bioproduct markets. An outcome of the project was the development of a baler for forest residues that might be a useful first step in other systems using forest residues. Demonstrations of the three process systems provided the information needed to evaluate costs and identify efficiency factors. The reported total system costs of producing biochar, biomass briquettes, and torrefied briquettes were too high to be useful in supporting the achievement of the bioenergy cost goals of BETO, though information was gained on improving efficiencies of the systems. The biochar product was the most interesting product because it might have a bioproduct market in some locations, and it has strong environmental benefits (soil remediation and carbon sequestration in the soil).

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# CEMAC: EVALUATION OF AGRICULTURAL EQUIPMENT MANUFACTURING FOR A BIO-BASED ECONOMY: NREL

### National Renewable Energy Laboratory

### **PROJECT DESCRIPTION**

This study analyzes agricultural and preprocessing equipment and manufacturing requirements to support the mobilization of the projections in the DOE 2016 Billion-Ton Report using the conventional supply chain logistics. The report discusses the required number of agricultural machines and their market values, the drivers and barriers of the transition in agricultural equipment, the potential economic impacts to the United States associated with this transition, and the factors that impact the transition in agricultural machinery to support the growth of a largescale biofuel and bioproduct industries.

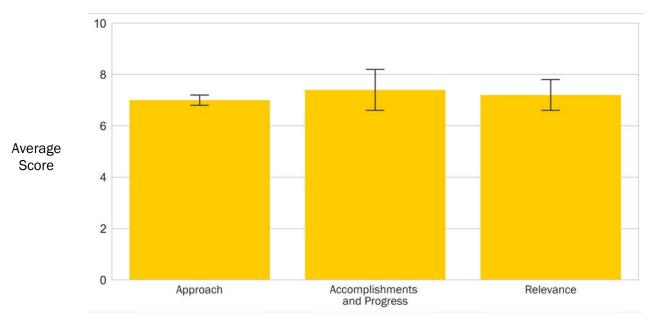
| WBS:                      | 6.3.0.8             |
|---------------------------|---------------------|
| CID:                      | NL0030036           |
| Principal Investigator:   | Dr. Chad Augustine  |
| Period of<br>Performance: | 10/1/2016-3/31/2018 |
| Total DOE Funding:        | \$93,900            |
| DOE Funding FY16:         | \$50,000            |
| DOE Funding FY17:         | \$6,000             |
| DOE Funding FY18:         | \$37,900            |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

Five major biomass resources are selected for the analysis

of feedstock equipment and manufacturing requirements to support the mobilization of commercial quantities of biomass resources using the conventional supply chains: corn stover, switchgrass, miscanthus, coppice woody crops, and non-coppice woody crops. Based on the *2016 Billion-Ton Report*, 304 million–652 million tons per year of these biomass resources are available from agricultural lands in the United States. Using the Oak Ridge National Laboratory Supply Characterization Model, the selected biomass resources could support an estimated 240–358 potential biorefineries that convert 230 million–340 million tons of selected biomass resources to biofuels annually. In the short term, it is estimated that approximately 280,000 pieces of

### Weighted Project Score: 7.2

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

equipment with a market value of \$36 billion would be required to harvest and deliver the biomass to the biorefineries. In the long term, this number is estimated to be approximately 380,000 pieces with a market value of more than \$47 billion. Analysis of the current U.S. agricultural equipment manufacturing industry suggests that approximately 70%–80% of total U.S. agricultural equipment demand is supplied from domestic manufacturers. Assuming that U.S. agricultural equipment manufacturing under the *2016 Billion-Ton Report* scenarios are similar, the sum of direct long-term employment impacts from U.S. agricultural equipment manufacturing is more than 56,000 full-time equivalent job years, and the sum of the total long-term impacts is more than 340,000 full-time equivalent job years. The domestic manufacture of the required equipment would result in almost \$11 billion in direct value added (contribution to the gross domestic product [GDP]) and nearly \$40 billion in total value added (contribution to the gross domestic product) during the long term. These are upper-end estimates because they assume that 75% of all agricultural equipment is manufactured domestically and that all required agricultural equipment is newly manufactured.

The study identifies and studies several recent transitions that took place in the agricultural farm machinery and the preprocessing equipment. These transitions are evaluated to outline the drivers and barriers of these new pieces of equipment. These transitions also provide insights into the transition needed from existing biomass supply chain systems to advanced supply chains. The project team completed this task by contacting and interviewing the companies behind the development of these pieces of equipment. Farm machinery supply chains need strong signals from biomass producers, biomass logistics companies, and biomass end users to tackle the barriers for the adoption of new technologies.

### **OVERALL IMPRESSIONS**

- Understanding the harvesting equipment needs to satisfy a hopeful large buildout of biomass production is important to educating the suppliers as well as the users. The project used several very key assumptions to scope the work that, once built out, paints a relatively clear picture for the future.
- The SOT moves toward blended feedstocks, pelleting, ownership, and other cost drivers, however, will likely significantly change the conclusions of this study, and as a result should also be modeled to fully build out the equipment supply picture.
- This was a straightforward, well-focused project addressing relevant and important questions about potential equipment manufacturing requirements as well as potential impacts on jobs and GDP. The approach was excellent in terms of using expertise from the DOE laboratories involved in considering feedstock supply issues and in communicating discussions of the issues together with industry stakeholders. The objectives of the project seemed to be totally addressed, the results were presented very clearly, and a well thought out interpretation of the results was included in the presentation. This analysis is a good complement to the Feedstock Supply Chain Analysis and the Supply Scenario Analysis projects also funded by BETO. As with all these modeling efforts, the results are useful for planning and communicating what a future situation might look like but are not predictive with the many changes in supply chain details that will inevitably occur.
- This project provides insight into how the feedstock supply chain could positively impact equipment manufacturing and jobs.
- I think interfacing more with industry would have helped clarify the size of this potential requirement as it relates to the existing agricultural equipment market. For example, although the tractor market in North America is some 280,000 units, only 10% of these are in the high-horsepower category, the size needed to operate the various implements in either the baling or chopping scenario. Therefore, in the baling scenario, estimates are for approximately 50,000 units in the short-term, early-development phase, equal to +/- 200% of today's production. This could also be said of the balers and forage choppers. Depending on the ramp-up of the industry, this could put tremendous pressure on the industry in terms of

manufacturing capabilities on all fronts: manufacturing facilities, engineers, steel fabricators, labor, dealers, and parts manufacturing, to name a few.

• This project made a first attempt to estimate the machinery requirements for bioenergy feedstock harvesting and handling in agricultural systems across the United States and to estimate the economic impact this might have on the country. Assumptions made to model this impact are enumerated, so adjustments can be made if different assumptions are deemed to make more sense.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

TECHNOLOGY AREA

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# INTRODUCTION

The Feedstock-Conversion Interface Consortium (FCIC) Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place on March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of nine projects were reviewed in the FCIC session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$40,274,601 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 2% of the BETO portfolio reviewed during the 2019 Project Peer Review. During the Project Peer Review meeting, the principal investigator (PI) for each project was given 20 to 40 minutes (the presentation length was shortened for the consortium overview presentation) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, and relevance to BETO goals. An additional presentation was dedicated to future work and plans of the FCIC. This section of the report contains the results of the Project Peer Review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the FCIC, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Mr. Beau Hoffman as the FCIC Technology Area review lead, with contractor support from Mr. Andrew Kobusch (Allegheny Science & Technology). In this capacity, Mr. Hoffman was responsible for review planning and implementation with support from Dr. Mark Elless and Ms. Liz Moore, who represent the Feedstock Supply and Logistics (FSL) and Advanced Development and Optimization (ADO) programs, respectively.

# FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM OVERVIEW

Many process bottlenecks and difficulties experienced in the nascent bioenergy industry are centered on feedstock handling and preprocessing operations. These issues often arise from the complexity in feedstock physical, chemical, and mechanical attributes that are present in lignocellulosic biomass feedstocks. The FCIC seeks to quantify, understand, and manage variability in biomass feedstocks, from field through downstream conversion, and to understand how biomass composition, structure, and behavior impact system performance. The FCIC ultimately aims to develop first-principles-based knowledge and tools for technology development firms to use when designing, building, and operating biorefineries and to develop a framework through which technology developers can assess the quality and value of streams to achieve successful operations.

The FCIC began as a virtual consortium incorporating research-and-development (R&D) efforts from BETO's FSL, conversion, and ADO programs. Several projects from the FSL and conversion programs were integrated into this consortium. The consortium at its inception in FY 2018 focused on six key tasks: Feedstock Variability, Feedstock Physical Performance Modeling, Process Integration, System-Throughput Analysis, Process Controls and Optimization, and Industry Engagement/Project Management. Building on experimental and modeling developments, in FY 2019, the FCIC reorganized to focus on five tasks dedicated to various steps in the process chain: Feedstock Variability, Materials Handling, Preprocessing, Low-Temperature Conversion, and High-Temperature Conversion; as well as three enabling tasks that crosscut these unit operations: Materials of Construction, Data Integration/Management, and Crosscutting techno-economic analysis (TEA) and life cycle assessment analyses. These R&D efforts feed into a quality-by-design approach to ultimately manage variability and process risk in a systematic manner.

The FCIC Peer Review Panel reviewed the original six key tasks. The panel also reviewed future plans that cover the current quality-by-design approach and the eight tasks that are currently being pursued.

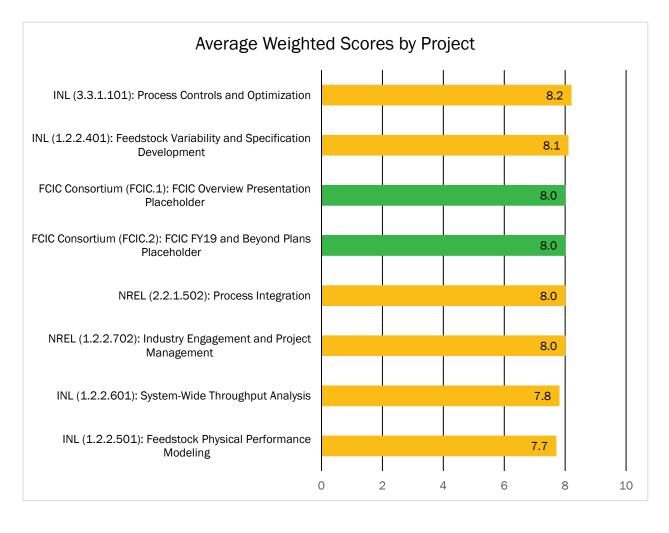
## FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM REVIEW PANEL

The following external experts served as reviewers for the FCIC Technology Area during the 2019 Project Peer Review.

| Name           | Affiliation                     |
|----------------|---------------------------------|
| Brandon Emme*  | ICM, Inc.                       |
| Andrea Slayton | Slayton Technical Services, LLC |
| Glenn Farris   | AGCO Corporation                |
| Lorenz Bauer   | LJB Chemical Consulting         |
| Benjamin Levie | Seattle City Light              |

\* Lead reviewer

## **TECHNOLOGY AREA SCORE RESULTS**



Sunsetting Ongoing New

## FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM REVIEW PANEL SUMMARY REPORT

#### Prepared by the Feedstock-Conversion Interface Consortium Review Panel

Realizing high uptime at pioneer commercial cellulosic facilities has continued to be a monumental challenge. Current technologies for delivering the feedstock to the reactor throat based on pulp and paper industry experience has proven to be insufficient for agricultural residues and similar materials. Feedstock characteristics such as tramp, ash, and variable moisture cause disruptions in feeding systems (plugging and abrasion) and induce conversion variations. The FCIC was created to identify and address these challenges though a crosscutting effort leveraging the skill sets of the DOE national laboratories supported by an industry advisory board (IAB).

#### IMPACT

Knowledge attained by the FCIC projects informs equipment suppliers servicing the lignocellulosic industry, reduces risk and promotes improved process reliability, especially at the reactor throat, as a result of feedstock variability. The capabilities of both the Biomass Feedstock Process Development Unit (PDU) at Idaho National Laboratory (INL) and the Integrated Biorefinery Research Facility at the National Renewable Energy Laboratory (NREL) provide scalable information on equipment and process performance for both thermochemical and biochemical processes for relevant feedstock qualities (e.g., high- and low-moisture and ash). The comprehensive national laboratory crosscutting project management structure of the FCIC projects further augment the tools and knowledge base.

The panel received a good impression that the projects were well designed to meet the goals of the FCIC and further identified which questions to explore next (e.g., advanced controls, improved equipment design). The characterization database is a useful tool for industry. Increased communications of the FCIC project results could increase visibility in the industry, especially around priority specifications.

#### **INNOVATION**

The FCIC projects provide several significant findings, including:

- X-ray diffraction methods for looking at feedstock and determining ash content
- System-wide throughput analysis, including process reliability impacts. Quantification of the impact of feedstock moisture and ash content on plant uptime as well as human intervention was relatively similar for both low- and high-temperature processes.
- Demonstration of improved feedstock milling through an adaptive control strategy was able to show high uptime but at the cost of less than design capacity.
- TEA models with the capability to include unit operation uptime reliabilities lead to the identification of system-wide throughput for pioneer plants.
- Material flow modeling in bins and hoppers (although many results are too complicated for a layperson to understand).

#### **SYNERGIES**

The FCIC project portfolio represented a concerted effort to integrate development efforts, most notably by characterizing feedstock moisture and ash variation from the field through the PDUs at INL and NREL and by integrating process data into the TEA analysis modeling system-wide throughput. Further computational modeling of biomass flow in bins and hoppers was also performed but was not able to adequately predict flow

reliability. In support of synergy, the national laboratories also produced a primer glossary to align nomenclature for industry.

#### FOCUS

The future strategy to refocus the FCIC on the development of first-principles-based knowledge and tools for technology development firms to use when designing, building, and operating biorefineries has the potential to cross over and illuminate empirically based equipment choices. The output value could be increased by simultaneously developing a framework that technology developers could use to assess the quality and value of streams to design at a broader systems level.

#### COMMERCIALIZATION

The FCIC portfolio was narrowed following the recommendations from the 2017 Project Peer Review. This resulted in more direct understanding of the impacts of feedstock moisture and ash content on the process uptime and human intervention, although full clarity was not attained as a result of other uncontrolled/uncontrollable processing factors at the PDU scale. The findings of the FCIC projects are useful, and as such the panel encourages the national laboratories to create more visibility of the results through a more deliberate marketing strategy, especially if this could also be used to create collaboration opportunities among the FCIC teams and industry.

#### RECOMMENDATIONS

Following are recommendations from the review panel:

- Integrate as many developments included in the state of technology (SOT) into the FCIC demonstration/benchmarking runs as possible. In particular, the impact of blending depot and pellets on plant reliability and uptime should be quantified as well as mitigation strategies should be developed for controlling moisture and ash content in the reactor feedstock.
- Ensure that the goals of the quality-by-design/first-principles focus will result in commercially relevant process reliability and demonstration by stretching the success rate target and timing.
- Create more industry immersion experiences for the national laboratories/BETO to ensure relevance to pioneer plants/industry. Continue to leverage the value of the IAB to support project relevance when direct feedback from pioneer plants is not available. Consider innovative methods for getting industry knowledge into the national laboratories (fellowships, analytical loaners, FCIC meetings on-site at industrial entities, etc.).
- As part of the first-principles strategy, establish quality specifications on feedstocks as they pertain to reliable delivery to the reactor throat along with mitigation methods in design, storage, and operations for high-moisture content.
- Develop a clear marketing plan to aggressively promote FCIC projects and output on a widespread basis to achieve greater industry adoption. Increase visibility through road shows at relevant industry conferences and pioneer plants. Consider whether a skill/resource map of the national laboratories might support this.

## FEEDSTOCK-CONVERSION INTERFACE-CONSORTIUM PROGRAMMATIC RESPONSE

#### INTRODUCTION/OVERVIEW

The FSL, Conversion R&D, and ADO programs thank the five reviewers for their time and careful review of the portfolio. We recognize that many technical disciplines are represented in the work of this consortium, thereby requiring a multidisciplinary panel. We also recognize that it is a difficult review processes because additional projects relevant to this work are present in many different sessions. Across the BETO portfolio, we have been working to adjust the format of the Project Peer Review to best communicate the efforts ongoing within our national laboratory consortia.

The following sections specifically address the recommendations from the review panel.

#### Recommendation 1: Quantify blending, depot, ash, and moisture impacts.

The programs concur that quantifying the technical, economic, and sustainability impacts associated with any process change or feedstock attribute is a critical first step. In reorganizing the FCIC in FY 2019 and FY 2020, the programs have established a designated crosscutting analysis task to perform these cost-benefit and trade-off analyses. The programs have communicated the need to maintain adequate resources to be responsive to these process changes and feedstock attributes. Feedstock processing strategies that are employed to manage critical material attributes (e.g., inorganic species, intrinsic moisture) will be evaluated to investigate the costs associated with that unit's operation and to quantify the impacts for other unit operations both upstream and downstream. These technical performance experiments will be subjected to TEA to ensure that feedstock processing choices lead to systems-level techno-economic and sustainability improvements.

In response to the desire to explore blending options, the programs agree that there is economic opportunity associated with this strategy and will consider this in the future. Blends will not be explored in the first 3 years of this consortium. At present, the focus of the consortium is on understanding the physical, chemical, and mechanical effects imparted by single feedstocks (i.e., corn stover and forest residues). The rationale is that through a fundamental science-based understanding of the physical, chemical, and mechanical effects of individual feedstocks, the identification of critical material attributes and the impacts of processing on product quality can be identified and quantified. Once the critical material attributes are understood for individual unit operations, we might investigate other feedstocks or blends.

In response to the desire to explore depot processing, the programs believe that a depot concept could support commoditizing lignocellulosic biomass feedstocks; however, given the nascent nature of the lignocellulosic biomass supply chain, these activities are not currently prioritized. Through the success of the consortium, the programs strongly feel that lessons learned about critical material, process, and quality attributes will inform how a depot could operate.

#### Recommendation 2: Stretch the consortium end goals.

The programs concur that more ambitious goals (e.g., 1,000 hours of continuous operations vs. 500 hours) would have a positive effect on the broader bioeconomy in several ways. At present, and subject to budget levels, the programs plan to retain the 500-hour objective. The programs feel that being able to achieve required quality attributes despite variable-feed properties during this time will achieve the major consortium goal: to demonstrate a comprehensive understanding of the impacts of feedstock variability through the process supply chain such that it can be managed by adjusting processing steps or processing conditions.

# Recommendation 3: Develop innovative ways to immerse the national laboratories with industry.

The programs fully concur with this recommendation to develop innovative methods for getting industry knowledge into the national laboratory consortium. The programs hope to implement this recommendation in several ways:

- FY 2020 work in the consortium has heavily stressed the need for the national laboratory consortium to develop tools that are meaningful to industrial problems. Examples include feedstock attribute data sets, open-source code that can be used by external models, and publicly available TEA.
- The programs could employ additional funding opportunities and formal collaborations between the national laboratories and industry, including Energy I-Corps and consortium-led funding opportunities.
- Creating a more structured engagement and communication strategy with the IAB.

#### Recommendation 4: Establish quality specifications on feedstocks.

Implicit to the quality-by-design approach is an understanding that feedstock quality will propagate through the entire process supply chain. The programs are prioritizing the identification of "critical material attributes" under the Feedstock Variability task, including variability as a function of storage, harvesting method, and environmental conditions. In FY 2020 planning, the consortium is developing deliverables and outcomes to make these data publicly available, including the metadata associated with downstream processing. It is envisioned that standardizing the terminology around these critical material attributes would enable technology developers to consistently communicate their feedstock quality requirements or specifications to feedstock providers.

## Recommendation 5: Aggressively promote the Feedstock-Conversion Interface Consortium results and visibility.

The programs fully concur and are implementing ways to improve the visibility of this consortium. The consortium is finalizing a communications plan that will include the use of best practices developed and employed by other consortia. This plan could include regular external webinars on special technical topics, colocating consortium listening days at key conferences and trade meetings, and dedicating a portion of the budget to maintaining a website with the consortium's accomplishments and capabilities. In addition, and when possible, FY 2020 planning includes the dissemination of deliverables and outcomes that are publicly available, such as models and scripts as digital appendices associated with peer-reviewed journal articles.

## FEEDSTOCK VARIABILITY AND SPECIFICATION DEVELOPMENT – INL

#### Idaho National Laboratory

#### **PROJECT DESCRIPTION**

Co-PI contributors: A. Hoover, R. Emerson, J. Klinger, T. Westover, L. Williams, M. Ramirez-Corredores (Idaho National Laboratory [INL]); D. Tanjore (Lawrence Berkeley National Laboratory [LBNL]); T. Semelsberger (Los Alamos National Laboratory [LANL]); E. Webb (Oak Ridge National Laboratory [ORNL]); B. Donohoe, N. Nagle, E. Wolfrum (National Renewable Energy Laboratory [NREL]); K. Sale (Sandia National Laboratories [SNL]); J. Collett (Pacific Northwest National Laboratory [PNNL]); G. Fenske, O. Ajayi (Argonne National Laboratory [ANL])

| WBS:                      | 1.2.2.401           |
|---------------------------|---------------------|
| CID:                      | NL0033424           |
| Principal Investigator:   | Dr. Allison Ray     |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$15,538,832        |
| DOE Funding FY16:         | \$6,535,000         |
| DOE Funding FY17:         | \$4,636,332         |
| DOE Funding FY18:         | \$4,367,500         |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

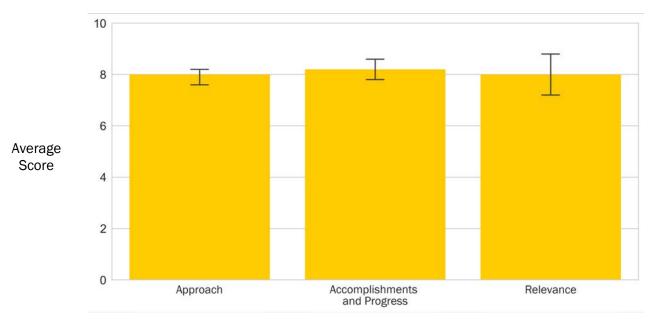
Biomass variability has proven to be a formidable

challenge to the emerging biorefining industry, impeding continuous operation, equipment uptime, and required throughput for economic production of lignocellulosic biofuels and chemicals at the commercial scale. Inconsistent feeding and handling operations at integrated biorefineries (IBRs) have been identified by the DOE BETO as a limiting factor in the conversion of lignocellulosic biomass to fuels and value-added coproducts. IBR development and operation have suffered from failing to account for the complexity and variability of lignocellulosic biomass.

The Feedstock Variability and Specification Development project aims to quantify the variability in chemical, physical, and mechanical properties of corn stover and loblolly pine residues and conduct fundamental

#### Weighted Project Score: 8.1

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

characterization required to understand property impacts on feeding, handling, preprocessing, operational reliability, and conversion performance in both low- and high-temperature conversion pathways. Understanding the magnitude and sources of variability will enable the development of technological solutions to integrate feedstock supply, storage, preprocessing, and conversion and improve operational reliability and, ultimately, maximize yields. This project generates foundational knowledge and develops methods required to contribute to the FCIC's goal of identifying and addressing the impacts of feedstock variability. This presentation outlines project accomplishments toward: (1) biomass supply for the FCIC's experimental baseline runs for preprocessing, low-temperature conversion, and high-temperature conversion; (2) fundamental characterization to quantify variability and to identify critical factors that affect reliability from preprocessing through conversion; and (3) methods development tailored to lignocellulosic biomass.

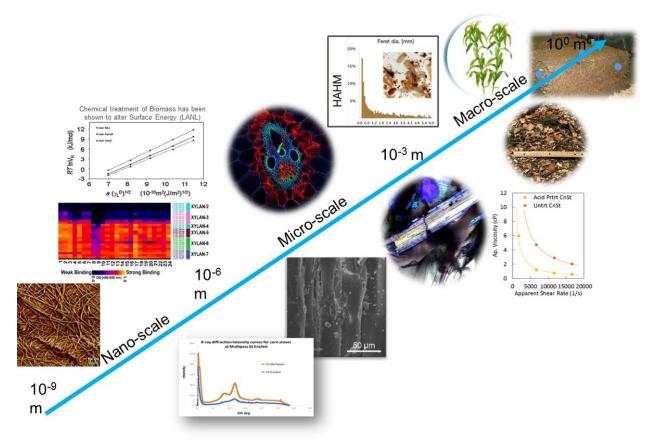


Photo courtesy of Idaho National Laboratory

#### **OVERALL IMPRESSIONS**

- This work is critical to organizing, categorizing, and characterizing feedstocks. It looks to be a good framework and will benefit from new methods of property analysis.
- Great work establishing and characterizing relevant feedstock ranges that are largely industry-relevant baseline causes of variation in the incoming material. It includes new methods implemented and shown to describe "cleanliness" of the feedstock, which will help support industry. Data are collected and organized in an open-source format that will make it easier for public access and use.
- The objective of this project is good. By design, the project looks at two feedstocks; however, it would be beneficial to expand this research to multiple feedstocks. For agricultural waste in particular, an aging

feedstock affects use and changes in the characteristics would be very difficult to quantify. The scope of this project was limited because of the complexity of the subject matter; understanding this is not a criticism of this project, but instead a statement that more work should be done to expand knowledge of feedstock characteristics on the processes and processing equipment.

- This project has many important aspects, such as the development of a database for industry to call upon for design information when contemplating the cost and operation of a commercial project. Development of a common language and principles of biomass from a technical basis will help accomplish this as well. Lacking, however, is a more detailed quantitative discussion of what a successful project here means. For example, how much can a developer be expected to save in testing costs by having this database available or knowing which variables must be planned for when designing a feed hopper?
- The feedstock variability and specification project is an important accomplishment and provides basic information that will useful to all those working in the biomass conversion field, both the actual data collected and as a model of the type of characterization work needed. Efforts should be taken to make these data more accessible to biogeotechnology developers and to continue to add more data, particularly on underreported properties such as ash characterization. The Chemical Catalysis for Bioenergy Consortium data hub would be a good model. It should be possible to reach out to land grant colleges and state agriculture organizations to aid in the collection of useful data that could expand the database. The FCIC primer is a useful document that provides a means for more uniform and effective communication about feedstock properties.. The X-ray diffraction analysis of biomass is a novel way to speciate metals and other ash materials.

- We appreciate the reviewer's comments. Likewise, we believe that some of the new approaches and methods developed and applied for property analysis offer significant potential for quantifying biomass quality and elucidating property-driven impacts on preprocessing and conversion.
- We appreciate the reviewer's comments. We certainly agree and will plan to expand the scope of our feedstock variability analyses as the consortium progresses and as funding allows. Moving forward in FY 2019, FCIC 2.0 will develop a fundamental understanding of how aging impacts biomass properties. Controlled studies under conditions that simulate aging of agricultural residues will be conducted to improve deconvolution of the complexities of resulting alterations in multiscale chemical, structural, and physical properties and how interactions among properties translate to behavior of these materials. Although this project focused on corn stover and pine residues, the consortium has industry collaborative projects under the direct funding opportunity that focus on diverse feedstocks, such as municipal solid wastes and almond wastes.
- We appreciate the reviewer's input. In FY 2018, the goal of the feedstock variability project was to quantify variability in physicochemical and mechanical properties of biomass for the FY 2018 experimental baseline runs. The culmination of knowledge derived from all the FCIC projects was aimed at solving challenges related to the design and identification of critical properties. Although FY 2018 FCIC represents a 1-year effort, these data sets provide a basis for informing FCIC 2.0 and the quality-by-design approach that is tailored to identifying critical attributes and process variables that are requisite for improving equipment operation and design.
- Thank you for this feedback. Data sets generated from the FY 2018 experimental baseline runs are available through the Bioenergy Feedstock Library (BFL), and the FCIC primer, which was developed as part of this project, is also available through the BFL (https://bioenergylibrary.inl.gov/Home/Home.aspx).

## FEEDSTOCK PHYSICAL PERFORMANCE MODELING – INL

#### Idaho National Laboratory

#### **PROJECT DESCRIPTION**

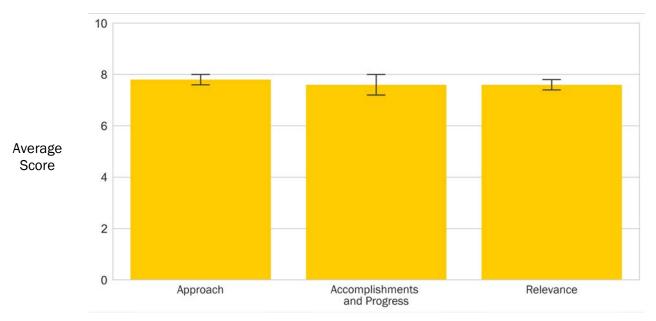
Feeding and handling represent a substantial challenge in biomass feedstock supply systems. Conventional systems for dry bulk solids are generally not suitable for lignocellulosic biomass, which typically exhibits large particle size variations, low density, and high compressibility. Methods do not yet exist to either physically characterize or computationally model the complex mechanical response of such materials. The primary objective of this project is to develop physicsbased computational models that reliably predict the mechanical behavior of a loblolly pine residue and a corn stover sample in a lab-scale direct axial shear test. These models are then used to identify critical material attributes

| WBS:                      | 1.2.2.501           |
|---------------------------|---------------------|
| CID:                      | NL0033425           |
| Principal Investigator:   | Dr. Tyler Westover  |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$2,115,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$650,000           |
| DOE Funding FY18:         | \$1,465,000         |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

that impact feeding and handling performance. Two types of physics-based models were pursued. First, the discrete element method (DEM) was applied to develop high-fidelity particle-based simulations that capture interactions between representative particles. Although DEM models can robustly capture all dominant particle flow mechanics, they are extremely expensive in terms of computation time and memory and are difficult to scale to industrial applications. Therefore, the necessary scaling is achieved by developing reduced-order continuum finite element method (FEM) models that essentially average over many particles to reduce computational cost. The robustness of the FEM models was verified using physical experiments and by comparing their predictions to those of the DEM models. Particle-based DEM models are essential for

#### Weighted Project Score: 7.7

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

developing and verifying FEM models to ensure that the FEM models capture appropriate functional relationships between key parameters. In many cases, these functional relationships cannot be measured experimentally (for example, the relationships between internal material stresses, strains, dilation, and shear strength) because the needed sensors do not exist or lack enough accuracy.

The objective of the project was accomplished by achieving greater than 80% agreement between the lab-scale direct axial shear test and computational simulations. Results of the flow tests and simulations using different geometries indicate that flow modes of biomass materials are coupled, resulting in highly complex flow that cannot be fully understood using classical continuum methods. Future effort will focus on developing more advanced continuum FEM flow models based on results of DEM particle models.

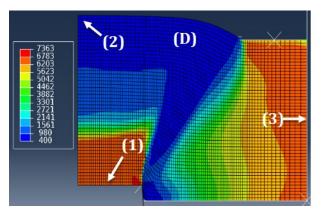


Photo courtesy of Idaho National Laboratory

#### OVERALL IMPRESSIONS

- This is ambitious work that has high use to industry if it can be understood and general enough.
- The early cellulosic biorefineries experienced significant problems in the interface of feedstock handling and conversion. The modeling created in this project suggests that if a project developer understands the physical properties of the feedstock in their plan, the proper feeding and handling system could be designed and hopefully not have the same sorts of problems that the industry presently faces. This could be an important step forward in the SOT as it exists today.
- This project undertook a very challenging application, and, not surprisingly, it found that several models need to be applied simultaneously to get reasonable system models. Congratulations on the frontier-type work; the reviewer anticipates that it will lead to new concepts for improving biomass flow through hoppers and screws.
- Relevant industry partners were involved in the project, but it was not clear where they had vetted the modeling analysis or this had been done only on the flow characterization methods. The reviewer suggests this is done as part of fully completing the work and helping to ensure its value to equipment designers.
- The presentation did a good job of providing a general understanding of the complexity of the problem; however, the details needed to be explained in plain language.
- A variety of flow modeling methods were applied, although the details were difficult to follow. This is an interesting project, but a model with a goal of an R-square of 0.8 might not be able to drive significant improvements. The results of the project are of limited impact on the overall biorefining industry. This is because a new set of tests would likely be required depending on the equipment and feedstock used. Unfortunately, the calculation approach failed to provide usable results.

- Agreed. The advanced simulation and characterization methods will enable consulting firms in bulk solids handling to properly advise industrial biorefineries, and the rapid and reduced-order models will be directly useful for industrial biorefineries to better understand the effects of feedstock variability.
- Exactly. It is also understood that the project developer will likely need to consult with firms that specialize in handling bulk solid (particulate) materials to appropriately apply advanced methods developed by this project.
- Industry partners primarily assisted by helping with the flow characterization methods and early discussion of simulation options. As the models develop and additional results are obtained, input will be sought from a wide range of industry and academic experts. This input will be sought through subcontracts and through the Particle Technology Forum within the American Institute of Chemical Engineers.
- For general understanding, complex models and characterization methods must be simplified to low-level reduced-order models. Please see responses 1 and 2.
- We agree that being able to predict flow behavior with 80% accuracy might not be adequate for the industry. Current advanced models that we have tested exhibit errors that are greater than 100% for key multidimensional predictions. We believe that the models can be improved substantially, which will lead to improved understanding and more reliable designs. Efforts at adapting advanced continuum and particle models are still in their relative infancy and will be pursued further in a future project to provide useful results.

## SYSTEM-WIDE THROUGHPUT ANALYSIS – INL

#### Idaho National Laboratory

#### **PROJECT DESCRIPTION**

Recent evidence indicates that the operational performance of the DOE's cofunded pioneer project on integrated biorefineries (IBRs) is significantly impacted by variability in feedstock properties and composition. This is a highimpact problem because several IBRs have already failed largely because of underestimated operational issues related to this variability. Thus, a timely solution to these operational issues is essential if second-generation biofuels are to be commercialized in any significant volume, allowing the economic benefits of new jobs and improved security of our fuel supply to be realized. The remaining IBRs are trying to solve these operational upsets; however, solving one issue invariably creates or reveals others

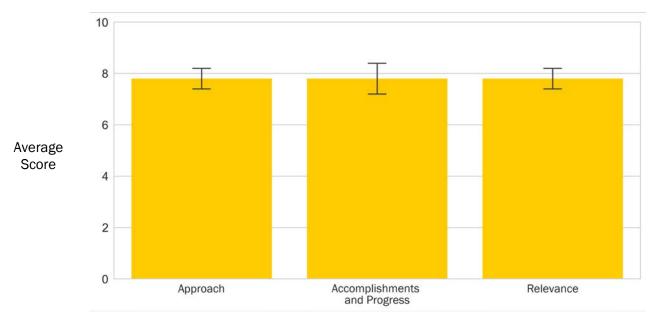
| WBS:                      | 1.2.2.601           |
|---------------------------|---------------------|
| CID:                      | NL0033426           |
| Principal Investigator:   | Dr. David Thompson  |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$3,477,499         |
| DOE Funding FY16:         | \$1,050,000         |
| DOE Funding FY17:         | \$950,000           |
| DOE Funding FY18:         | \$1,477,499         |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

because of interactions across the system and or the masking of downstream issues by upstream problems. It is well known that compositional variability can have significant impacts on titer, rate, and yield from conversion processes; however, the system-wide impacts and trade-offs of variation in feedstock physical properties on first-plant scales are not well understood.

The objective of this project is to provide analyses that identify and quantify specific impacts that feedstock properties have on feedstock handling, processing, and conversion unit operation performance and how these impacts cascade throughout the system and impact the attainment of 90% uptime and design biofuel yields and costs. This project uses a combination of discrete event modeling and modified steady-state process simulation

#### Weighted Project Score: 7.8

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

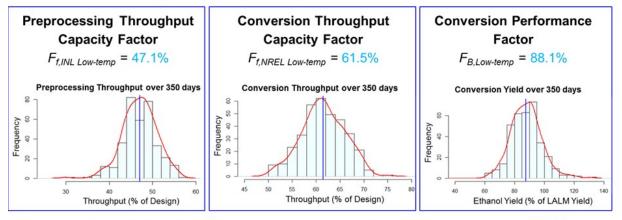
to model the dynamic throughput and conversion process performance impacts of feedstock properties across the field-to-biofuel system. We define the operational reliability of a system to include the feedstock attributederived impacts of below-design throughput (including downtime, or zero throughput) and yield (i.e., conversion performance). This operational reliability is then used to estimate annual capacity, productivity, process economics, and sustainability metrics. To accomplish this, we use throughput analysis combined with existing and developing knowledge of the sources and impacts of variable feedstock properties on operational reliability.

To maximize the potential impact of our analyses to current pioneer biorefinery processes, the analyses focused on conventional feedstock supply systems used by the pioneer biorefineries. Additionally, past conversion platform design cases that were reasonably representative of pioneer biorefinery technologies were used. These included biochemical (fermentative, low-temperature) conversion of nonpristine corn stover biomass to ethanol (2011 biochemical corn stover-to-ethanol design case) and fast pyrolysis of nonpristine southern pine residues to hydrocarbon fuel products (2013 pyrolysis and upgrading to hydrocarbons design case).

This project fulfills a critical role for DOE and industry stakeholders by developing and using an approach for the early identification of bottlenecks and pinch points across the entire field-to-biofuel system as well as quantifying their relative impacts on achievable throughput, yield, process economics, and sustainability metrics. Using input data generated during the experimental baselining of the preprocessing and conversion deconstruction process development units, this project developed modeled operational reliability baselines for the two feedstock conversion systems operated during a year's time. The modeled baselines agreed well with the experimental observations, allowing for the generation of the distributions of expected throughput and conversion yield that would have resulted from the given feedstock property input distributions.

#### FY18 GOAL: LOW-TEMPERATURE MODELED BASELINE FOR FCIC

- Ties together Low-temp information/data from all other FCIC activities
- Provides a bridge to quantify the implications around economics/LCA metrics



• Operational Reliability:  $R_{sys,Low-temp} = F_{f,INL \ Low-temp} \times F_{f,NREL \ Low-temp} \times F_{B,Low-temp} = 25.5\%$ 

**GHG Emissions:** Preprocessing =  $15.462 \text{ kg CO}_2\text{e}$  / dry ton feedstock

Scaled conversion = 1.935 kg CO<sub>2</sub>e / gal ethanol

Photo courtesy of Idaho National Laboratory

#### OVERALL IMPRESSIONS

- The system-wide view is important in integrating all the other parts of the FCIC work. The work is important in determining the overall capacity of a plant in terms of where the bottleneck is and which parameters in the biomass cause capacity to be diminished.
- Models such as those created by this project—which capture both operating reliability and production throughputs based on the effects of feedstock variability—will have significant advantage to inform both commercial and R&D activities. Currently, the main weakness is the lack of data for parts of the modeling, such as the scale-up cost for low-throughput systems and operating reliability data for high-throughput systems. This is not a fault of the PIs but a weakness, nonetheless, limiting the models' use and value. Over time, however, as more data become available, dynamic models like these will become a valuable tool.
- This project is a great new way to apply the Aspen/TEA models because it incorporates relevant highly variable unit operation capacities/uptime such that the model was able to predict which steps of variation are the true rate-limiting steps to the plant. Modeled uptime for pioneer plants was reasonable but still needs to be validated against industry when data are available.
- Use of the models to help direct future work will need to include broader mitigation options. It is suggested to use the FCIC/FSL IABs and industry interviews to help define some of the more relevant approaches to bring into the model. Moisture control should be a focus topic.
- This was not an easy topic to present because of the need to really think about what was being presented. It is an interesting approach to looking at plant reliability and thus profitability by getting the most out of what a plant has and directing money toward improvement; however, it would have taken much long than a half hour of time to show the strength of the models.
- System-wide throughput analysis is a critical part of improving the efficiency of biofuel production. This type of stepwise analysis is the foundation of Six Sigma and other process design analysis approaches. The results of the analysis reflected the poor throughput of both the low- and high-temperature processes related to equipment reliability. This information confirms the importance of the FCIC to the overall success of biofuel production. There is a clear need to include equipment performance data in the TEA analyses, as discussed in the project. The problem is the lack of availability of these data, particularly at the commercial scale. Unfortunately, these data are considered highly proprietary; however, I believe that NREL has a larger unit that might also be able to provide data. Operational data should be included in the TEA evaluation of projects to provide a better estimate of early plant performance.

- Throughput analysis is usually applied in supply system optimization and in manufacturing industries, and to date it has not been applied to any great extent in the chemical industry. Generally, classical reliability and use approaches are followed to maximize time on stream, whereas mismatches of capacity are solved through the insertion of material flow buffers between mismatched equipment. Although this approach has been shown to be successful for liquids and gases, bulk solids such as biomass that have a range of structural and mechanical properties that depend on hard-to-control variables (such as moisture and ash) present challenges that cannot simply be solved by inserting material flow buffers. Including throughput capacity use and conversion performance in an operational reliability metric provides an approach to solving these challenges.
- We previously used this method along with observational and experiential data to develop estimates of equipment-level at-scale downtimes and performance impacts. In that case, we were able to produce results that were consistent with the observations of the DOE tiger team that worked with the pioneer biorefineries to identify reasons for much longer than expected startup times and feeding system-derived

conversion system upsets. Through that analysis, we were able to identify which unit operations and high-level feedstock properties (moisture and particle size) were most impactful to the operation of the preprocessing system. As we learn more fundamental causes of impacts, we will be able to integrate those into the models. Additionally, first-principles modeling in other FCIC projects will directly inform both equipment and system designs.

• The objective of the analysis during FY 2018 was to define modeled operational reliability baselines for the systems that the FCIC have access to (i.e., data sources that were available). The prior estimates for at-scale impacts from the previous analysis were not used for these baselines because they were not directly measured. We believe that as we gain a better understanding of the fundamental (i.e., feedstock property-based) mechanisms of impacts to individual PDU-scale equipment through the efforts of the FCIC, there will be a better basis for predicting impacts to larger scale equipment through fundamental modeling, which can then be applied to throughput modeling of the system. In this way, the redirected FCIC efforts will improve the modeling approach for system-wide throughput/cost/sustainability analysis, fill in identified data gaps, and develop tools/models that are focused on helping industry.

## **INDUSTRY ENGAGEMENT AND PROJECT MANAGEMENT – NREL**

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

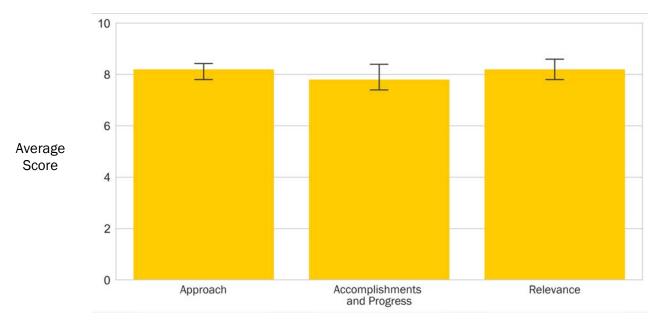
Industry Engagement and Project Management aims to coordinate and manage FCIC R&D activities and to promote interactions with IAB members and stakeholders to deliver technological solutions developed within the FCIC for industry adoption. This project consists of three tasks: industry engagement, industry collaborative R&D, and project management. INL and NREL will serve as two lead institutions for the FCIC efforts and will work proactively with PNNL, ORNL, LANL, LBNL, ANL, and SNL to develop and execute work plans, to prioritize and coordinate R&D activities, to establish communications pipelines and leadership teams for the different FCIC R&D projects, and, finally, to engage industry to solicit

| WBS:                      | 1.2.2.702           |
|---------------------------|---------------------|
| CID:                      | NL0033723           |
| Principal Investigator:   | Dr. Michael Resch   |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$824,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$824,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

significant input and translate FCIC innovations for industry adoption. In the industry engagement task, the project management team has engaged with industry stakeholders and established an IAB. The goal of these actions is to ensure more efficient communications and, ultimately, to promote and enable industry national laboratory collaborations that will be effective in helping industry overcome technical barriers, thereby improving operational throughput and, thus, profitability. Communication of FCIC accomplishments and capabilities has been largely through the development of the FCIC website (www.fcic.inl.gov). The industry collaborative R&D task has promoted industry national laboratory collaborations by funding \$8 MM in R&D projects through FCIC directed funding opportunity awards. A web-based process tool was also established to

#### Weighted Project Score: 8.0

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

manage the funding opportunity program's proposal submission, review, approval, award process, and project execution. In the project management task, a sensible project management structure, workflow system, and reporting process was put in place to ensure that the FCIC will continue to be efficient and effective. This task focused on global FCIC integration and coordination of activities to ensure rapid and efficient progress toward goals. The FCIC project management team ensured that deliverables were provided to DOE in accordance with the approved work plan and budget. The FCIC project management team also coordinated establishing a leadership team comprising representatives from DOE and national laboratories to establish the vision and define the strategy of the R&D focus as well as to approve the direction of and changes to the R&D focus as the FCIC evolves.

The objectives of this project were to: (1) ensure the effective management of the consortium to achieve FCIC objectives and outcomes using scientific expertise and core capabilities of the national laboratories, (2) establish a functional FCIC IAB representing the broad range of stakeholder interests and an active FCIC industry engagement team, (3) complete at least two industry collaborative projects, and (4) engage and promote partnerships that translate FCIC innovations to industry. This project will ensure the accomplishment of overall FCIC goals through active project management, industry engagement, and outreach activities with R&D projects that address the development and optimization needs of bioenergy industry stakeholders. Industry engagement will include activities that provide industry input to FCIC annual operating plans, communication of FCIC capabilities and accomplishments to industry, and the transfer of technical knowledge developed by FCIC research to industry via technical reports and presentations. R&D projects will include strong potential for industry adoption and industry collaborative R&D projects that are competitively awarded through a FCIC directed funding opportunity. The intended outcomes of this work include industry input on FCIC direction, active and diverse partnerships with industry, and industry use of FCIC innovations.



Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

• The FCIC was an important industry-driven effort by BETO to address real needs of pioneer biomass plants. The focus areas were based on what was indirectly known to be the challenges at the pioneer plants during their commissioning phases, although direct participation by pioneer companies was not possible, and in lieu of that the decision to use an IAB for this purpose was helpful if not directly executable.

- Obtaining results from the consortium in only 2 years was exceptional, and all consortium members should be commended. Inclusion of the full breadth of national laboratories was useful to deliver a more diverse knowledge and skill set to the projects, even when only a few of the laboratories needed to do the majority of the project execution. This approach should be replicated in the future whenever possible.
- The main aim of the FCIC was to establish high reliability of feedstock delivery to the reactor throat; however, a set of quality specifications was not a highly visible output of much of the work. Moisture and ash were identified as significant impact variables, but no clear guidance has yet been given to drive upstream control methods. If pellets of blended feedstocks are a viable option, there should be some analysis/scoring of how well they meet the reliability specifications, not only the cost targets.
- Managing a consortium such as the FCIC is not only an important undertaking but also a complex task. The work of the FCIC will prove to be a necessity to the success of a robust cellulosic bioenergy business. It is difficult to assess this project through this presentation, however, because we now know that FCIC work has been completely refocused in approach although how and why this happened is not entirely clear. Therefore, the FCIC's overarching goal was not attained. The original progress of the FCIC technology area would suggest that the program very likely would have been successful. The goals as set out in this presentation were achieved, and individual program goals were achieved for the most part. Therefore, it is difficult to reconcile the two positions, whether they were successful or not.
- The consortium is a good way to organize industry and national laboratories, and this one seems to be doing that well, with lots of cooperation and contribution from members.
- Engaging industry that is attempting to implement biotechnologies provides key feedback concerning their problems and concerns. The concept of addressing the cross-biomass conversion operability problems because of feedstock variability addresses a major issue that had previously received little attention. Many biorefineries have failed because of problems related to feed handling. It is difficult for people developing new technologies to address these issues. This project is the first concentrated effort to apply a manufacturing science approach to biofuel production. Some high-quality projects with commercial groups were launched by the project team. These industry-driven projects will help keep the FCIC relevant.

- We appreciate the support for this work from the reviewer's comments. We agree that a great outcome from this work would be to develop feedstock specifications and ranges of material and chemical properties that would be acceptable and beyond those ranges would be detrimental to throughput and conversion. We will work toward approaching feedstock quality metrics to help guide current and future use of lignocellulosic feedstocks in a biorefinery. Blended and pelleted feedstocks were not evaluated within the current FCIC projects; the related pellet studies are funded under the FSL Program and the FCIC's industrial collaborative research. We will leverage those research results in the future for analysis of reliability specifications.
- We thank this reviewer's acknowledgement of how difficult and complex managing a multi-laboratory consortium is. Much of the first-year accomplishments resulted in newfound collaborations among national laboratories and team formation. The first-year objectives were met as we demonstrated a high-and low-temperature experimental and modeled baseline. We also set up research teams and reviewed and funded the directed funding opportunities to foster industry-national laboratory collaborative projects. These successes will be built upon in the next iteration of the FCIC.

## **PROCESS INTEGRATION – NREL**

#### National Renewable Energy Laboratory

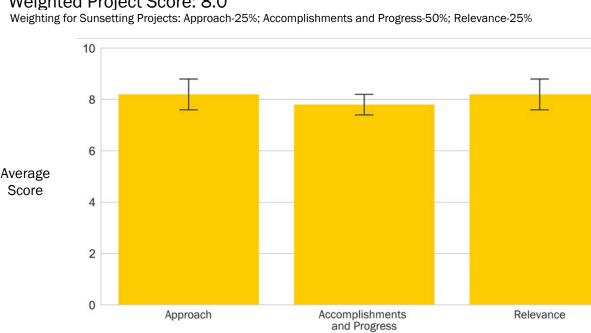
#### **PROJECT DESCRIPTION**

The Process Integration project is part of the FCIC, an integrated and collaborative network of eight national laboratories (ANL, INL, LANL, LBNL, NREL, ORNL, PNNL, and SNL) dedicated to identifying and addressing the impacts of feedstock variability-chemical, physical, and mechanical-on biomass preprocessing and conversion equipment and system performance to move toward a target of 90% operational reliability. In FY 2018, the Process Integration project supported this overall FCIC goal of improving operational reliability and conversion performance of low-temperature and high-temperature integrated processes through laboratory and processrelevant experiments to document and mitigate the negative effects of feedstock variability.

| WBS:                      | 2.2.1.502           |
|---------------------------|---------------------|
| CID:                      | NL0033394           |
| Principal Investigator:   | Dr. Ed Wolfrum      |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$7,422,970         |
| DOE Funding FY16:         | \$1,275,000         |
| DOE Funding FY17:         | \$871,970           |
| DOE Funding FY18:         | \$5,276,000         |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

The key objective of the Process Integration project in FY 2018 was to execute robust, industrially relevant baseline experiments that document process reliability and conversion performance across biomass preprocessing and both low- and high-temperature conversion performance

Because this project encompasses a substantial portion of the feedstock logistics and conversion value chain, it addresses a number of Multi-Year Plan (MYP) barriers: Ft-E: Terrestrial Feedstock Quality, Monitoring, and Impact on Conversion Performance; Ft-G: Biomass Physical State Alteration; Ft-I: Overall Integration and



Weighted Project Score: 8.0

 ${\mathbb I}$  One standard deviation of reviewers' scores

Scale-Up; Ct-A: Feedstock Variability; Ct-C: Efficient Preprocessing; Ct-D: Efficient Pretreatment; Ct-I: Product Finishing Acceptability and Performance; and Ct-J: Process Integration.

#### OVERALL IMPRESSIONS

- The work done makes good use of the strengths of the two national laboratories and was performed with a high degree of consistency.
- Benchmarking is a key activity of scale-up, thus the baselining of 2016 SOT variance performance was absolutely a key activity, especially because such work in the national laboratories had not been executed to date. The project demonstrated several operational challenges also seen at pioneer plants and underscored the importance of the identification and quantification of process variation (as seen through uptime/capacity).
- Use of wear-sensitive equipment in portions of the process introduced some additional levels of variation that make it difficult to parse out the impact of the feedstock quality against equipment performance. In any future benchmarking runs such as was conducted here, it would be advisable to implement a well-defined feedstock control (i.e., cellulose powder) that can be run before and after each case to establish the "plant health" to decouple from the feedstock itself. It would also be advantageous to run more than one run of each feedstock if time and budget allow.
- This project was well managed and thorough. It would be wonderful if every project could have such extensive work done to improve operations. It would be useful to target other feedstock characteristics as well as downstream processing.
- This project is a solid contributor to the FCIC team and developed significant data, but more detail on the conclusions or summary is needed. For example, the presentation makes the conclusion that some sources of variability in biomass cannot be controlled. In a presentation of findings, a list of those would seem to be a necessity. But overall, this is good work that I am sure informed the decision-making process in the new FCIC move toward the quality by design as seen in future work for FCIC.
- The process integration project provided the operational data for use in the other FCIC programs, including pretreatment and conversion. It was the first attempt to obtain controlled data on the integrated operation of all the unit operations of the process and as such provides unique data for use by the remainder of the groups. The data collected on operability, including the number of times human intervention was required, is particularly useful information about equipment reliability. The development of a rapid way to predict wear will be a great assistance to engineers selecting the material of construction.

- We thank the reviewers for their comments. This project was challenging because it was split across two laboratories (INL, NREL) for the actual experimental baseline runs, with work at two other laboratories for the equipment wear portion (ORNL, ANL). It was as rewarding as it was challenging, however.
- We agree that the lack of a "feedstock control" will make the information collected harder to interpret. We will consider options to add such a control in future benchmarking experiments. We also agree that multiple runs of each feedstock would have provided additional information, but we were limited by time and budget. In the end, we chose to perform single runs on multiple feedstocks rather than repeated runs on a single feedstock.
- We appreciate the reviewer's comments on the project management. We had very strong teams, which simplifies project management.

- We agree that more detail should have been included; the milestone reports we submitted in FY 2018 were quite detailed, but this level of information was not presented in the presentation because of time constraints. We stated that "biomass is variable, and many sources of variability cannot be controlled" on Slide 31. That was imprecise, however. We should have said that upstream processes (harvesting/storage/transport) can result in significant variability that the preprocessing and conversion processes cannot predict and must be able to address. In future years, the FCIC will be looking upstream from first-stage deconstruction to understand the source(s) and effect(s) of this variability and developing science-based solutions to the problems caused by this variability.
- We are pleased that the reviewers found our results to be valuable, both the operability and the conversion data. We believe they are already helping to inform work in the FCIC in FY 2019.

## **PROCESS CONTROLS AND OPTIMIZATION – INL**

#### Idaho National Laboratory

#### **PROJECT DESCRIPTION**

The Process Controls and Optimization project studied the impact of biomass properties on the performance of preprocessing and primary deconstruction process and equipment and developed strategies and methods to achieve greater than 90% operational reliability while meeting the specifications of feedstock quality. The Process Controls and Optimization project is part of the FCIC, an integrated and collaborative network of eight national laboratories: ANL, INL, LANL, LBNL, NREL, ORNL, PNNL, and SNL.

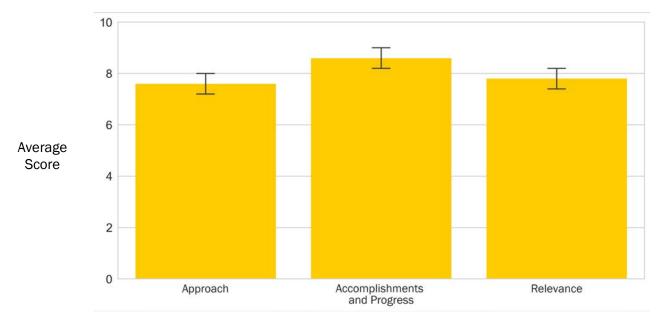
| WBS:                      | 3.3.1.101           |
|---------------------------|---------------------|
| CID:                      | NL0033726           |
| Principal Investigator:   | Dr. Quang Nguyen    |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,896,300         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$1,896,300         |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

For IBRs to achieve reliable process operability through feed handling, preprocessing, and conversion operations, it

is essential to control processing equipment to accommodate a wide range of feedstock properties that affect the operation of the equipment. These properties include moisture content, ash content, fiber integrity, and particle size distribution. The project focused on the development and application of in-line sensors and adaptive control systems that enable reliable operation of feedstock preprocessing equipment as well as lowtemperature and high-temperature primary deconstruction operations while maintaining downstream conversion performance with wide-ranging feedstock properties.

#### Weighted Project Score: 8.2

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

The project successfully demonstrated that an autonomous adaptive control system achieved 90% operational reliability for the two-stage grinding of baled corn stover. The study of comprehensive FCIC project data from the baseline runs yielded correlations among parameters collected across laboratories, including:

- Physical properties for input biomass materials
- Process control data collected from preprocessing along with low- and high-temperature conversion
- Properties and conversion yields of output materials from those same processes.



Photo courtesy of Idaho National Laboratory

#### OVERALL IMPRESSIONS

• The demonstration of a method for increasing the uptime of the front end of the biomass process was a valuable approach to supporting pioneer plants struggling with grinder uptime. The implementation of advanced control methods and instrumentation allowed for the project team to not only address downtime issues but also develop a practical method of online compositional analysis to further guide plant operations. The reviewer recognizes the successful approach of adaptive control to solve the particular issue with the INL scale and setup, but benchmarking the solution against other alternative approaches (i.e., bale full/partial rejection, oversizing of grinding) might have further increased the industrial value/relevance of the work.

- The key findings that further input homogenization of bales and practical capacity limits to the grinding operation are both relevant for industry and should be considered by equipment suppliers. The scalability of the INL system will be a secondary activity to realize the full impact of the project work.
- This project appeared to be hugely successful in meeting its objectives. It is easy to see how the results could be applied to commercial applications. Good project execution appeared to yield excellent results.
- The PIs developed a robust autonomous feed-forward operating system, and such systems are relevant for successful bioeconomy projects. They were successful in obtaining solid data about the impacts of feedstock variability on equipment performance. This is a sunsetting project but will provide good baseline information to inform the new FCIC activities in this area of work and continue the progress this work represented.
- I believe that controls are a critical part of the FCIC, and the work here has done much to show its value overall to reducing material variability impacts.
- Process control and optimization provides key tools improving the throughput of biofuel production. The project was conducted using a sound approach the impact on biofuel product seems to be limited to providing proof of the performance of in-line sensors with an adaptive control loop for a single piece of equipment. It is a good example, however, of how adaptive control can predict operational problems before they happen and adjust the parameters to prevent shutdowns. The model developed illustrates the impact of feed variability and control methods on yields and operability and how focusing on a single unit can produce significant improvements. It is not clear, however, whether the specific results will be widely transferable.

- We agree with the reviewer's comment regarding benchmarking the use of the adaptive control system to maintain the equipment online against alternative approaches of rejecting off-specification bales (e.g., high moisture) or oversizing the equipment because these latter methods result in high biomass loss and increased capital and operating costs.
- We appreciate the reviewer's comment. We expect that additional work in developing an adaptive control system will be required for new unit operations and equipment as the FCIC 2.0 R&D activities progress.
- We appreciate the reviewer's comment. We believe that having the adaptive control system will allow the avoidance of downtime and, possibly, the need for additional processing steps.
- The adaptive control logics should be applicable to most, if not all, biomass preprocessing systems as well as downstream unit operations. The specific results are applicable to the equipment studied (hammermill, screw conveyors). Different equipment will have different performance characteristics. For example, moisture content of biomass has less impact on the capacity of rotary shear devices than hammermill.

## FCIC OVERVIEW PRESENTATION

#### Feedstock-Conversion Interface Consortium

#### **PROJECT DESCRIPTION**

| Many of the serious bottlenecks being experienced in the nascent bioenergy industry are centered on feedstock |
|---|
| handling and preprocessing operations. Further, these   |
| bottlenecks directly affect the process of feeding  |
| feedstocks into the conversion process, conversion  |
| equipment operation, and process integration. The   |
| complexity and variability in feedstock physical, chemical,   |
| and mechanical attributes directly relate to the operational  |
| difficulties encountered with handling the elastic solid  |
| materials, the recalcitrance of feedstocks to efficiently   |
| convert into products, and the inhomogeneity of   |
| intermediates resulting in nonuniform conversion. All   |
| these issues tend to occur where the feedstock supply   |

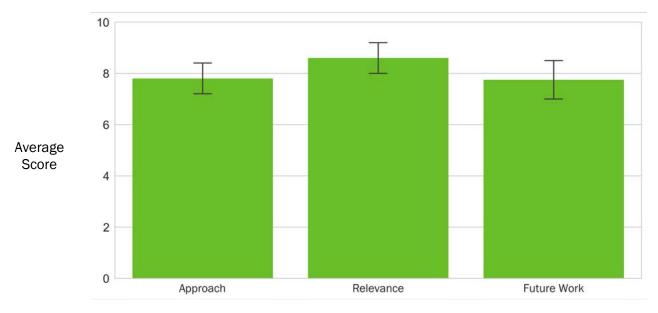
| WBS:                      | FCIC.1              |
|---------------------------|---------------------|
| CID:                      | NLOOFCIC1           |
| Principal Investigator:   | Dr. Michael Resch   |
| Period of<br>Performance: | 10/1/2017-9/30/2019 |
| Total DOE Funding:        | N/A                 |
| DOE Funding FY16:         | N/A                 |
| DOE Funding FY17:         | N/A                 |
| DOE Funding FY18:         | N/A                 |
| DOE Funding FY19:         | N/A                 |
| Project Status:           | New                 |
|                           |                     |

system couples with the conversion process, referred to as the feedstock-conversion interface. These issues are then largely responsible for the problematic operation of the integrated biorefineries. This is a big, complex problem that requires robust solutions involving extensive testing and R&D.

because of the increasing importance of these issues, the existing feedstock-conversion related efforts are being organized into a FCIC, which became fully integrated and functional in FY 2018. This consortium is funded by the three BETO programs: FSL), Conversion, and ADO. The FCIC goals are to identify and address the impacts feedstock chemical, mechanical, and physical variability have on supply logistics, storage handling, preprocessing, conversion equipment operation, and process integration to develop and demonstrate improved



Weighting for New Projects: Approach-25%; Relevance-25%; Future Work-50%



 $\square$  One standard deviation of reviewers' scores

integrated feedstock conversion. The DOE national laboratories possess unique and differentiated capabilities in biomass characterization, preprocessing of various biomass into on-specification feedstocks, high- and lowtemperature conversion technologies, physical and mechanical modeling, and integrated analysis of economic and sustainable impacts. All these capabilities will be leveraged to establish a consortium that surpasses what an individual laboratory can deliver. The FCIC consists of six projects with an integrated and collaborative network of eight national laboratories (ANL, INL, LANL, LBNL, NREL, ORNL, PNNL, and SNL). The FCIC R&D efforts are focused on five primary areas: (1) Feedstock Variability and Specification Development, (2) Feedstock Physical Performance Modeling, (3) Process Integration, (4) System-wide Throughput Analysis, and (5) Process Controls and Optimization, with a sixth area related to industry engagement and project management.

The reliability issues addressed by the FCIC projects are significant barriers to the growth and success of the biofuel industry. The FCIC was set up to develop scientific knowledge and solutions needed to overcome these barriers and will work with industry to translate FCIC outputs to industry operations. Meeting the FCIC goals will lead to consistently functioning biorefineries, improved profitability, and increased investment and use of the billion tons of available biomass resources. This presentation provides an overview and scope of the consortium and highlights the interactions among the five R&D projects.

#### **OVERALL IMPRESSIONS**

- The FCIC has been valuable to validate main feedstock factors facing pioneer plant operations through a comprehensive approach of characterization, modeling, and demonstration. Use of the full breadth of the national laboratories through higher levels of inter-laboratory coordination has been useful to leverage unique knowledge and skill sets available within the greater national laboratory network that longer term will create increased value to taxpayers. BETO should continue to look for industry roadblocks where the consortium (and inclusion of IABs) can have this kind of positive impact within such a short development cycle.
- The FCIC consortium and funding are correctly targeted at a key factor that has prevented biofuel refineries from achieving the target performance predicted by the laboratory experiments. The lack of consistent feedstocks and equipment reliability have been the reasons for failure on many projects and have suppressed interest by investors in the bioeconomy. It is difficult for groups attempting to commercialize biorefineries to perform this type of basic research. Any work providing high-quality data in this area is critical to future success. The work this year was to establish baseline information that will be useful for future work. The projects from this year are not being renewed, except for the annual operating plan projects with industry partners. The FCIC area is being refocused on a more fundamental approach. I believe that the 2017 projects were all worthwhile, however, and would have provided results that would have helped many biotechnology developers. One limitation was the focus on a limited range of processes and conditions. The planned refocusing on fundamentals might provide information with a wider impact.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

## FCIC FY 2019 AND BEYOND PLANS

#### Feedstock-Conversion Interface Consortium

#### **PROJECT DESCRIPTION**

| Many of the process bottlenecks and difficulties           |
|--|
| experienced in the nascent bioenergy industry are centered |
| on feedstock handling and preprocessing operations, the    |
| process of feeding feedstocks into the conversion process, |
| conversion equipment operation, and process integration.   |
| These specific issues-including the complexity and         |
| variability in feedstock dimensional, physical, chemical,  |
| and mechanical attributes; the operational difficulties    |
| encountered with handling solids; recalcitrance of         |
| feedstocks to be efficiently converted into fuels and      |
| products; and inhomogeneity of intermediates resulting in  |
| nonuniform conversion-all mostly occur where the           |
| feedstock supply system couples with the conversion        |
|  |

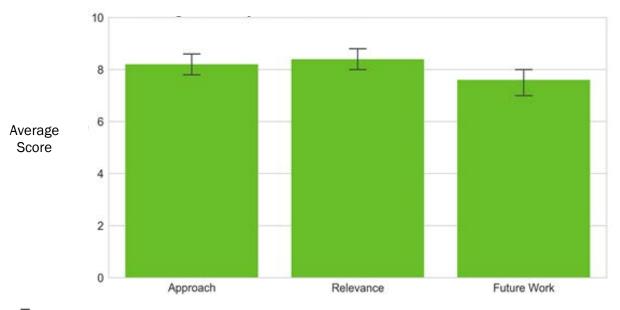
| WBS:                      | FCIC.2              |
|---------------------------|---------------------|
| CID:                      | NL00FCIC2           |
| Principal Investigator:   | Dr. Zia Abdullah    |
| Period of<br>Performance: | 10/1/2018-9/30/2020 |
| Total DOE Funding:        | \$9,000,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$9,000,000         |
| Project Status:           | New                 |
|                           |                     |

process. This is referred to as the feedstock-conversion interface, and this is where problematic operation of the integrated biorefineries is experienced. To address this, the FCIC was formed, leveraging core capabilities at ANL, SNL, LANL, LBNL, INL, NREL, ORNL, and PNNL.

Presently, biorefineries are designed and built by firms that have engineered equipment mostly for the mature agricultural and pulp and paper industries, where the processes are well understood. The approach used for mature industries is usually incremental, and it is not suitable for new industries, where the physics of conversion processes, the impact of feedstock variability, and scale-up rules are not well understood.

### Weighted Project Score: 8.0

Weighting for New Projects: Approach-25%; Relevance-25%; Future Work-50%



 $oxed{I}$  One standard deviation of reviewers' scores

A key hypothesis underlying FCIC's framework is that poor quantification, understanding, and management of variability in biorefinery streams contributes significantly to the inability of biorefineries to operate continuously and profitability. To address this problem, the FCIC will employ the quality-by-design approach originated by the pharmaceutical industry to manage variability in process streams in a very disciplined manner.

The objectives of the FCIC are to:

- 1. Develop knowledge and tools that will help technology developers so that with improved design, as well as process specifications, a greater number (~70%) of biorefineries will succeed through startup and continuous operation.
- 2. Develop a framework through which technology developers will be able to assess the quality and value of various streams in their processes for the purpose of using that valuation to make decisions to achieve Objective 1.

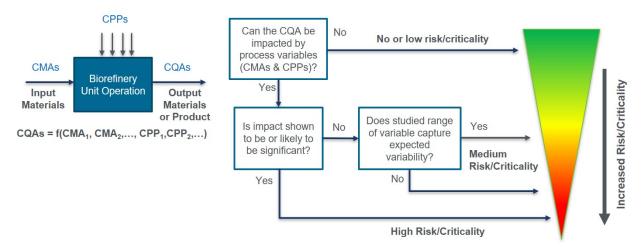


Photo courtesy of Feedstock-Conversion Interface Consortium

#### OVERALL IMPRESSIONS

- Future FCIC efforts to scale down integrated processes by developing transfer functions between unit operations is a good approach to not only better understanding each block but also allowing for easier assimilation of local process developments into holistic process operation. It would be good to create some visualization/training on how these would be used by equipment manufacturers so that those who are not familiar with the method would be able to use the results and hence also provide relevant feedback to the projects.
- The 500-hour integrated run goal is a good way to establish validity of both the development methodology as well as the actual process improvements; however, only a 70% success rate is not, so what that means to industry/investors needs to be clarified.
- This FCIC FY 2019 proposal is a major improvement over the 2018 plan. It includes more specific milestones and objects. It describes a new overall approach based on focusing on fundamentals and the quality-by-design approach. The critical success factors are clearly identified. The FCIC has the potential to greatly impact the biomass-to-fuel and renewable chemicals process by addressing an area that has been neglected in the past. It would be useful if the impact on improvements related to the FCIC program could be estimated. What is the sensitivity of throughput on the price of the product? Most continuous chemical technologies assume a 90% operational uptime. How much was conversion improved by monitoring feedstock quality? One concern is that the use of a pharmaceutical approach for

a low-margin, high-capital process might not be a good fit. What is the effect on feedstock costs? The TEA analysis is critical and needs to be considered in all the project work.

- There is much to like in this presentation of the reboot and rethinking of the approach of the FCIC; however, the central piece to this plan being the adoption of the quality-by-design product development approach used in the pharmaceutical industry might prove to be both the strength and weakness of the project. Only time will tell. We will learn a great deal by using this design philosophy to produce commodity fuels and chemicals instead of medicine. I do believe that there needs to be rigorous controls in place to not slip into making designer biomass feedstocks. Trying to reduce variability could easily lead one down that path.
- The new approach outlined will be a good new perspective, but much of the actual work will remain similar to before. I like the focus on making sure first principles are mostly used and that the product quality defines the design.

- Thank you for the suggestion to create a visualization-based training tool. This is a good idea, and we will explore opportunities for implementation.
- The success rate of 70% was chosen as an aspirational goal to acknowledge the significant challenges that face biorefineries. We agree that this will be very difficult to measure but hope that this will inspire our research teams to make great strides to improve the success rate. By significantly improving the success rate, we will identify the largest impacts on failure and focus on further increment improvements in the future.
- Thank you for the feedback. We plan to conduct extensive TEA and use the results to guide research priorities, the impact of performance improvements, as well as uptime.
- Task 8 will include TEA activities for the key areas of preprocessing, low-temperature conversion, and high-temperature conversion. We recognize that constraining downstream critical material attributes (CMAs) too tightly will simply result in shifting apparent costs upstream, so Task 8 includes the development of process-wide TEAs to minimize costs at the system level.
- We also appreciate the relative insensitivity of the pharmaceutical approach to cost and will strive to adjust our approach to high-capital, low-margin processes.
- Thank you for the feedback. We plan to conduct extensive TEA and believe that this will enable us to focus on improving the conversion processes.
- Because we will be constrained by the final product cost targets, the TEA will prevent us from defaulting to the solution of "designer feedstock," which will tend to be too expensive to allow us to meet those product cost targets.

# **ADVANCED ALGAL SYSTEMS**

PROGRAM AREA

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## INTRODUCTION

The Advanced Algal Systems (AAS) Program Area was reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review. The review took place March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 36 projects were reviewed in the AAS session by a review panel of five external experts from industry.

This review addressed a total federal share of approximately \$108,000,000 (Fiscal Year [FY] 2016–FY 2019 obligations) in financial assistance awards and national laboratory direct funding, which represents approximately 14.1% of the dollar value of the overall BETO portfolio reviewed during the 2019 Project Peer Review. During the Project Peer Review meeting, the principal investigator (PI) for each project was given 30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were independently evaluated and scored by the review panel plans using one of three standard review criteria and scoring rubrics (see introduction of report) depending on the age of the project—e.g., new start, ongoing, and sunsetting. Scoring criteria included the project approach, technical progress and accomplishments, relevance to BETO goals, and future work. This section of the report contains the results of the Project Peer Review, including average score by criteria for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the AAS Program, scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

## ADANCED ALGAL SYSTEMS OVERVIEW

The mission of the AAS Program is to reduce the cost of algal biofuels through public/private partnerships for early-stage research and development (R&D) on sustainable algae production, logistics, and conversion to biofuels. Projects presented within the AAS session address a diverse range of topics, including algal biology; algal cultivation; harvest and processing logistics; conversion interfaces and conversion technologies; and analyses of high-value coproducts, techno-economics, sustainability, and resource availability.

AAS R&D focuses on showing progress toward achieving high-yield, low-cost, environmentally sustainable algal biomass production and logistics systems that produce algal feedstocks well suited for conversion to fuels and other valuable products. Algal biomass includes micro- and macroalgae as well as cyanobacteria. Algal feedstocks include concentrated whole algal biomass, fermentable substrates, extractable lipids, secreted metabolites (alcohols or others), or biocrude resulting from hydrothermal liquefaction (HTL). These feedstocks must be upgraded, blended, and/or purified to produce a finished fuel or bioproduct. Developing algal feedstocks to achieve BETO's advanced biofuel price goals requires breakthroughs along the entire algal biomass supply chain.

#### ADVANCED ALGAL SYSTEMS SUPPORT OF OFFICE PERFORMANCE GOALS

The AAS Program performance goal is to deliver technologies that can enable the verification of technical performance of algae cultivation, harvesting, and conversion processes at the engineering scale capable of converting algal feedstocks to biofuels and bioproducts in support of BETO's goals for the mature modeled minimum fuel selling price (MFSP) of \$2.5/gallons gasoline equivalent (GGE) for biofuels by 2030. For details on the program's technical goals and milestones, please review BETO's *Multi-Year Plan* (MYP).

#### ADVANCED ALGAL SYSTEMS APPROACH TO OVERCOMING CHALLENGES

The AAS Program approach to overcoming challenges and barriers is outlined in the work breakdown structure (WBS), organized around five key activities. Current activities are focused on:

• Algal strain improvement

- Cultivation system improvement
- Improving the capacity and efficiency of harvesting, preprocessing, storage, and handling
- Characterizing algae to interface appropriately with conversion methods
- Integrating algal R&D systems.

These activities are performed by national laboratories, universities, industry, and consortia teams.

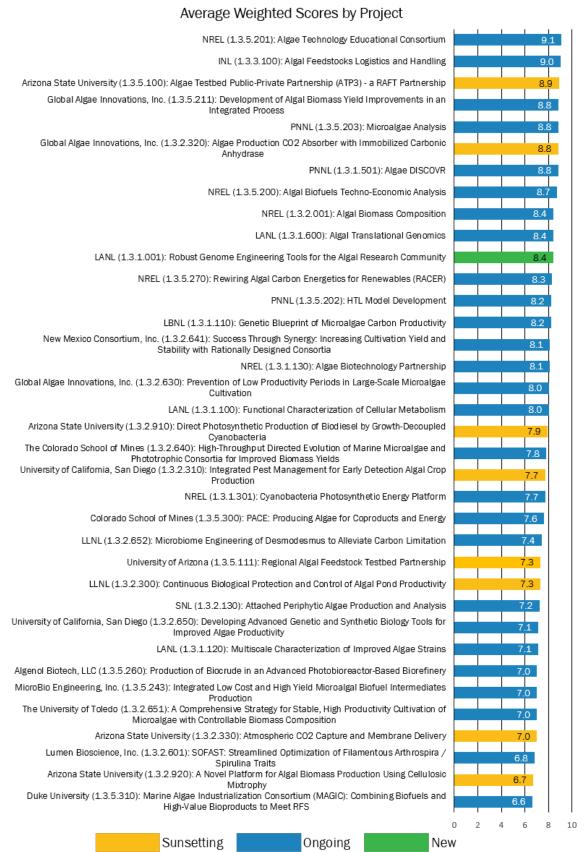
## ADVANCED ALGAL SYSTEMS REVIEW PANEL

The following external experts served as reviewers for the AAS Program during the 2019 Project Peer Review.

| Name              | Affiliation                         |
|-------------------|-------------------------------------|
| Toby Ahrens*      | Larta Institute                     |
| Louis Brown       | Synthetic Genomics                  |
| Michelle Legatt   | Patagonia                           |
| Jose Olivares     | Elsevier & Biologic Energy Partners |
| Becky Ryan        | Indigo Agriculture                  |
| w Lagal variances |                                     |

\* Lead reviewer

## **TECHNOLOGY AREA SCORE RESULTS**



## ADVANCED ALGAL SYSTEMS REVIEW PANEL SUMMARY REPORT

#### Prepared by the Advanced Algal Systems Review Panel

BETO's AAS Program provides funding for a range of disciplines necessary for advancing energy production from algae at commercially meaningful scales. Project performance appears to be in good alignment with MYP goals, and state-of-technology (SOT) estimates of the cost of algal-based fuels (\$/GGE) continue to trend toward meeting mid- and long-term BETO goals. Projects span a broad range of disciplines, including applied genetics, crop stability, engineered systems, logistics, and conversion, among others. Funded projects address individual bottlenecks as well as larger integrated efforts. Funding for continued incremental advances appears to be balanced with earlier stage high-risk/high-reward projects with transformative potential. Continued investment across the supply chain is still warranted.

The projects receiving the top four overall scores across the rating categories (i.e., approach, accomplishments, relevance, future work) reflected the institutional diversity and breadth of disciplines supported by the program. The top projects included two national laboratories, a university, and a private company. The highest ranked project targeted education and workforce development, followed by projects on logistics, public-private test beds, and large-scale integration.

- National Renewable Energy Laboratory (NREL), Algae Technology Educational Consortium (ATEC): This project reported broad-reaching impacts through curriculum development and coursework delivery for K–12 schools, community colleges, and continuing education.
- Idaho National Laboratory (INL), Algal Feedstocks Logistics and Handling: This well-managed project used a unique approach to address the stability of seasonal storage of algae. Improved storage could allow for processing in a lower cost facility designed for average annual production rather than a larger, more expensive facility designed for peak productivity but with spare capacity much of the rest of the year.
- Arizona State University, Algae Testbed Public-Private Partnership (ATP3) a Regional Algal Feedstock Testbed (RAFT) Partnership: This public-private partnership provided access to a network of test beds and supported many studies that fed into BETO's SOT and other modeling efforts. Project participants included industry, academic, and laboratory partners. A wide range of efforts included education and training, high-quality publicly available cultivation data, method harmonization, and benchmarking/validation of many cultivation and conversion technologies.
- Global Algae Innovations, Inc. (GAI), Development of Algal Biomass Yield Improvements in an Integrated Process: This project integrated several innovations in an industrial setting, including improved contamination control, development of a low-energy harvester, and optimized drying and extraction. Reductions in cost across the supply chain resulted in a modeled selling price of \$2.51/GGE.

Overall, the AAS Program is on track to address critical technology barriers and to meet MYP goals. Projects continue to report productivity improvements, and there appears to be good communication and coordination among national laboratories, public-private test beds, and industry partners. Interconnectivity among laboratory-led research projects was noted as a weakness in the prior program review but is one of the strengths and portfolio highlights in this current review. Continued advances in productivity improvements, culture stability, and coproduct development remain high priorities.

#### IMPACT

Progress is being made on many barriers and technical challenges identified in the MYP, and similar to conclusions from the previous peer review, government funding continues to play a critical role in de-risking technologies prior to significant private capital investment.

Several projects warrant specific mention. First, the effort on microalgae analysis led by Pacific Northwest National Laboratory (PNNL) continues to improve industry standards for biomass quantification and has provided recommendations that are widely disseminated and easily accessible. The project has improved confidence in data underpinning the SOT and techno-economic analysis (TEA), which are used to prioritize program funding. Method standardization across projects in the portfolio contributed to vast improvements in the clarity of methodologies used for productivity reporting in this current review, which had been noted as a point of confusion in previous reviews.

Notable progress has also been made on algal productivity, including understanding genetic traits for productivity (e.g., NREL's Rewiring Algal Carbon Energetics [RACER] project, Lawrence Berkeley National Laboratory's [LBNL's] Genetic Blueprint of Microalgae Carbon Productivity, the Colorado School of Mines project on High-Throughput Directed Evolution of Marine Microalgae and Phototrophic Consortia for Improved Biomass Yields) as well as demonstrated improvements in measured productivity in an outdoor, integrated industrial environment (e.g., GAI's Development of Algal Biomass Yield Improvements in an Integrated Process). The program's understanding of microbial diversity continues to expand (e.g., New Mexico Consortium's Success Through Synergy: Increasing Cultivation Yield and Stability with Rationally Designed Consortia project, Lawrence Livermore National Laboratory's [LLNL'] microbiome work), which will be critical for designing strategies for large-scale culture stability and integrated pest management strategies (e.g., University of California San Diego's project on Integrated Pest Management for Early Detection Algal Crop Production).

Other impactful projects have focused on specific bottlenecks in the supply chain, such as GAI's project on carbon dioxide (CO<sub>2</sub>) capture and delivery (Algae Production CO<sub>2</sub> Absorber with Immobilized Carbonic Anhydrase) and INL's project focused on seasonal storage to enable consistent year-round biomass supplies for conversion facilities. INL's project feeds nicely into other downstream processing efforts, such as PNNL's work on HTL model development.

The NREL-led ATEC project was also notable in terms of the breadth of its impact on K–12 and continuing education students and programs.

#### INNOVATION

Advances are still needed across the supply chain, and BETO is supporting innovation through an appropriate mix of steady incremental advances and high-risk, high-reward opportunities. Funding for novel approaches is encouraged if kept at a small number of projects, as is the case in the current portfolio. Notable innovations included:

- Carbon capture and delivery: GAI, Algae Production CO<sub>2</sub> Absorber with Immobilized Carbonic Anhydrase
- Microbiome: New Mexico Consortium, Success Through Synergy: Increasing Cultivation Yield and Stability with Rationally Designed Consortia; and LLNL, Microbiome Engineering of Desmodesmus to Alleviate Carbon Limitation
- Diverse genetic improvement methods supported by strong justifications for target strains: NREL, RACER; LBNL, Genetic Blueprint of Microalgae Carbon Productivity; and Colorado School of Mines, High-Throughput Directed Evolution of Marine Microalgae and Phototrophic Consortia for Improved Biomass Yields
- Coproduct development: Arizona State University, Direct Photosynthetic Production of Biodiesel by Growth-Decoupled Cyanobacteria; and Duke University, Marine Algae Industrialization Consortium (MAGIC): Combining Biofuels and High-value Bioproducts to Meet Renewable Fuel Standards (RFS).

Several projects targeted innovative approaches to coproduct valorization, but some lacked techno-economic considerations comparable in quality to the SOT and TEA efforts for transportation fuels. For example, coproducts could require downstream processing steps such as separations, drying, purification, and/or formulation steps, and they might have additional regulatory considerations. Several projects reported exciting potential for novel coproducts, but one or more considerations in the preceding list were not included.

The proportion of risk in the portfolio appeared to be appropriate. In addition, projects should be encouraged to share challenges broadly to help accelerate the pace of the program's innovation, especially for high-risk efforts. Learning from these challenges could serve as an important foundation for future work.

#### SYNERGIES

In general, national laboratories provided clear articulation of multi-investigator and cross-laboratory collaboration, and these harmonization efforts contributed to the national laboratories receiving 7 of the highest 10 scoring projects. However, high ratings were not distributed evenly among all national laboratories. Interconnectivity among laboratory-led research projects associated with technology, life cycle assessment (LCA), and TEA appears to be strong, such as research feeding modeling efforts supported by PNNL, Argonne National Laboratory (ANL), and NREL.

Another improvement from the previous peer review was industry engagement through formal collaboration and industry advisory board (IAB) involvement. Two large national laboratory-led projects—the PNNL-led Development of Integrated Screening, Cultivar Optimization, and Verification Research [DISCOVR] project and the NREL-led RACER project—included IABs that appeared to convene on a regular basis and were engaged with project leadership. Industrial strains were also included in standardized productivity tests in laboratory-led projects (e.g., strains shared by Algenol).

There seem to be several opportunities for improved collaboration with other U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) programs. First, the AAS Program has funded innovative work in carbon capture and use for many years, and carbon use efficiency efforts in other EERE programs are encouraged to work openly with the AAS Program to build on these strengths. Second, if the AAS Program de-emphasizes large-scale demonstrations, the Advanced Development and Optimization Program appears to be a logical partner to fund critical pilot- and demonstration-scale activities in continuous, outdoor environments. Third, the portfolio includes many diverse approaches for genetic improvement of various strains, and there might be opportunities for collaboration on approaches used in other EERE programs focused on improvement of industrial microbes.

#### FOCUS

The peer review covered 36 projects, including 21 projects from national laboratories, 11 university-led projects, and 7 projects led by private companies. Many included multi-institutional collaborations. Funding was provided through a broad group of funding opportunity announcements (FOAs), ranging from opportunities to address specific bottlenecks, larger integrated multi-institutional efforts, and a call for innovative approaches that were not covered by previous FOAs. Reviewed projects included new efforts, projects in the middle of their funding period, as well as sunsetting projects. Funding covered the full supply chain—from genetic improvement of crops, crop stability, scale-up and production, harvesting, and logistics, through conversion and final products. The breadth of the portfolio was reflected in national laboratory-led projects, which included research on education, standards development for analyses, genetic improvement, culture stability, screening and scaling, logistics, conversion, and large-scale techno-economic modeling.

Funded projects appear to be well-aligned with the barriers and technical challenges outlined in the MYP. One gap noted in the previous peer review was a lack of interaction with end users of products and coproducts. This gap remains, and the program is encouraged to prioritize involvement with end users of all products that contribute significantly to financially viable approaches.

#### COMMERCIALIZATION AND RECOMMENDATIONS

The AAS Program has made consistent progress on MYP goals, and the quality of data underpinning the SOT and TEA continues to improve. After hearing progress from portfolio projects, the peer review panel has several recommendations that it feels will help the program continue its path to supporting cost-competitive energy production from a commercial algal industry.

Coproduct valorization appears to continue to be critical to support viable techno-economics for large-scale energy applications. Development efforts must include explicit product targets, including product specifications, downstream processing costs (separation, purification, formulation), supply chain logistics, and pricing assumptions. In addition, SOT models assume coproducts will play an important role in fuel technoeconomics, but there is little consensus on whether early reliance on high-value coproducts can be easily transitioned to mid-value or commodity-scale coproducts. Future efforts will need to be explicit in identifying product targets, pricing, and processing assumptions to maintain relevance. Related TEA should be integrated throughout projects and used to prioritize effort when appropriate.

Another area for improvement includes further definition of what "outdoor conditions" mean to BETO and future commercialization efforts. If a future algal industry depends on production in large-scale open ponds, then testing in conditions that will be representative of environmental exposures is critical. Many projects acknowledged this challenge but defined outdoor conditions in different ways, with some addressing one specific environmental exposure and others addressing many variables. Program guidance for this stage of testing is suggested. Outdoor test bed facilities are critical, and the program currently relies heavily on a small number of test beds. The program is encouraged to maintain funding for current test beds and consider adding additional sites to capture additional variability in climate, source water, and pest pressures, which will be important for broad industry deployment. The scope of research in exposed environments should also include iterative outdoor-indoor testing, such as pond forensics, quality verification, ecology, and efforts to learn from stable outdoor cultures.

Promising results from early-stage genetic improvement work are being scaled up for continued testing in outdoor conditions, and use in test beds or industrial environments requires appropriate regulatory compliance. Several groups have worked hard to ensure current compliance, but these efforts will likely increase in number and scale in the future. The program is encouraged to support funding for risk assessment tools to inform future regulatory compliance.

Although the quality of data is improving overall, many projects could still benefit from improved experimental design. Objectives should be quantitative and defined prior to the experiment, the scale and duration of tests should match the question being asked, and data should be reported with appropriate statistics (*n* values, error bars, significance). Statistical standards should be encouraged for data integrity in modeling efforts such as the SOT and TEA.

The program is advised to encourage open discussion of lessons learned with funding recipients. Insights from challenges could be as valuable as filtered reporting of positive results.

Finally, the AAS Program has been a leader in carbon capture and use innovation, and the program is encouraged to have open and direct collaboration with carbon use efficiency efforts in other EERE programs.

## ADVANCED ALGAL SYSTEMS PROGRAMMATIC RESPONSE

#### INTRODUCTION/OVERVIEW

The AAS Program staff thanks the review panel for commending the strategic direction of the program as well as the technical progress of AAS projects. The AAS Program strategy for prioritizing R&D gaps identified by the rigorous national laboratory-led analysis portfolio and working to close them with targeted calls for proposals has proven successful. We will continue to work along the supply chain to bring about foundational and impactful R&D to support BETO's goals. Although the AAS Program has a clear technology pathway of focus for benchmarking success, we make room in our portfolio for opportunities for innovation and novel technologies. BETO thanks the panel for acknowledging how critical government funding is in supporting this innovative technology area to reduce risks for private investors. We closely coordinate with industry and stakeholders through advisory groups, in-person meetings at DOE, workshops, Requests for Information, and conferences to ensure that the R&D we fund is relevant, necessary, and well planned. The review panel recognized the improvements we have made in national laboratory coordination and in industry engagement since the 2017 review. The AAS Program is well positioned to help accelerate the growth of the U.S. bioeconomy by filling a key role in the portfolio of domestic bioenergy feedstocks.

#### Recommendation 1: Coproduct valorization.

The AAS Program recognizes the key role that coproducts play in reducing the MFSP of algal biofuels. AAS continues to work toward better incorporation of technical standards for products within FOAs to ensure that selected projects understand product targets, pricing, size of market, adjacent markets, and processing assumptions to support commodity-scale production volumes and make appropriate contacts with downstream product users. AAS continuously improves the methodology for competitive project technical and financial verifications at the initiation, midpoint, and end of projects to ensure that projects are both disciplined and agile in responding to R&D learnings as projects progress.

#### **Recommendation 2: Support outdoor testing.**

The AAS Program agrees with the review panel that testing algal systems in conditions representative of commercial outdoor exposure remains a critical area of emphasis to continue making progress in overcoming challenges to algal fuel and products. AAS continues to develop strategies that are informed by outdoor testing requirements so that projects consider methodologies informed by minimum requirements to test outdoor deployment readiness. AAS also notes the panel's comment that publicly funded outdoor test bed facilities are a critical resource for high-impact R&D developments and data generation. AAS might continue to pursue test beds and could consider incorporating additional sites to add geographically diverse data points to support broad industry deployment in the United States. The FY 2019 AAS area of interest in the larger BETO-wide competitive FOA topic aligns with the panel's specific request to increase iterative indoor-outdoor-indoor testing of algal strain and cultivation technologies to identify and improve upon highly productive and robust mass cultures. Although the AAS Program's mission space does not include setting national regulatory policies and standards, the program remains informed of developments in this area through its involvement in the federal Biomass R&D Board Algae Interagency Working Group that includes representatives from federal agencies that are in this space.

#### Recommendation 3: Improve data quality.

With each competitive funding opportunity, AAS strives to improve upon the rigor of the technical verification process. These verifications help projects improve their experimental designs before work commences and understand progress toward projects' interim and final targets. AAS will continue to consider how projects are incorporating appropriate experimental designs, controls, and statistics as well. Within the national laboratory analysis portfolio, AAS can encourage all BETO-funded analysis projects to consider their statistical standards.

#### Recommendation 4: Share lessons learned.

The review panel suggestion to encourage open discussion of lessons learned, including insights from challenges and failures, is a broadly applicable suggestion. AAS will continue to request that project performers publish, present at conferences, and amplify success stories as well as lessons learned to ensure that government-funded work informs future technical efforts throughout the field. AAS has published scale-up challenges and lessons learned from the algal process development scale and integrated biorefineries within the *National Algal Biofuels Technology Review*.<sup>1</sup>

#### Recommendation 5: Carbon use efficiency.

AAS notes the review panel's recognition of the program's leadership in carbon use innovation. As we continue to execute our strategies for carbon use in algal systems, we will continue efforts to coordinate within BETO and with the DOE Office of Fossil Energy on CO<sub>2</sub> management R&D. We will work to investigate other potential collaborations within EERE and DOE to further algal systems potential to contribute to advancements in circular carbon economy strategies.

<sup>&</sup>lt;sup>1</sup> U.S. Department of Energy. 2016. *National Algal Biofuels Technology Review*. U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Bioenergy Technologies Office, 66–71. https://www.energy.gov/sites/prod/files/2016/06/f33/national algal biofuels technology review.pdf.

# ROBUST GENOME ENGINEERING TOOLS FOR THE ALGAL RESEARCH COMMUNITY

#### Los Alamos National Laboratory

#### **PROJECT DESCRIPTION**

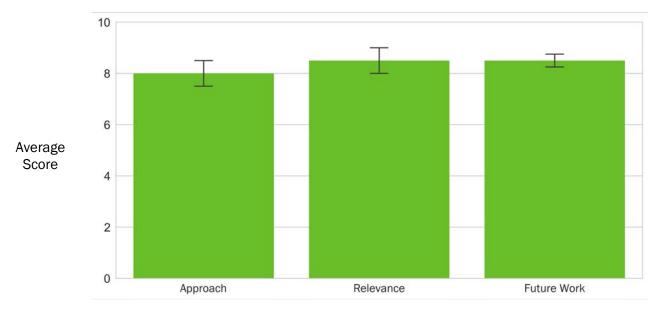
To achieve target levels of biomass and biofuel production, it would be beneficial to greatly increase the number of genetically engineered algal strains under development to maximize algal biomass and improve biofuel and highvalue bioproduct yields. This increase, however, requires changing algal genome editing and metabolic engineering experiments from a slow and arduous process, developing and testing only one or a few mutants at a time, to a more rapid "prototype"-focused (i.e., characterization of large numbers of genetically engineered strains) endeavor. The algal community needs a better set of molecular tools. This project aims to address two of the biggest problems hampering genome and metabolic engineering efforts

| WBS:                      | 1.3.1.001           |
|---------------------------|---------------------|
| CID:                      | NL0034646           |
| Principal Investigator:   | Dr. Blake Hovde     |
| Period of<br>Performance: | 10/1/2018-9/30/2020 |
| Total DOE Funding:        | \$200,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | New                 |
|                           |                     |

across the algal research space. The first problem is the lack of available resources regarding promoter choice in genetic engineering expression cassettes for algal production strains. Currently, only a handful of extremely strong promoters are being used to drive gene overexpression for products of interest. Although these promoters will work to improve algal productivity in certain cases, researchers recognize that a wider variety of promoter sequences can be used to fine-tune expression with the potential to improve algae as a production platform, as demonstrated in current bacterial and yeast systems. The second problem is a lack of precise and rapid generation of new genetic mutants. Currently, most of the time spent on genome metabolic engineering



Weighting for New Projects: Approach-25%; Relevance-25%; Future Work-50%



 ${f I}$  One standard deviation of reviewers' scores

projects is simply generating the desired mutants. This leaves little time for characterizing mutant properties, let alone generating many mutants for characterization. To address these issues, we are performing two tasks during this seed project to model a rapid approach for generating engineering toolboxes for algal production strains:

- Task 1: Transcriptomic evaluation of *Nannochloropsis salina* in multiple environments for identification of variable-strength constitutive promoters and inducible promoters.
- Task 2: Validation and curation of a promoter library for inducible and variable-strength promoters for *N. salina*.

The output of this project will directly benefit BETO MYP barrier Aft-C: Biomass Genetics and Development, specifically regarding more control of synthetic biology and algal metabolic engineering efforts and significantly increasing the throughput of genetic engineering targets chosen as objectives for upcoming efforts to improve algal production. The investment in developing these tools now will pay dividends in upcoming years by removing large technical hurdles that currently hinder many projects. This work will provide access to an initial curated promoter library for *N. salina* that will be available to the algal genome engineering research community. This work will also provide a road map for the rapid development of molecular toolboxes for additional algal production strains.

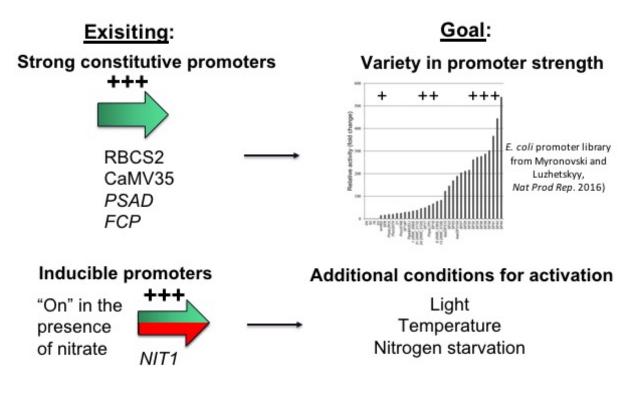


Photo courtesy of Los Alamos National Laboratory

#### OVERALL IMPRESSIONS

- This project's genetic engineering methodology strives to accelerate the time to identify and verify promotors and promotor strengths. If successful, the team will establish an important baseline for future applications.
- The project is clear and concise with reasonable goals for a 1-year project.

- This kick-starter project is a nice complement to the portfolio of BETO projects. The project team is working toward opportunities to make connections across the portfolio of projects. There is a clear focus on the rapid development of a genetic tool for use in an industrial relevant algal strain. Successful completion of the project will positively impact strain and tools development in alignment with MYP targets.
- This is a small, targeted project with clear direction and good relevance to the BETO mission and concurrent projects at national laboratories. The project is early in its merit review cycle, and initial accomplishments are on track. Future work tied to original project objectives appears to have a high chance of success.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Our team appreciates the positive feedback and the review committee's recognition that this work will improve the rate at which new algal genetic strains can be generated and improved. In addition, the reviewers recognized that the scope of work presented was appropriate for the project timeline and budget as a proof-of-concept task. Upon successful completion of this project, the applied model of using transcriptomic data to rapidly develop native promoter libraries for immediate use will be presented and expanded upon to (1) quickly generate useable promoter libraries for current and new BETO algal production strain candidates and (2) release a public-facing tool for users to generate candidate promoter libraries from their own transcriptomic data collections for new algal species of interest. These outcomes are synergistic with other BETO projects through leveraging existing or planned data collection as inputs. Expanding this project would likely provide beneficial outputs for other advanced algal system endeavors.

## FUNCTIONAL CHARACTERIZATION OF CELLULAR METABOLISM

#### Los Alamos National Laboratory

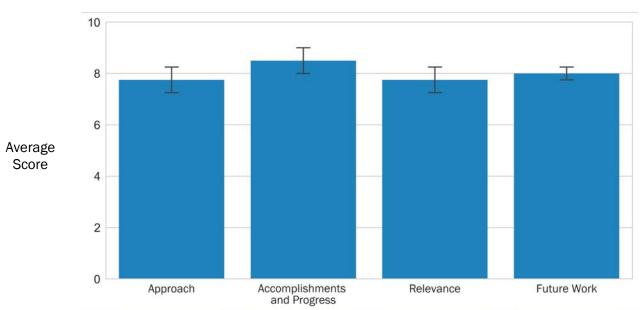
#### **PROJECT DESCRIPTION**

The objectives of this project are to integrate biotechnology and genomic developments for improved algal lines coordinating multiomic characterizations, genetic engineering, and flow cytometry phenotyping for universal applications to algal strain productivity and robustness improvements. We will directly focus on engineering nitrogen regulatory responses altering carbon dynamics to optimize biomass and product flux, developing flow cytometry tools for rapid physiological characterization and the development of robust strains, and developing novel epigenetic understanding of physiological regulation to develop techniques for accelerated strain improvement through an integrated

| WBS:                      | 1.3.1.100           |
|---------------------------|---------------------|
| CID:                      | NL0026328           |
| Principal Investigator:   | Dr. Scott Twary     |
| Period of<br>Performance: | 10/1/2016-9/30/2020 |
| Total DOE Funding:        | \$2,950,000         |
| DOE Funding FY16:         | \$1,000,000         |
| DOE Funding FY17:         | \$650,000           |
| DOE Funding FY18:         | \$650,000           |
| DOE Funding FY19:         | \$650,000           |
| Project Status:           | Ongoing             |
|                           |                     |

improvement platform. This work will develop novel capabilities through an expanded suite of flow cytometry physiological assays, expanding the molecular engineering toolbox of *Nannochloropsis salina* to include Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) and CRISPR-associated (Cas), and defining and regulating epigenome responses. These developments will identify key functional pathways and regulatory mechanisms as targets for advanced improvement strategies. We have currently adapted six physiological assays for multiple algal species characterizing intracellular pH, cellular actin structure, metabolic activity, reactive oxygen species, DNA ploidy, and lipid accumulation. These assays have also been applied toward population sorting to create more robust lines. We have characterized the methylation profile of

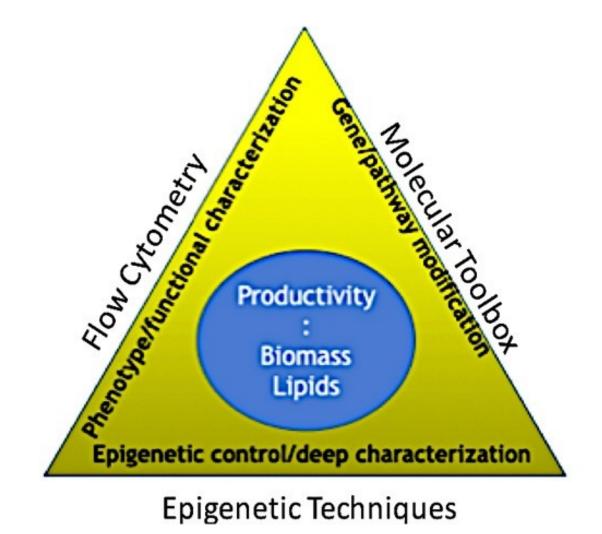
#### Weighted Project Score: 8.0



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

 $\square$  One standard deviation of reviewers' scores

the epigenome in two algal species: *N. salina* and *Picochlorum soloecismus*. The percentage of the genome methylated under nitrogen replete (nonstress) conditions is less than 2%, significantly less than most species. The epigenome responds to both epieffector molecules and nitrogen stress with significant reductions in genome methylation. These changes result in increased lipid accumulation, suggesting that regulation of lipids can be controlled by these mechanisms. We developed constitutively expressing Cas9 and Cas12 lines in *N. salina* for targeted gene editing. Initial targets include regulatory genes involved in nitrate uptake and signaling. New targets will be derived from the metabolic responses of these knockout systems. All three capability advancements will be integrated to create a complementary approach for more powerful strain improvement.



#### Photo courtesy of Los Alamos National Laboratory

#### OVERALL IMPRESSIONS

• The goals, technical, and management approaches of this project were clearly articulated. The team has made great progress on all project objectives, and objectives are related to the BETO mission. The team is encouraged to focus future efforts on the portions of the project with the greatest potential impact.

- This multifaceted project attempts to integrate different components into a single platform to establish a better understanding of genetic pathways involved in nitrogen's influence on algal growth—an ambitious goal with lots of coordination.
- This project is designing an integrated strain improvement platform using environmental, epigenetic, and genetic factors for targeted advances with rapid, comprehensive phenotyping leading to increased understanding of these modifications. The techniques being established and optimized for algal strains in this project will add significant value to future strain characterization projects. Large-scale testing will be needed to confirm the 50% increase in lipid formation.
- The project team is employing innovative approaches to improving strain characteristics targeted toward value drivers in algal production systems. The accomplishments to date and their connection to the BETO MYP targets were clearly communicated by the presenter. Of note, the improvements on methods to transform algae and modify methylation are demonstrating great potential value. There is an opportunity to expedite outdoor testing of the modified strains to validate the laboratory results.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Our team greatly appreciates the reviewers' critique of our technical approach and impacts. These inputs will be incorporated into improving our experimental plan. The primary focus is on nitrogen stress induction of lipid accumulation. Biomass productivity is defined by ash-free dry weight. Lipid productivity correlating to boron-dipyrromethene (BODIPY) staining is validated by gas chromatographic/mass spectrometry fatty acid methyl esters analysis. Increased strain productivity is assessed against parent lines grown under conditions ranging from the laboratory scale to greenhouse 50-L raceways. Potential collaborations are established for permitted outdoor genetically modified organism (GMO) trials to correlate laboratory results to outdoor production, if time and funding allow.
- The three-pronged approach integrating flow cytometry, epigenetics, and genetic engineering relies on critical achievements in assay optimization and dye viability effects, methylation assays and methylome sequencing analysis, and CRISPR-Cas editing stability and effectiveness.
- The initial component development focuses on identifying and advancing strengths that can be leveraged into the integrated system. The most effective and relevant results will be the focus for future investigations. For example, multiple epigenetic regulators will be screened for evaluating efficacy and phenotypic responses. The flow assay portfolio can be expanded as novel experimental developments are analyzed. We are reducing stable transformation selection cycles from weeks to days through coordinated flow cytometry sorting of fluorescent reporter genes linked to antibiotic selection. Population sorting into multiple or single-cell transformants can facilitate rapid transgene characterizations. This work demonstrates the value of integrating multiple tool kit developments into one enhanced strain improvement method. Manipulation and evaluation of phenotype using three different molecular approaches (phenotype, genotype, epigenome) increases the probability of generating a highly productive strain and generating a (more) holistic understanding of both physiological and epigenetic changes that occur from targeted genetic engineering strategies. This more comprehensive analysis allows greater elucidation of both primary and secondary responses, enriching the knowledge base to further advance the field.

## GENETIC BLUEPRINT OF MICROALGAE CARBON PRODUCTIVITY

#### Lawrence Berkeley National Laboratory

#### **PROJECT DESCRIPTION**

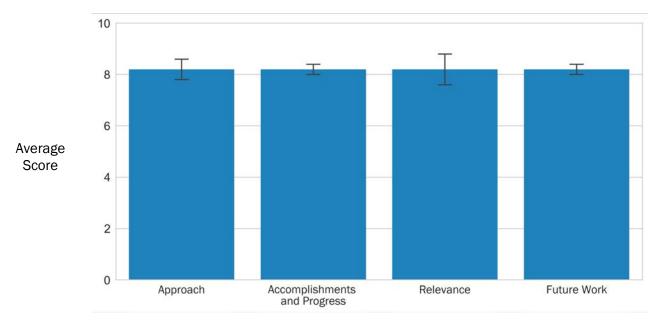
The potential of microalgae to emerge as major biofuel producers is limited by the fact that maximal internal carbon accumulation (lipids and/or carbohydrates) in algae occurs at the expense of cell growth. Further, different strains of algae have adapted and evolved in various environmental conditions, and thus rotation of specific "seasonal" strains is required to maximize stabilize biomass production throughout the year. A better understanding of algal biology—in particular, mechanisms (1) regulating carbon production and switches from rapid growth to stress-induced carbon storage and (2) growth responses at varied temperatures—is critical to overcoming these limitations. Improving the productivity and

| WBS:                      | 1.3.1.110           |
|---------------------------|---------------------|
| CID:                      | NL0032266           |
| Principal Investigator:   | Dr. Igor Grigoriev  |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$1,050,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$350,000           |
| DOE Funding FY18:         | \$350,000           |
| DOE Funding FY19:         | \$350,000           |
| Project Status:           | Ongoing             |
|                           |                     |

robustness of algal strains against perturbations will require extensive advanced genetic, genomic, and molecular biology tools, which are currently lacking for most algal species. This project directly addresses barriers to Aft-3: Genetic Modification and Development. Combining expertise in algal genomics, transcriptomics, metabolomics, and gene editing to characterize novel algal strains with the highest potential as third-generation biofuels will improve biomass production rates and decrease the lag time for genetic modification by 50%.

#### Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $\square$  One standard deviation of reviewers' scores

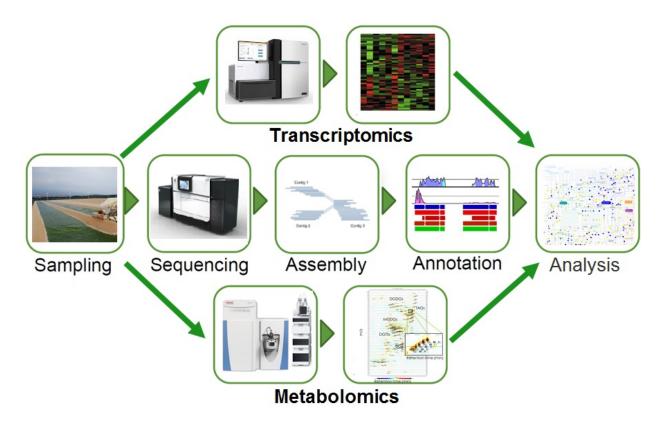


Photo courtesy of Lawrence Berkeley National Laboratory

#### **OVERALL IMPRESSIONS**

- Significant value has been realized through the development of a functional genomics pipeline designed to evaluate multiomic data relevant to algal production in real field stresses. Progress to date has identified drivers of cold stress tolerance and potential targets for modification. This project demonstrates the potential to use highly advanced genetic tools and machine learning in application toward commercial targets. Given the accomplishments to date, I expect the team to be successful in continuing to improve the efficiency and value of the omics toolbox.
- This annual operating plan (AOP) project is in the final year of its merit review cycle. The project appears to be managed well and is on track to meet the original project objectives. The project has clear relevance to the MYP goals, the BETO portfolio, and the broader algal industry.
- This project demonstrates the value of a functional genomics development pipeline to identify gene targets with the potential to increase algal productivity to achieve MYP goals. Accelerating the development pipeline during the next fiscal year will be incredibly beneficial.
- A 50% decrease in the time required for this level of carbon pathway mapping is an ambitious task but essential in propelling the overall field research forward. Several national laboratory teams, in addition to private companies, are working on this research path, and it will beneficial to harmonize efforts so no time is wasted or work is doubled.
- The team is developing an algal functional genomics pipeline for the production and interpretation of multiomic measurements from multistate perturbation experiments to identify gene targets for strain improvement and commercialization at an accelerated (50% reduced) development time. They will be using the newly developed pipeline to identify gene targets for strain improvement in *Scenedesmus sp.*

NREL 46B-D3 (NREL) within the first 2 years and then in *Monoraphidium minutum* 26B-AM (PNNL) within 1 (the third) year, achieving the target identification at 50% time reduction. The approach is reasonable and focused on two very relevant strains for the program. The team has sequenced and annotated the genome for *Scenedesmus sp.* and has constructed a metabolic model and curated it. They have also profiled the transcriptome and lipidome under cold and heat shock and done some gene network analysis to map genetic responses. The progress is deemed reasonable and impactful. Genomebased strain improvement is key to the MYP performance goal to increase seasonal areal productivity. These genetic improvements rely on well-sequenced, annotated, and understood genomes. This project helps advance the knowledge of individual key organisms associated with the BETO program. The team will move to sequencing the genome and transcriptome of *Monoraphidium minitum* next. After FY 2019, the team will optimize, enrich, and apply the Blueprint functional genomics pipeline to produce genomes, multiomes, and customized modeling/analysis tools for additional BETO-approved strains.

• No major weaknesses are noted.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Many thanks for your thoughtful review. Because algae have adapted and evolved in many environments, we hypothesize that the genetic basis of these adaptive traits can be identified and exploited to maximize biomass production throughout the year, particularly by improving productivity at the crossover points when "summer" strains are rotated in favor of "winter" strains. By measuring the systems-level responses with modern omics tools under heat and cold stress conditions, we were able to identify many genes that were differentially transcribed and verify the impact of these transcriptional responses by measuring the downstream impact within the lipidome and metabolome. In partnership with algal molecular biologists, we plan to validate our findings by modifying the expression of several differential expressed genes to preadapt the algal strains to a wider temperature range to improve productivity. Additional outdoor cultivation tests will be needed to fully validate the impact of any genetic modifications. Going forward, we plan to validate and refine our functional genomics pipeline on a diverse set of algae to build a solid understanding of algal physiology for each evolutionary distinct lineage and fold in additional omics measurements to improve the metabolic models and regulatory networks that control growth and biomass composition of industrially relevant production strains.

## **MULTISCALE CHARACTERIZATION OF IMPROVED ALGAE STRAINS**

#### Los Alamos National Laboratory

#### **PROJECT DESCRIPTION**

Algae have the potential to be cost-effective and sustainable organisms for the production of renewable fuels and chemicals; however, several challenges must be overcome to realize the full potential of algal feedstocks. First, techno-economic analysis (TEA) of algal biofuels continues to point to algal productivity as a major contributor to biofuel costs. Second, although freshwater strains such as *Chlorella* and *Scenedesmus* routinely demonstrate high performance in laboratory screens, the use of large-scale freshwater systems for algal biofuels and bioproducts is not an acceptable approach from both a sustainability and a human agriculture competition perspective. Third, the relationship between indoor

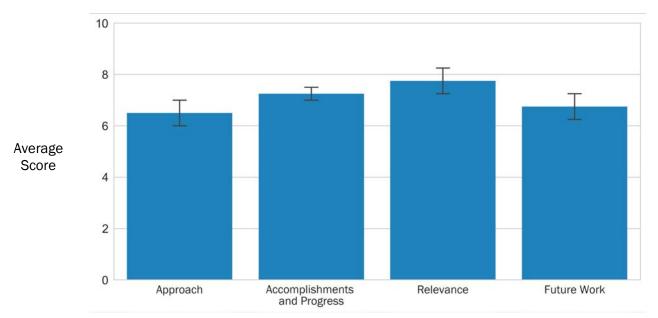
| WBS:                      | 1.3.1.120           |
|---------------------------|---------------------|
| CID:                      | NL0025841           |
| Principal Investigator:   | Dr. Taraka Dale     |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$2,300,000         |
| DOE Funding FY16:         | \$500,000           |
| DOE Funding FY17:         | \$600,000           |
| DOE Funding FY18:         | \$600,000           |
| DOE Funding FY19:         | \$600,000           |
| Project Status:           | Ongoing             |
|                           |                     |

phenotypes of improved strains and outdoor phenotypes is still relatively poorly understood.

Our working hypothesis is that algal strains with improved outdoor productivities can be generated indoors by using a suite of algal strain improvement strategies. Thus, our goal is to develop this suite of improvement approaches using cell sorting, adaptation, and genetic modification techniques, and we focus specifically on tools for generating algal strains with increased biomass and carbon storage as well as environmental robustness (e.g., salinity tolerance). In this presentation, we share our progress on developing these tools and testing these strains across a range of scales, from indoor flasks to outdoor ponds.

#### Weighted Project Score: 7.1

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores



Photo courtesy of Los Alamos National Laboratory

#### OVERALL IMPRESSIONS

- This is a broad and ambitious project with clear relevance to MYP goals. Team members are encouraged to add clarity and specificity to the objectives and project management structure to ensure progress is made toward project goals.
- This project focuses on developing strain characterization and improvement techniques that are proven to successfully identify strains that translate desired performance from lab bench to outdoors. The unique indoor-outdoor-indoor approach will be incredibly valuable across the industry once it is optimized.

- The project has a great balance between lab-scale and outdoor testing, which is essential in the progress of the entire biofuel field. The project seems to be on two distinct paths: the non-genetically modified and genetically modified, with minimal synergy between the two. It could be beneficial to integrate both paths, resulting in a comprehensive improvement of strains that could be leveraged for outdoor scale-up.
- The multiscale characterization of the algal strains project clearly aims to connect the indoor assessment of strain performance with outdoor demonstration data. The project team has identified a promising strain with the potential to improve productivity and stress tolerance in the field. Improved methods to select for valuable-strain characteristics are also under development. Connecting these tools to realize the iterative feedback loop of lab to field and back to lab testing is critical to fully realizing the project value.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Our project management approach does have more detail than time would permit in the presentation. That said, we take your point and will review our objectives and project management structure and look for improvements to increase our chances of success.
- Thanks for the positive feedback.
- Our two strain improvement approaches are, in fact, currently distinct; however, we agree that in the future it would be valuable to integrate them. Of course, if each new strain is a genetically modified strain, that would entail getting regulatory approval every time we went outside, which would slow our ability to move outdoors. We have been involved in the successful preparation and approval of a Toxic Substance Control Act Environmental Release Application (TERA) for a different project, however, and we are actively considering writing a TERA for at least our most characterized genetically modified *Picochlorum* strain.
- We agree that the feedback from outdoor work is important. We do have specific examples of using outdoor data to inform our indoor work, but we opted to focus on other strain improvement successes in this particular presentation. We look forward to further tightening this interaction between the field and lab, and we will consider this comment as we move forward.

## ALGAE BIOTECHNOLOGY PARTNERSHIP

#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

The development of advanced genetic and genomic tools for targeted algal metabolic engineering pursuits will be integral to achieving target biomass productivity and, ultimately, the BETO goal of cost-competitive biofuels derived from algal biomass by 2022. At present, however, broad host-range tool development is currently hindered by strain-specific negative regulatory mechanisms. Indeed, the biological processes controlling algal transcription and translation are subject to complex host regulation, which often presents hurdles for targeted genetic engineering strategies. Advanced genetic approaches, such as CRISPR mediated genome editing offer a means to rewire these regulatory systems and/or introduce novel functionality

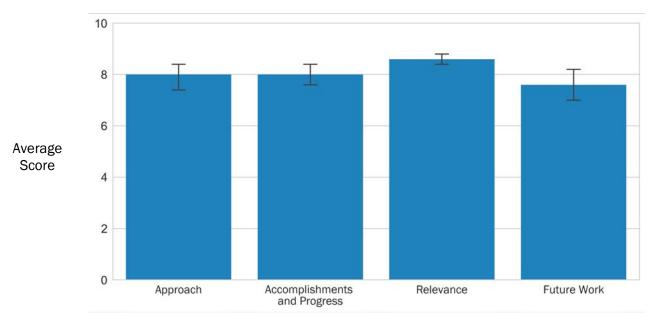
| WBS:                      | 1.3.1.130             |
|---------------------------|-----------------------|
| CID:                      | NL0028812             |
| Principal Investigator:   | Dr. Michael Guarnieri |
| Period of<br>Performance: | 10/1/2015-9/30/2021   |
| Total DOE Funding:        | \$1,560,236           |
| DOE Funding FY16:         | \$200,000             |
| DOE Funding FY17:         | \$500,000             |
| DOE Funding FY18:         | \$430,236             |
| DOE Funding FY19:         | \$430,000             |
| Project Status:           | Ongoing               |
|                           |                       |

into algal biocatalysts. Synthetic systems biology approaches also present a means to construct novel genetic regulatory networks and rewire natural biological systems to establish orthogonal networks wherein nonnative control elements are introduced into or evolved in host microbes for bypass of host control.

The Algae Biotechnology Partnership aims to develop advanced genetic editing tools, synthetic and orthogonal genetic regulatory systems, and functional genomic pipelines to enable universal metabolic engineering strategies in top-candidate deployment algal strains. Successful development will ultimately open the door for targeted strain-engineering strategies, aimed at maximizing algal outdoor biomass production, composition, and strain robustness. The project will initially develop orthogonal tools in *Picochlorum sp.* 39-A8, which is a



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

top-candidate, halotolerant strain that was downselected and evaluated for outdoor production capacity. The strain displays a rapid maximum growth rate (less than 3-hour doubling time, among the fastest reported to date for eukaryotic algae) and high biomass accumulation capacity, superior to the current SOT. Our 3-year project objective is to demonstrate multistrain applicability of orthogonal tools in concert with genome editing capabilities.

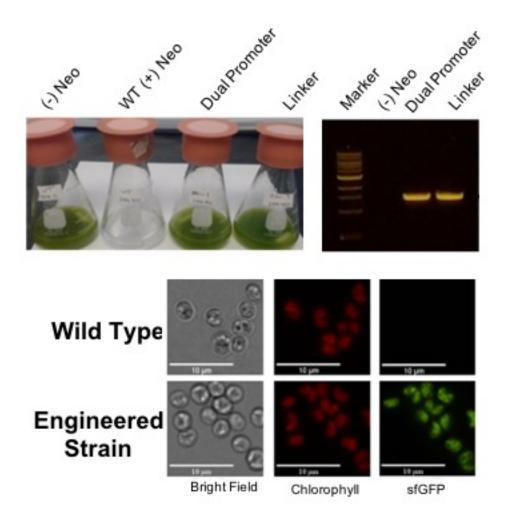


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This is an ambitious project leveraging the core capabilities of participating organizations to develop a genetic engineering toolbox with broad applicability to improve strain productivity. This project's toolbox has the potential to drastically reduce the amount of time and resources to apply these techniques to different algal strains.
- The project is making a pivot from their previous work in strain development to focus on developing tools for most of the project timeline. Although it is imperative for the entire industry to have a robust genetic toolbox, by focusing only on developing genetic tools for the first 2 years and then deploying these tools to five different strains in year three seems potentially risky. Working toward alleviating issues regarding TERA permitting is essential for the entire biofuel program.

- The project team is transitioning focus from the identification of a highly productive halotolerant strain to the development of a universal toolbox for strain improvement. A significant accomplishment of the project was the completed screening of more than 300 strains under high temperature and salt, which led to the identification of a highly productive strain relevant to targeted field conditions. The current project goal to identify a broad host-range genetic tool kit is ambitious and potentially challenging to complete as defined. A universal system for improving strains has high potential value, especially given the increasing diversity in algal strains of commercial interest.
- This is an ongoing AOP project at the beginning of a new review cycle. The team provided an overview of previous work with a strong justification of the focus for future efforts. The project has clear relevance to BETO priorities, MYP goals, and the algal industry. The project appears to be managed well, and a clear technical approach is supported by quantitative objectives.
- The aim of the project is to develop advanced algal genome editing tools, including synthetic and orthogonal genetic regulatory systems with broad-host range applicability and functional genomic pipelines in top-candidate deployment algal strains. The goal is to demonstrate integrated system "universality" via targeted integration and orthogonally regulated gene expression of native and heterologous fatty acid biosynthetic pathway genes in five candidate deployment organisms. The approach is deemed to be reasonable. The accomplishments to date are deemed to be appropriate. The work addresses the industry-wide need for genetic tools in nonmodel systems—including tools, strains, and metadata—that will be publicly disseminated to enable rapid adoption by the algal industry for targeted enhancement of deployment strains. If successful in developing universal genetic manipulation tools and will demonstrate tunable gene expression and CRISPR-Cas9 editing. The final step will be testing the "universality" of the tools on five representative organisms.
- No major weaknesses are noted.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the review panel for their encouraging and constructive critique as well as their recognition of the potential impact of our pursuits. We agree with the reviewers' assessment that although this work presents an ambitious and potentially challenging path forward, is also presents a potentially transformative route to address the industry-wide need to for broad host-range genetic tools in nonmodel, deployment-relevant systems. We are optimistic that the genetic tools pursued on this project have the potential to substantially increase the throughput of algal metabolic engineering pursuits targeting enhanced microalgal productivity, and thus we believe this work has clear relevance to BETO priorities and MYP goals. We also agree with the panel's assessment that working to alleviate issues regarding TERA permitting will be essential for the entire algal biofuel program; we are actively engaging on this front to ensure the work conducted here is compliant with regulatory guidelines and also hope our findings can help inform these guidelines moving forward. Related, we are actively deploying our topcandidate strains at various domestic test beds in coordination with other projects in the BETO algal portfolio (e.g., DISCOVR); and we will strive to deploy engineered variants of these, or other topcandidate engineered strains, within the current period of performance to evaluate outdoor performance and provide a proof of concept for the deployment potential of strains engineered with our team's novel genetic tools. We believe our progress to date to identify high-productivity, halotolerant algal strains, and to develop associated genetic and genomic tool kits therein, represents a critical advancement for the BETO algal portfolio and the larger algal research community. We look forward to continued efforts to enhance productivity in top-candidate strains via the further development of robust genetic and functional genomic tools amenable to phylogenetically diverse algal strains.

## CYANOBACTERIA PHOTOSYNTHETIC ENERGY PLATFORM

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

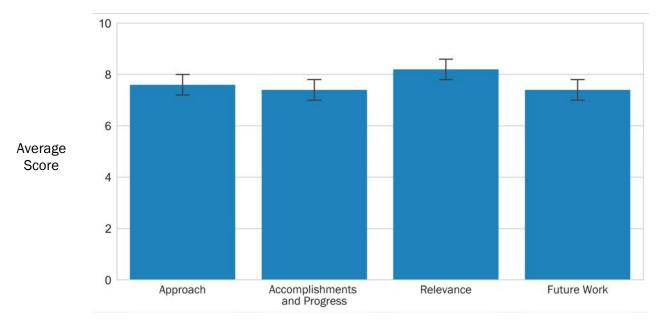
The objective of this project for the new FY 2019–FY 2021 merit review cycle is to develop a cyanobacteria platform with the goals of exploiting photosynthetic energy conversion and carbon use for ultimate use in the fundamental biochemical targets to improve biomass productivity. This project leverages years of research and an excellent publication track record at NREL in photosynthesis and carbon and energy metabolism in the model strain *Synechocystis* and will translate and project this knowledge base to the cyanobacteria of industry interest, such as species from the *Synechococcus* and *Arthrospira* genera. In FY 2019, the target is to verify the successful modulation of gene expression of the identified

| WBS:                      | 1.3.1.301           |
|---------------------------|---------------------|
| CID:                      | NL0022533           |
| Principal Investigator:   | Dr. Jianping Yu     |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$1,600,000         |
| DOE Funding FY16:         | \$400,000           |
| DOE Funding FY17:         | \$400,000           |
| DOE Funding FY18:         | \$400,000           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

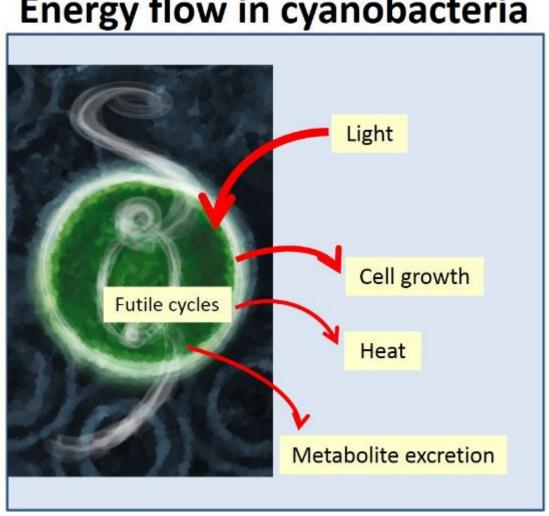
metabolic switch in *Synechocystis*, showing biomass productivity enhancement of at least 10% relative to the wild-type grown under diurnal light conditions in benchtop photobioreactors (PBRs). By the 18-th month midpoint, this project will have demonstrated a 20% increase in biomass productivity using engineered *Synechocystis* strains and will deliver a strategy to transfer the technology to production-relevant species. The end of the project will be a successful platform for rapid testing of photosynthesis and biomass improvement hypotheses in cyanobacteria, including strains of industrial relevance, as well as the development of a route to implement these strategies in selected eukaryotic systems.

#### Weighted Project Score: 7.7

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $\square$  One standard deviation of reviewers' scores



## Energy flow in cyanobacteria

Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- The end of the project will be a successful platform for the rapid testing of photosynthesis and biomass improvement hypotheses in cyanobacteria, including strains of industrial relevance, as well as the development of a route to implement these strategies in selected eukaryotic systems. Overall, I think this is an interesting project that is dealing with an important attribute in improving biomass productivity by improving photosynthetic productivity.
- This project is an AOP project at the beginning of its merit review cycle. The project appears to have ٠ appropriate technical and management approaches and good alignment with the MYP goals. Team members are encouraged to reach out to industry partners that have more direct experience with a focus on future planned research.
- This project leverages past research to further improve the photosynthetic efficiency of engineering algal ٠ strains. If successful, it will increase biomass productivity and contribute to BETO goals.

- The Cyanobacteria Photosynthetic Energy Platform project is focused on modifying the expression of photosynthetic pathways that have a high probability of impacting algal growth and productivity. The clear objectives and underlying data on gene targets are a strength of this approach. The upcoming completion of the proteomics and transcriptomics analysis will also be interesting to further the options for targets of modification. Additionally, the project team has outlined the potential partners for strain testing and potential commercial utility. Taking the next steps in evaluating these modifying strains in outdoor trials and assessing biomass quality will be critical to realizing the utility of the concept.
- The aim of the project is to develop genetic tools for cyanobacteria to improve photosynthetic efficiency through carbon pathway engineering, leading to improved biomass productivity and ultimately to reduced cost for fuels and chemicals. The target is to improve biomass productivity in cyanobacteria by 25%. The team will take a synthetic biology approach to manipulate the carbon sink in cyanobacteria by expanding the sink via ethylene production promoted by the insertion of the efe gene and overexpress/upregulate the photosynthetic apparatus. At the same time, the glycogen synthesis pathway will be blocked. The hypothesis is that this will increase biomass productivity for the organism. To do this, the team will develop new genetic manipulation and phenotyping tools. The project is very focused and has previous experience manipulating the organism with the efe gene. The project is initiating but has previous experience inserting the efe gene into cyanobacteria. Developing tools in model organisms allow for rapid hypothesis testing and then provide options for application to production cyanobacteria and eukaryotic species. The hope is to generate a small set of genetic manipulation tools applicable to cyanobacteria, which will enhance the carbon sink in biomass production. This could possibly generate a high-biomass-productivity organism. If successful, the project could advance BETO goals for high productivity and resilient algal crops. The project has recently been initiated and will be working on photosynthetic overdrive by PII overexpression and energy balancing by down-regulating the glycogen or sucrose flux using a weak promoter to drive glgC and sucrose-phosphate synthase expression. This is a simple strategy that can be demonstrated.
- No major weaknesses are noted.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

## ALGAE DISCOVR - PNNL

#### **Pacific Northwest National Laboratory**

#### PROJECT DESCRIPTION

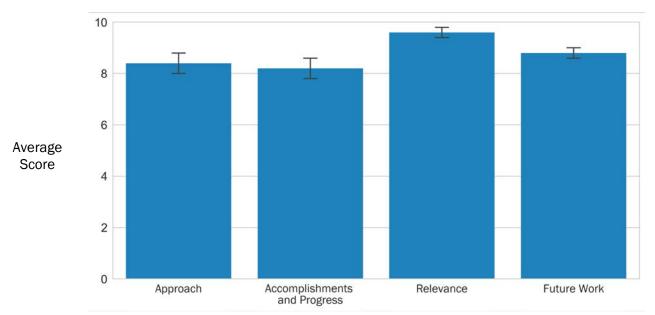
New cultivars are needed for robust year-round algae cultivation. In addition, benchmarking and tracking the state of algal cultivation is a responsibility of the BETO. We are developing and applying an integrated platform and workflow for standardized, deep characterization of highly productive and resilient microalgal strains. Four national laboratories—PNNL, Los Alamos National Laboratory, NREL, and Sandia National Laboratories (SNL)—are collaborating to combine unique capabilities to significantly improve the TEA feasibility of algaederived biofuels and products, as demonstrated in the context of SOT experimentation at the test bed of the Arizona Center for Algae Technology and Innovation (AzCATI).

| WBS:                      | 1.3.1.501             |
|---------------------------|-----------------------|
| CID:                      | NL0032208             |
| Principal Investigator:   | Dr. Michael Huesemann |
| Period of<br>Performance: | 10/1/2016-9/30/2019   |
| Total DOE Funding:        | \$6,780,000           |
| DOE Funding FY16:         | \$0                   |
| DOE Funding FY17:         | \$1,500,000           |
| DOE Funding FY18:         | \$2,390,000           |
| DOE Funding FY19:         | \$2,890,000           |
| Project Status:           | Ongoing               |
|                           |                       |

New strains are screened using five consecutive tiers in a conceptual downselection funnel to arrive at the most promising strains. In Tier I, strains obtained from culture collections and industry partners are screened on gradient incubators to determine their temperature and salinity tolerance range. In Tier II, the strains' winter and summer season biomass productivities are quantified in the Laboratory Environmental Algae Pond Simulator (LEAPS) PBRs, biomass harvested from the LEAPS is analyzed for biochemical composition (lipids, protein, carbohydrates) and conversion susceptibility, and the resistance of strains to common grazers and pathogens is assessed in laboratory-scale stress tests. In Tier III, downselected strains are concurrently

#### Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

improved by cell-sorting and adaptive evolution and evaluated in terms of culture stability in indoor test beds. In Tier IV, the best winter and summer season strains are evaluated in outdoor raceway ponds to confirm high-productivity biomass and culture stability and to provide biomass for detailed compositional and coproduct analyses.

The top strains are then evaluated in Tier V in seasonal SOT outdoor pond culture campaigns at AzCATI, the dedicated BETO SOT test bed. The core team supervises and coordinates the BETO algal SOT campaign at AzCATI. Management activities include the detailed experimental design of field trials, implementation of harmonized protocols and data management, and test bed oversight.

Major accomplishments so far include the successful execution of the DISCOVR strain downselection pipeline, starting with more than 40 initial strains; the identification of strains with biomass productivity up to 34% more than the benchmarks; the development of quantitative strain downselection decision rules based on maximum specific growth rate versus temperature data, LEAPS productivity, biomass composition, and grazer resistance; and the performance of 11 outdoor pond culture campaigns. Most importantly, a 13.6% increase in annual SOT biomass productivity (relative to 2017) was demonstrated at AzCATI, equivalent to a reduction in the biomass selling price of 10%, from \$909 per ton to \$824 per ton.

DISCOVR research direction and priorities are guided by a technical advisory board that convenes on a quarterly basis. A DISCOVR website has been designed and posted (https://discovr.labworks.org/), providing an overview of research activities and unique technical capabilities. To further solicit high-impact ideas to help reduce algal biofuel costs, we are requesting research proposals in a call for collaboration.

In summary, DISCOVR is a streamlined, coordinated, synergistic effort that leverages the member laboratories' complementary core capabilities in environmental simulation and productivity prediction, robustness evaluation, biomass valorization, and strain improvement. DISCOVR addresses several key research needs stated in BETO's MYP with the goal of delivering high-productivity biofuel-relevant algal strains through a standardized process for characterizing and comparing potential biofuels and bioproduct strains.

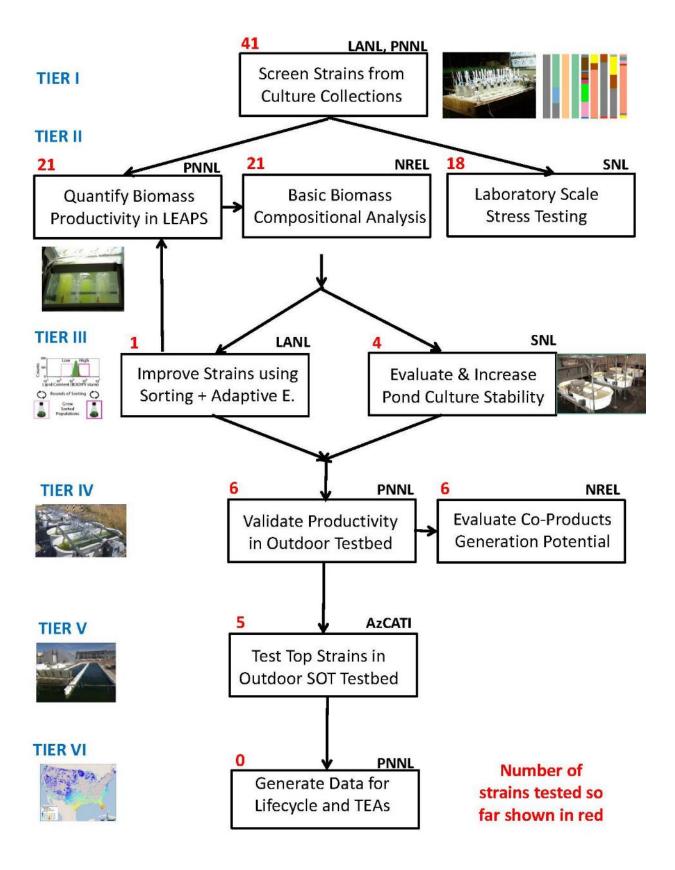


Photo courtesy of Pacific Northwest National Laboratory

#### OVERALL IMPRESSIONS

- The DISCOVR project team has established a highly integrated and collaborative process leveraging the expertise and capabilities of each member. The productivity targets, associated goals, and process for downselecting promising strain candidates is very clearly defined. The focus on field-relevant conditions in the laboratory testing and strains of highest interest for biomass production is also a strength of the approach. Significant learning has been achieved in the results shared to date. This project might benefit from additional outdoor testing capabilities in relevant, diverse environments.
- This project comprehensively aligns advanced technologies and analytic methods in a wholistic approach to evaluate, identify, and optimize high-potential algal strains. The goal for this pipeline approach is to contribute to the SOT annually because the summer productivity must improve 10% year over year to achieve the MYP 2025 target.
- This project is a large consortium focusing their efforts on a detailed and thorough strain characterization system, LEAPS, and validating their data by deploying their optimized strains to several large-scale sites. Future efforts need to focus on TEA/LCA modeling, but overall their efforts and results will become the next baseline for future projects.
- This was an incredibly ambitious project from its inception, and the team appears to be managed well, making great progress, and meeting its milestones. The broad collaboration has strong project management and is maintaining relevance to the algal industry and BETO's mission.
- The project aims to decrease the cost of biofuel production by screening and identifying highproductivity microalgae strains for biofuels and bioproducts that are resilient in year-round cultivation. To do this, the team has taken the approach of screening relevant strains from collections and submitted by industry collaborators through a complex six-tier selection, characterization, and identification pipeline, from which the best strains are downselected for outdoor trial cultivations and final TEA/LCA to determine their influence on the SOT. The project is very complex and includes selection, screening, productivity assessment, compositional analysis, stress testing, strain improvement, pond culture stability, outdoor testing, and coproduct evaluation; thus, it is a very thorough screening and identification process. The team management is well defined with participants from four national laboratories and the AzCati test bed, each bringing core expertise and capabilities to the project. The team has defined a set of key challenges and related success factors to ensure that strains are relevant and feed into BETO's other algal projects. The approach overall is seen to be very strong. The grazer testing, for cultivation resilience, is seen as an excellent component of the overall assessment of the resilience of strains. The project provides a direct interface to the development of BETO's MYP productivity goals, and it provides a method to show how new strains can be identified that will evolve and improve the SOT targets for BETO. Most importantly, the team is collaborating with several industry partners to test strains specific to their programs and has recently placed an open call for collaborations. The team is poised to continue strain characterization, LEAPS testing, biomass characterization, strain improvements, resilience testing, and further outdoor testing in test bed facilities. Thus, the project will increase the number of strains that go through the full screening, improvement, and valorization pipeline.
- The team is encouraged to consider adding tests to determine if the predefined screening protocols are biasing and predisposing the high-performing selected strains.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the complimentary feedback on this project and the team's progress. We appreciate the opportunity to respond to some of the points raised here.
- We want to add that we are continuously using TEA as an underlying driver to prioritize the different research areas. The TEA integration is in collaboration with the algal TEA project (WBS: 1.3.5.200),

specifically to the farm modeling, which calculates improvements in minimum biomass selling price (MBSP). For example, TEA has identified productivity as a critical driver of biomass production costs, and this area is the primary target pursued for strain comparison and improvement for the DISCOVR consortium. Our productivity measurements are integral aspects of the annual SOT framework. For example, in FY 2018, a 13% improvement in productivity yielded a 10% reduction in MBSP.

• It is a fair concern that the current screening protocol might be biased, and we are actively considering potential modifications to the initial wide-net screening approach to reduce the bias. Reducing the bias and making the selection procedures more relevant to selecting strong outdoor performing candidate strains will be a priority of our work moving forward. One bias that we recently realized is in favor of oxygen-sensitive strains because of the continuous stripping of photosynthetic oxygen out of the medium during the measurement of maximum specific growth rate, whereas in pond conditions, oxygen buildup to supersaturating levels is a common and nearly daily occurrence. High oxygen levels are problematic for photosynthetic biology, so mechanisms to tolerate high oxygen levels are critical to survival in outdoor ponds. Therefore, in the next 3-year cycle, we will add a screen for oxygen tolerance. Ultimately, all screening protocols need to deal with false positives and false negatives. The former adds to the burden of larger scale confirmation, and the latter results in missed leads. The true test of our screening protocol will come from outdoor trials as we continue to pursue our goal of annual quantified improvements in productivity.

## ALGAL TRANSLATIONAL GENOMICS

#### Los Alamos National Laboratory

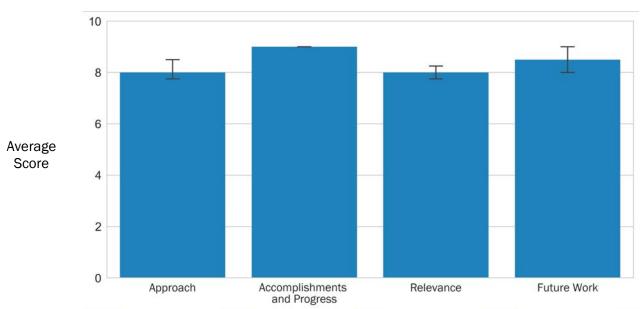
#### **PROJECT DESCRIPTION**

The primary goal of this project is to curate and expand the genomic information housed in the algal Greenhouse knowledge base to accurately characterize the metabolic potential of leading production strains to enable performance improvements. A significant barrier to advancing applied algal systems is that genome-wide metabolic models and regulatory networks are lacking, stemming from a dearth of knowledge of gene function for most production strains. Our research will focus on sequencing complete genomes and curating gene annotations through *in silico* and experimental approaches to expand fundamental knowledge of production strain physiology with a primary focus on inorganic and organic

| WBS:                      | 1.3.1.600             |
|---------------------------|-----------------------|
| CID:                      | NL0029949             |
| Principal Investigator:   | Dr. Shawn Starkenburg |
| Period of<br>Performance: | 10/1/2015-9/30/2021   |
| Total DOE Funding:        | \$1,750,000           |
| DOE Funding FY16:         | \$350,000             |
| DOE Funding FY17:         | \$350,000             |
| DOE Funding FY18:         | \$600,000             |
| DOE Funding FY19:         | \$450,000             |
| Project Status:           | Ongoing               |
|                           |                       |

carbon assimilation and metabolism. Building on previous genomics efforts, we will accomplish the following major technical objectives: (1) maintain and expand the Greenhouse knowledge base; (2) develop and deploy new assembly methods to construct complete genomes; (3) curate carbon metabolism pathways for leading production strains, beginning with *Scenedesmus*; and (4) phenotype *Scenedesmus* inorganic and organic carbon use to functionally validate genome annotations. Understanding the molecular mechanisms of carbon assimilation and sequestration in eukaryotic microalgae as well as advancing our basic knowledge of biophysical and biochemical components of carbon uptake will generate useful hypotheses to enable strain improvement through downstream genetic and systems engineering. Further, exploiting the ability of

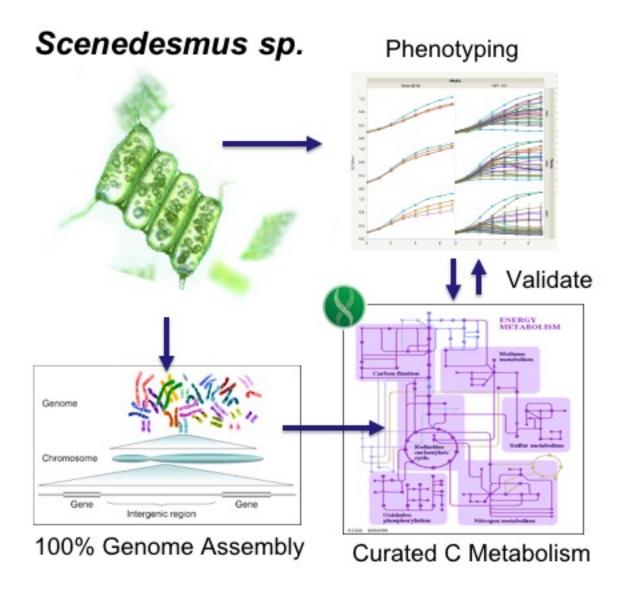
#### Weighted Project Score: 8.4



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

 $oldsymbol{I}$  One standard deviation of reviewers' scores

microalgae to grow mixotrophically on light and organic carbon has the potential to greatly improve productivity when grown in nonpotable, organic-rich wastewater sources, and improve carbon input cost sustainability through discovery and use of efficient carbon metabolism pathways.





#### OVERALL IMPRESSIONS

• This project has high potential to be a catalyst to the advancement of algal fuel production through deepening the omics toolbox. The focus on *Scenedesmus* for both relevance and pragmatic reasons is a strength of the approach. Given that the project has just begun, the team has created a strong foundation for their future work through the literature review process. If successful, the development of more efficient methods for complete genome assembly will be highly valuable. Focusing on carbon pathways for modification aligns with production cost targets to enable the use of wastewater for algal growth. The variability and complexity of the anticipated water sources in a production system should be considered when completing the phenotyping analysis.

- This project continues building on previous research by leveraging genomics to characterize the metabolic pathways of industrially relevant strains to farther enhance performance.
- This is a well thought out and ambitious project. The use of wastewater might be beneficial for this strain but not others, and that might limit the overall benefit of this project.
- This AOP project is early in its merit review cycle, and initial accomplishments are on track. The team provided clear justification for the work and strain of choice, and successful completion of this project should have strong relevance to the BETO portfolio and the broader algal industry. The objectives and approach appeared to be appropriate for the project goals around understanding carbon use and metabolism.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the thoughtful review and critique. Industrial-scale production of algal biomass using wastewater that is rich with organic matter would provide a cost-effective means to maximize productivity and improve biofuel yield. Unfortunately, the genetic basis for the use of reduced carbon from these waste streams is larger unknown for any candidate production strain. We agree that the variability and complexity of waste sources (carbon types, organisms, and additional dissolved materials) must be considered when assessing productivity improvements; however, the curated carbon use pathways will provide knowledge of which waste carbon streams are best suited for *Scenedesmus*, will guide genetic modifications that are required to enable metabolism of additional carbon sources, and determine which carbon sources are likely consumed by other cocultivated organisms in open systems.
- We agree that the type and degree of organic carbon use is most likely strain specific. We chose to focus on *Scenedesmus* because of its outdoor growth performance, abundance of genomic material, and known ability to be cultivated in a variety of nonpotable wastewater sources. Further, curating and validating the functional annotations of *Scenedesmus* will improve the genome annotations of other chlorophytes because this new information will be available for homology assignments as new algal genomes are sequenced. As resources allow, curating the genome annotations in other lineages (i.e., *Nannochloropsis*) will maximize the value of this project for the user community.

## ALGAL BIOMASS COMPOSITION

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

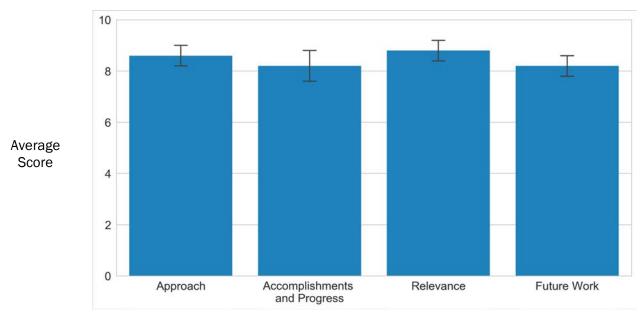
Addressing critically needed improvements in biomass, bioproduct, and biofuel productivity is a priority for algae commercial development and is guided by supporting economic and sustainability principles. Exploiting pathways for the integration of engineering approaches with fundamental biochemistry of photosynthetic organisms might help to unravel the contentious nexus of growth rates, biomass productivity and composition, and nutrient load. This project focuses on identifying critical factors for economic development and deployment of algal biofuels, biomass productivity and conversion efficiency, and compositional characteristics and then providing a robust set of tools to allow for an unambiguous biomass

| WBS:                      | 1.3.2.001           |
|---------------------------|---------------------|
| CID:                      | NL0025629           |
| Principal Investigator:   | Dr. Lieve Laurens   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$3,100,000         |
| DOE Funding FY16:         | \$850,000           |
| DOE Funding FY17:         | \$750,000           |
| DOE Funding FY18:         | \$750,000           |
| DOE Funding FY19:         | \$750,000           |
| Project Status:           | Ongoing             |
|                           |                     |

quality and compositional description. This project is highly relevant to the DOE multiyear program targets of reducing costs and integrating dynamic biomass composition with downstream process characteristics by providing options for the development of fuel-relevant products derived from either the lipid, carbohydrate, or protein fraction of algal biomass. This project directly addresses two BETO barriers: (1) lack of understanding of the value of the feedstock (in context of seasonality and environmental variability) and (2) lack of information on the physical, chemical, and biological quality of the biomass in the context of the impact on biorefinery operations and performance. To address these barriers, this project (1) builds on the standardization effort for compositional characterization of algal biomass by supporting and validating the implementation of

#### Weighted Project Score: 8.4

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

methods and (2) gathers an understanding of the dynamic biochemical composition and carbon allocation in terms of biomass value and conversion yields and selectivity. The goal for this project's merit review cycle is to build and show a coproduct portfolio that, when integrated in a conversion pathway, can increase the intrinsic value of algal biomass by at least 30% of biomass cost value for a set of model species. This goal will be achieved by increasing the value of biomass and supporting a dynamic biochemical compositional profile in a set of model algae to ultimately quantify the value of the biomass for conversion or upgrading pathways. To establish this conversion interface, a highly granular compositional profile should be established during a dynamic growth profile to link with lipid upgrading, nutrient and water recycling, and with integrated fuel and bioproduct conversion. As an outcome of the experimental valorization subtask, we will continue to drive toward an inherent value of the components in the biomass composition, providing a better link with biomass production costs and eliminating the potential conflict between maximizing biofuel yields and maximizing potential revenue, which provides a better sense of the path to commercialization. To date, this project has developed and is maintaining an online repository of robust standard analytic procedures. We added a sterol quantification procedure to support the development of sterol-derived coproducts as well as help to close the overall descriptive mass balance of algal biomass. We built an amino acid analytic pipeline to aid with the more rigorous assessment of protein and protein-derived high-value products. Through the development of an experimental data collection framework for the quantitative assessment of biomass composition, bioproducts, energy, and productivity in different indoor PBR cultivation conditions, we compared continuous and batch cultivation on overall measured growth rates and project algal farm productivity. We used this framework to select species, growth scenario, and bioproducts based on the overall value of the biomass. This allowed for tracking quantitative increases in intrinsic value, with the aim of adapting cultivation conditions to outdoor pond operations toward increased overall intrinsic biomass value.

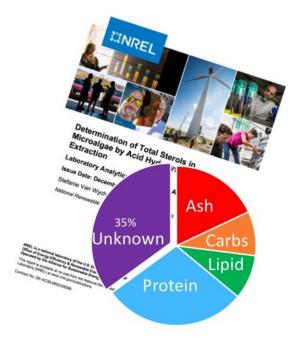


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• The group's best efforts are tied to developing innovative analytic techniques. The other aspects of this project are too big in scope and are loosely associated with each other.

- This project continues to have a clear benefit to the algal industry as a whole and is an important link to BETO priorities. Dr. Laurens continues to be a leader in biomass compositional analysis, and the team regularly interacts with industry and the modeling community to make sure critical compositional assumptions are clear. The project appears to be managed well, is meeting its milestones, and is maintaining its relevance to public and private algal research. The project is also commended for prioritizing information dissemination and community engagement.
- This project has the potential to, and likely will, dramatically reduce the cost of biofuels via understanding how to maximize the value of the coproducts. The current scope includes creating analytic techniques that accurately account for the entire biomass composition, cultivation variables impact on composition, as well as the downstream processing required to fully capture the value of the coproducts created.
- The development of methods to assess algal biomass composition in support of a developing bioproduct portfolio is critical to drive improvement in the economics of the production of fuel from algae. This project nicely combines novel methods to work toward closing the mass balance and enabling tools for novel compound discovery. In addition, the team has worked to define best methods for assessing algal product quality and made the physical materials available to the broader community. Continued work on biomass composition analysis under varied cultivation conditions will be critical to determining quality variance in real-world conditions.
- The projects goals are to reduce the cost of biofuels by increasing the algal biomass value and to reduce the uncertainty around process inputs and outputs. The first goal will be approached through a quantitative development of biomass composition, energy, and productivity for model algal species. The second goal will take an approach of standardized characterization and development of standards for the quantitation of properties. Therefore, the project helps address key barriers in sustainable production of algae, biomass characterization, and material properties. The project's main strength is in the development of robust standardized analytic procedures. This is seen through the large download of methods and the standardization of methods across the ATP3 partners. Further, the identification of key valuable products that can influence the overall valorization of the biorefinery process can provide incentives toward processes that help reach BETO's strategic goals in this area. The future work planned activities are deemed appropriate.
- A possible weakness is noted in the approach to use the tools generated to valorize biomass components because many factors affect the market value of raw components.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their complimentary feedback on this project. Several comments by the reviewers were reiterated, and we appreciate the opportunity to respond on the relevance of the compositional shift experiments. It is our primary goal to establish tools and techniques required to test whether there are cultivation conditions, light, temperature, or semicontinuous harvesting that impact composition without inhibiting overall biomass productivity. If we can unlock this potential in indoor PBR, we can implement this approach in relevant outdoor cultivation trials. Details on the cultivation strategies implemented to obtain shifts in biomass composition needed to be minimized, and we want to clarify that the growth experiments experienced high-incident light, which is likely one of the primary drivers of productivity. We have shown that maintaining high cell density cultures, by frequent harvesting, yielded higher storage products (carbohydrates and lipids), which translates to increased intrinsic value when following the novel TEA modeling approach. By comparing the rates of accumulation of storage products and shifting biomass composition in a consistent manner under respective strain optimized media and nutrient conditions, we aim to elucidate the differences in inherent capacity of the strains to adapt their underlying composition.

• In summary, we have developed an experimental setup that allows us to test hypotheses in PBRs, and we are making progress on using these experiments to provide biomass for biochemical mapping of metabolites and thus validating different valorization models. Since the peer review presentation, we have finalized our work with the TEA team on integrating compositional dynamics into a valorization framework. By setting up this conceptual process, we are now able to directly assess and leverage the impact of additional products identified in this project.

## ATTACHED PERIPHYTIC ALGAE PRODUCTION AND ANALYSIS

#### **Sandia National Laboratories**

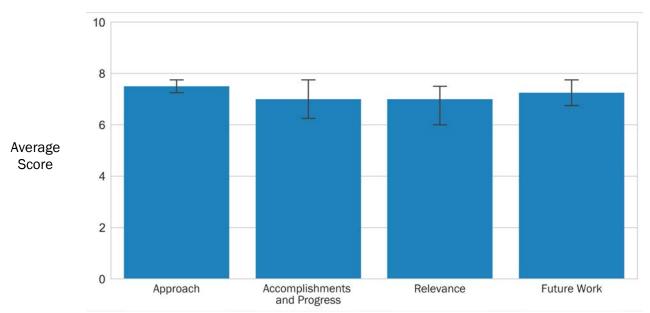
#### **PROJECT DESCRIPTION**

This project aims to test, evaluate, and show the proposition that attached periphytic algal polyculture systems are capable of achieving high annual average biomass productivities that at least equal production from raceway ponds and can exceed to  $24 \text{ g/m}^2/\text{day}$  (ash-free dry weight), thereby providing a path to 5,000 gal acreyear algae-derived fuel. The approach uses compromised surface waters with nutrient contamination (N, P, trace metals) concentrations that are much lower than those required for recirculating raceway pond production of planktonic algae. The same surface waters will also generally have adequate levels of carbon dioxide (CO<sub>2</sub>) and/or carbonate to avoid the need for supplying

| WBS:                      | 1.3.2.130           |
|---------------------------|---------------------|
| CID:                      | NL0027375           |
| Principal Investigator:   | Dr. Ryan Davis      |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$3,200,000         |
| DOE Funding FY16:         | \$950,000           |
| DOE Funding FY17:         | \$750,000           |
| DOE Funding FY18:         | \$750,000           |
| DOE Funding FY19:         | \$750,000           |
| Project Status:           | Ongoing             |
|                           |                     |

supplementary CO<sub>2</sub>, which is also otherwise required for recirculating raceway pond production of planktonic microalgae. By periodically pulsing the inflow, the shallow turbulent medium provides several mechanisms that contribute to the capability of an attached periphytic culture to achieve relatively high productivities despite lower nutrient concentrations. These include a high exposed surface-to-volume ratio of cultivation, turbulence-induced rapid light dark cycles that improve photon use efficiency of the cellular photosynthetic apparatus, and improved nutrient and gaseous exchange and breakup of boundary layer gradient limitations that otherwise exist among the algal cellular matrix, water, and atmosphere. These mechanisms are partially

#### Weighted Project Score: 7.2



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

 $oldsymbol{I}$  One standard deviation of reviewers' scores

shared with observations of high algal productivity seen using thin-layer cascading cultivation systems, which have system configuration and operational similarities.

To optimize yield and minimize ash based on new substrate materials and culture seeding processes, we apply SNL's computational fluid dynamics expertise and algorithms with experimental validation to predict the residence time of seed culture cells in the floway and substrate matrix in the absence and presence of an established turf. A key component of this R&D effort will be to evaluate whether culture seeding and substrate optimization can provide synergistic yield enhancement, minimize biomass productivity losses through maturation latency and sloughing, and reduce ash in the presence of a native (i.e., unseeded) periphytic turf because the native periphytic cohort is expected to confer the culture stability observed to date. As part of this work, we are evaluating the impacts of sloughing and evaporation losses based on changes to the substrate material and as a function of biomass yield because scale-up of this technology will likely face significant hurdles in arid regions, such as the U.S. Desert Southwest, if increased evaporation losses are incurred by the system compared to already existing surface waters. The current year goal is to demonstrate the ability for attached algal cultivation to simultaneous achieve  $24 \text{ g/m}^2/\text{day}$  and 25% ash using compromised surface waters. The 3-year goal of the project is to demonstrate attached algal cultivation coupled to water treatment with a net biomass cost of \$450 ton ash-free dry weight.

#### **OVERALL IMPRESSIONS**

- This AOP project includes a novel approach to low-input and low-cost production of algal biomass. The project appeared to be managed well and had clear relevance to the BETO mission and MYP goals. The new merit review cycle is building on directly relevant previous work. The team is encouraged to incorporate TEA results from a fully integrated process into the project's experimental design.
- This project strives to increase algal biomass productivity in environments with excess nutrients (from agriculture runoff) with as little additional infrastructure and equipment as possible. The project has made significant progress in baseline understanding and implementing work to overcome learnings and challenges.
- The attached periphytic algal project has been a successful collaboration between research and public offices to solve a very specific water contamination challenge. The team has developed a valuable data set in a relatively large production setting that can drive TEA assumptions and future work in this area. The challenges around biomass quality are significant and will require considerable effort to overcome for this system to be useful in the production of feedstock for fuel.
- The aim of this project is to develop cost-effective means for cultivating easily harvestable algal biomass using nutrients from compromised surface waters and attached algae cultivation methods. This project is currently working to couple remediation of agricultural/storm runoff with algal biomass production >24  $g/m^2/day$  and ash content <25%. Scale-up of a domestic algal biomass industry requires identification of value propositions, including remediation of runoff, to achieve production costs that are commensurate with high-volume commodities and energy. The high ash content of biomass from turf systems is a challenge that the project will be addressing. The team is using three facilities for turf algal growth but mainly focusing on the Salton Sea floway. Biomass from this system has been thoroughly characterized for chemical composition and microbial ecology. The team is working on ash reduction and reduced nonbiogenic ash by 77% using a mesh to filter waters and will be working on seeding the turf algal system with non-diatomaceous strains of algae. The approach is reasonable and should work as long as the system is not naturally reserved by diatoms. Although turf algal systems have challenges, as noted by the project team, the opportunity for high growth, biomass productivity, and water remediation are excellent. If the biomass productivities are achieved with reduced ash content, the project can help achieve productivity targets for the BETO program. The team will deploy flow-rate feedback, seed cultures with non-diatomaceous periphyton, evaluate species and biomass production, and quantitate evaporation. The approach is reasonable.

• The only concern noted is related to the possibility of natural reseeding by diatoms.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# CONTINUOUS BIOLOGICAL PROTECTION AND CONTROL OF ALGAL POND PRODUCTIVITY

#### Lawrence Livermore National Laboratory

#### PROJECT DESCRIPTION

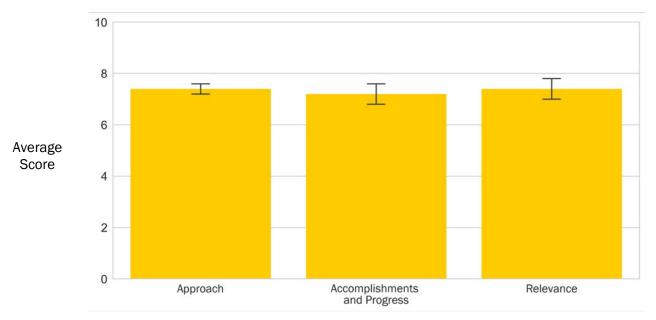
We present on two projects, one funded under the Targeted Algal Biofuels and Bioproducts (TABB) competitive FOA, concluding this year, and another follow-up project, funded as an AOP, beginning this year. The projects are aimed at improving algal cultivation through the application of microbes to protect algal crops from losses caused by predators and pathogens. Ultimately, both projects aim to increase annual algal biomass yields. Our

| WBS:                      | 1.3.2.300          |
|---------------------------|--------------------|
| CID:                      | NL0029886          |
| Principal Investigator:   | Dr. Michael Thelen |
| Period of<br>Performance: | 9/1/2015-9/15/2018 |
| Total DOE Funding:        | \$1,080,000        |
| Project Status:           | Sunsetting         |
|                           |                    |

projects address barriers from the TABB FOA of the high costs of producing biomass and low yields of target feedstocks and of translating laboratory success to outdoor cultivation environments. In addition, we focus on the MYP barriers Aft-B: Sustainable Algae Production and Aft-A: Biomass Availability and Cost. The TABB project team was led by LLNL and included SNL (Livermore), the University of California at Davis, and the microalgal development company Heliae, LLC (Arizona). Our goals were to identify probiotic bacteria that protect algae against predators and pathogens and rapidly test these bacterial applications at increasing scales. During our 3-year project, we identified both a bacterial isolate and consortium that protect against rotifer predation at the laboratory and mesocosm scales. This project highlights the importance of (1) leveraging the algal microbiome to increase algal resistance to predators and pathogens and (2) rapid translation from laboratory to outdoor testing. We performed a feasible industrial-scale (10,000 L) probiotic addition and incorporated laboratory and outdoor experimental data into a relevant TEA model to assess sensitivities and future opportunities. Our new project will apply what we have learned, addressing the sensitivities of the TEA

# Weighted Project Score: 7.3

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



L One standard deviation of reviewers' scores

model to make our probiotic application more economic. This new project forms a new collaboration with Lawrence Berkeley National Laboratory and aims to determine the mechanisms of bacterial protection and to induce the protective effect, increasing the efficiency and duration of the application.

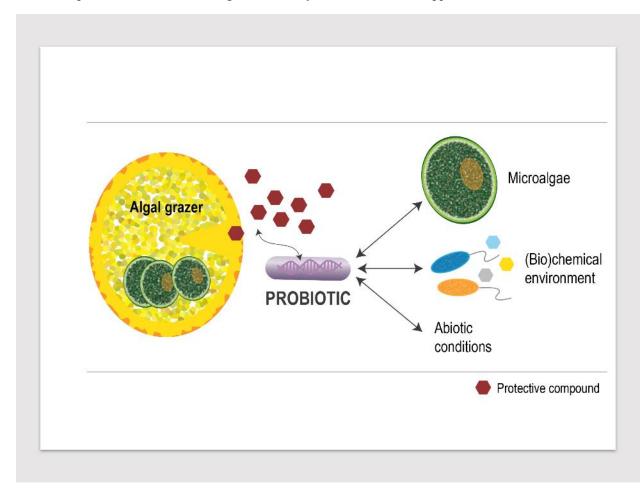


Photo courtesy of Lawrence Livermore National Laboratory

#### OVERALL IMPRESSIONS

- The next phase of this project continues to develop strategies for creating a "probiotic" that can be added to open pond algal raceways to improve the productivity and robustness of commercial farms.
- This project review is a combination assessment of the completed work and the new plan that is a continuation of this project. There were many key accomplishments exploring the use of probiotic bacteria in the cultivation of *Myrmica salina* as a protective approach to rotifer predation, including the development of a TEA around this strategy. The team is now building on this work to understand the potential mode of action and develop the process to scale. For the upcoming work, the project team will benefit from clarity on objectives in the outdoor trials to ensure project success.
- To reach the overall project goals of BETO, minimizing pond crashes is essential. This project has the potential to establish new and innovative solutions for pond pest management, but they seem to be focused only on mitigating saltwater rotifer. Rotifers are only one of many pests that hinder algal productivity. The project would make the most impact if the team focused on expanding their work of yearly sampling and characterizing the microbiome community to more sites while simultaneously using their techniques to find a solution for the different pests that arise during the different seasons.

- This project is focused on identifying, understanding, and scaling probiotic microorganisms for largescale outdoor production, which has clear relevance to the BETO mission and MYP goals. The project included an appropriate proportion of laboratory, mesocosm, and field-testing, with experimental design appropriate for each scale. The group has completed most objectives and will be building on these accomplishments in a future AOP merit review cycle. The team is encouraged to incorporate outdoor testing early in the project to ensure bench-level successes will have relevance in an industrial environment in the presence of more challenging ecological pressures.
- The aim of the project is to improve the resilience of algal crops to predators and pathogens by using probiotic bacteria that will increase annual algal biomass yields above the 2015 SOT baseline. The team plans to improve the protective effect of probiotic bacteria by demonstrating probiotic application regimes that significantly increase the magnitude and duration of the probiotic protective effect by 25% each, above the current baseline, and significantly decrease *in situ* algal carbon loss compared to untreated, ultimately contributing to improved algal cultivation yields. The approach involves studying single cultivation relationships between algae and bacteria and identifying microbial communities that enhance algal cultures and scaling these up in a stepwise fashion. In the new AOP, the team will take an approach to identify protective genes because they hypothesize that violacein is the compound produced by bacteria that infers protection. The approach is deemed reasonable. Progress in the previous AOP is deemed reasonable. Success in developing probiotic mesocosmsmecocosms for algal cultures could potentially enhance robustness of cultures and overall productivity, helping to meet productivity goals for the BETO program.
- The team should provide a vision on the use of the identification of the gene(s) responsible for violacein production.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# INTEGRATED PEST MANAGEMENT FOR EARLY DETECTION ALGAL CROP PRODUCTION

#### University of California, San Diego

#### **PROJECT DESCRIPTION**

Contamination of industrial-scale growth systems by pathogens, predators, and nonproductive contaminating species continues to be a major obstacle to the robust and economically sustainable production of algal biomass and bioproducts. Appropriate management of these pests requires a sensitive and continuous monitoring system that can detect and identify contaminants and competitors as early as possible. Compared to current detection

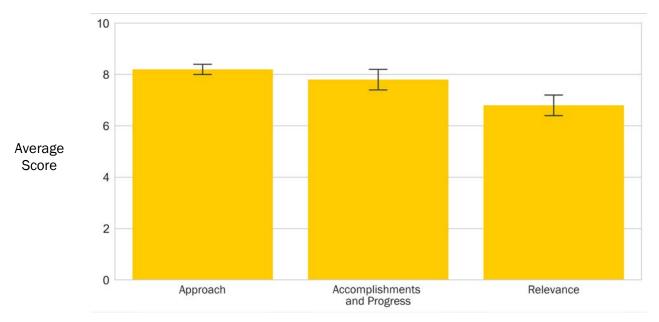
| WBS:                      | 1.3.2.310           |
|---------------------------|---------------------|
| CID:                      | EE0007094           |
| Principal Investigator:   | Dr. Robert Pomeroy  |
| Period of<br>Performance: | 10/1/2015-3/31/2019 |
| Total DOE Funding:        | \$820,327           |
| Project Status:           | Sunsetting          |
|                           |                     |

methodologies, such as quantitative polymerase chain reaction (PCR) or FlowCam monitoring systems, a mass spectrometry-based detection system is orders of magnitude more sensitive and can be readily automated for continuous monitoring of multiple production ponds.

We developed a chemical ionization mass spectrometry-based detection system capable of real-time monitoring of volatile compound abundances in the air over an algal culture. Using this system, we examined the headspace over healthy algal cultures throughout multiple growth phases, under abiotic stresses, and through culture crashes resulting from infecting the cultures with predators. The resulting data allowed us to confirm previously characterized molecular signatures derived from breakdown pathways occurring in the culture liquid. These experiments allowed us to expand our catalog of molecules that indicate the health of the algae or contamination as well as to determine thresholds for detection of contaminants and the kinetics of

# Weighted Project Score: 7.7

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

culture crashes post-infection. Altogether, this research is rapidly advancing the development of a field-deployable instrument for monitoring the contamination in algal cultures.

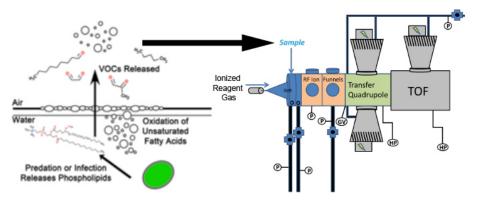


Photo courtesy of University of California, San Diego

#### **OVERALL IMPRESSIONS**

- Tools for integrated pest management are critical for large-scale stable outdoor production, and the relevance to the BETO mission, MYP goals, and the algae industry was clear. The team discussed a suite of promising results that aligned with originally planned objectives. The team is encouraged to think about how lower cost detectors might be able to build on these accomplishments and increase the potential for field deployment.
- This project demonstrates innovative use of already established instrumentation for early detection of contamination. This process, although interesting, is not viable at the production scale but could be used by other research groups that are working on contamination issues of outdoor systems.
- Significant expertise and progress were demonstrated evaluating samples and developing reliable analytic methodologies to predict pond crashes. Future work is required to further fine-tune a portable prototype.
- Crop protection at the commercial production scale will continue to be one of the most important areas for R&D to achieve reliable, high-quality algal biomass production. This project focused on very early identification of pest presence, which has very high potential, allowing algae farmers to act before the crop is lost. The team produced exciting results demonstrating the ability to detect pest pressure well before the health of the culture declines. The challenge in this system is the likelihood of success in scaling. There is a great opportunity to continue to use this method in laboratory work supporting the development of cultivation practices that mitigate biotic pressure in the algal field.
- The objective of this effort was to develop simple, automated, affordable, and robust technologies for the early detection and identification of pathogens, predators, and nonproductive competitors in algal cultures. The team used two major technologies in their approach: mass spectrometry and quantitative PCR with high-resolution melt analysis. This is a small project that is ending. To meet the goal of the project, the team developed mass spectrometric methods to evaluate possible signature compounds indicative of an imminent crash caused by a pathogen. They developed approaches to monitor cultures with molecular tools. The approach is deemed innovative and well implemented.
- Several weaknesses were noted associated with the implementation of the technology in the field.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their comments. In our detailed responses to scaling, costs, and alternative devices, we provide a detailed argument for continuing to develop this technology toward field deployment.
- We thank the reviewer for their acknowledgement of our project's successes.

# ALGAE PRODUCTION CO<sub>2</sub> ABSORBER WITH IMMOBILIZED CARBONIC ANHYDRASE

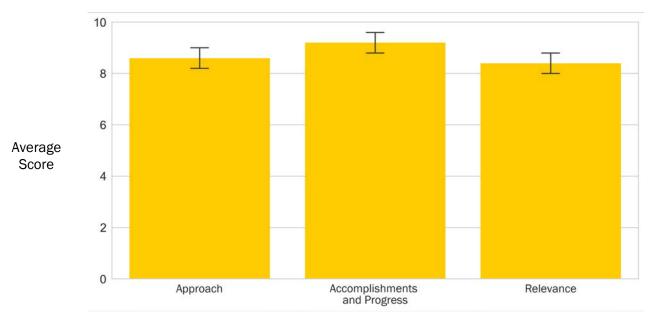
#### **Global Algae Innovations, Inc.**

#### **PROJECT DESCRIPTION**

GAI is a leader in low-cost algae production technologies. A suite of advances in open pond algal growth is being developed and demonstrated to achieve commercially viable production of oil and high-protein meal. An essential part of GAI's algae production method is the efficient and economic transfer buffering storage distribution of  $CO_2$  from power plant flue gas to the actively growing algae, ensuring an ample supply of  $CO_2$  for photosynthesis at all times.

| WBS:                      | 1.3.2.320            |
|---------------------------|----------------------|
| CID:                      | EE0007092            |
| Principal Investigator:   | Dr. David Hazlebeck  |
| Period of<br>Performance: | 10/1/2015-12/31/2019 |
| Total DOE Funding:        | \$998,962            |
| Project Status:           | Sunsetting           |
|                           |                      |

GAI is partnering with TSD to apply immobilized carbonic anhydrase and alternative absorber designs to improve the capture efficiency and reduce the cost of  $CO_2$  management in algae production. Additionally, the outdoor, open raceway cultivation methods will be developed to improve  $CO_2$  use efficiency. The capture and use improvements will be demonstrated in an integrated outdoor raceway testing with flue gas.



#### Weighted Project Score: 8.8

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%

 $oldsymbol{I}$  One standard deviation of reviewers' scores

#### **OVERALL IMPRESSIONS**

- This project focused on improved CO<sub>2</sub> capture and delivery using an industrial flue gas source and demonstrated performance in outdoor ponds. The relevance to the BETO mission, MYP goals, and the algal industry were clearly described. Project objectives were completed and TEAs were discussed and used to prioritize efforts. The project was well managed, and it appears that the technology could have wide applicability for a variety of flue gas sources.
- This is an innovative and detailed system for sites that will colocate with a power plant and have access to their flue gas.
- This project showed success in decreasing the cost of CO<sub>2</sub> captured; most advantages are attributed to alternative design, not the absorber material.
- The project team delivered on goals on time or early across all facets of the project objectives. An integrated system has been developed to significantly improve carbon use efficiency in a large-scale algal production facility. The improvement of CO<sub>2</sub> delivery and use is critical to achieving economic feasibility in algal production and directly addresses MYP goals. The cultivation system and design are directly linked to the methods employed in this process and will need to be considered holistically.
- The goal of the project was to use carbonic anhydrase and/or other absorbers to increase CO<sub>2</sub> capture use efficiency from flue gases. The team, including all industrial partners, operated the GAI facility in Hawaii near a power plant that provided flue gas, some of which can be used for algal cultivation. The approach taken was to capture CO<sub>2</sub> from the flue gas using an absorber, converting the CO<sub>2</sub> to a NaHCO<sub>3</sub> media that could be fed directly to a pond. The team faced major challenges in the complexity of the system and the efficiency and lifetime of carbonic anhydrase. The approach the team took was successful in implementing this CO<sub>2</sub> concentrating technology. The project defined the baseline and used it to determine success. The project set target goals, which have been met, showing high carbon capture and use efficiencies. The result is that the system indicates an ability to reduce the CO<sub>2</sub> supply cost significantly. The team showed 83% capture efficiency with more than 95% use efficiency for the algae. The team moved to a modified packed column for CO<sub>2</sub> capture that showed better capture efficiency and stability than carbonic anhydrase. The team plans to move into direct carbon capture from air. The organization of the project is deemed to be part of the success because the team was able to move the technology forward by redesigning the CO<sub>2</sub> absorber and increasing the overall performance.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# ATMOSPHERIC CO2 CAPTURE AND MEMBRANE DELIVERY

## Arizona State University

#### **PROJECT DESCRIPTION**

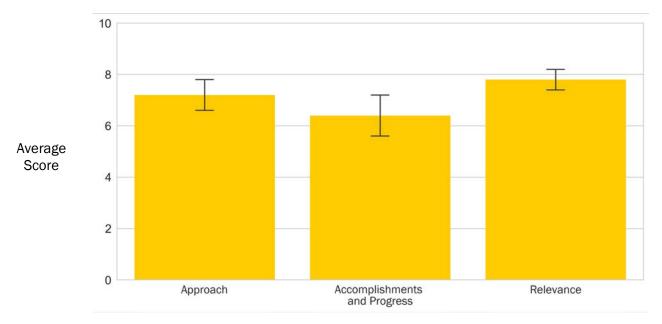
| A major bottleneck for growing microalgae as a                 | WB   |
|--|------|
| sustainable alternative to fossil carbon in economically       | CID  |
| producing fuels and chemical products is the cost of           | Prin |
| delivering $CO_2$ in enough concentrations for it not to limit | Peri |
| growth. This project sought to develop and integrate two       | Perf |
| innovative technologies for capturing and concentrating        | Tota |
| $CO_2$ from air and delivering it to microalgae with high      |      |
| efficiency into an Atmospheric CO <sub>2</sub> Enrichment and  | Proj |

| WBS:                      | 1.3.2.330           |
|---------------------------|---------------------|
| CID:                      | EE0007093           |
| Principal Investigator:   | Dr. Bruce Rittmann  |
| Period of<br>Performance: | 10/1/2015-9/30/2018 |
| Total DOE Funding:        | \$1,000,000         |
| Project Status:           | Sunsetting          |
|                           |                     |

Delivery (ACED) system. The CO<sub>2</sub> capture technology is based on moisture swing sorption, where specialized resin materials selectively capture CO<sub>2</sub> when dry and release it when wet into a confined space where the concentration can be increased up to 500-fold. The CO<sub>2</sub>-delivery technology is based on membrane carbonation, which uses hollow fiber membranes that allow CO<sub>2</sub> to diffuse into the algae-containing liquid without forming bubbles, achieving nearly 100% delivery efficiency.

#### Weighted Project Score: 7.0

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

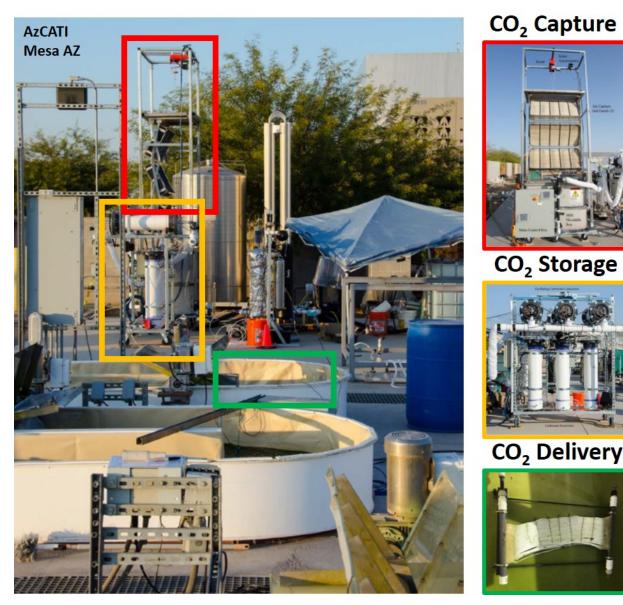


Photo courtesy of Arizona State University

## OVERALL IMPRESSIONS

- The purpose of this project was to understand and develop innovative ways to capture and deliver atmospheric CO<sub>2</sub> to pond culture. If successful, the study would have clear benefits to the algal industry and would align with BETO priorities and MYP goals. Unfortunately, the CO<sub>2</sub> capture portion of the study encountered hardware, software, and integration hurdles that were not able to be mitigated, combined with economics that did not appear to advance the SOT. Membranes used for CO<sub>2</sub> delivery appeared more promising, and the team indicated that the membranes met several performance targets during the study period.
- This is a novel approach but not a robust deployment of technology. It is very capital intensive, and it seems that the maintenance cost is very high as well.

- This project uses novel membrane technology previously developed for wastewater treatment and adapts it to capture and concentrate CO<sub>2</sub> from ambient air. The team successfully demonstrated the concept at commercially relevant scales, but further fine-tuning required for seamless integrated operations.
- The ACED projects aims to combine two independent systems to significantly reduce the cost of CO<sub>2</sub> delivery for algal biomass production. The atmospheric capture component of the project experienced significant challenges and will require additional effort to be evaluated. The membrane delivery system has shown promise in significantly improving the carbon use efficiency compared to the currently used system of CO<sub>2</sub> sparging. Because this project has closed, the evaluation of the membrane delivery at scale through modeling and large-scale evaluation should be considered for future work.
- The goal of this project was to design, build, and demonstrate a system to capture and concentrate CO<sub>2</sub> from ambient air and deliver the CO<sub>2</sub> to microalgae. The ACED concept uses anionic exchange resin sheets to capture CO<sub>2</sub> when dry and release when wet. The CO<sub>2</sub> is transferred to sodium carbonate/bicarbonate brines to buffer capture and demand rates; and it is thermally extracted and pressurized. This allows for nearly 100% CO<sub>2</sub> to be delivered on demand to microalgae using membrane fibers. The technology is very innovative. The team was able to develop mitigating approaches for most of the challenges faced in the development and deployment of the technology.
- A few minor weaknesses were noted related to the complexity of the technology and need for some simplifications.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the feedback.
- Although hardware and software issues limited the operation time of the CO<sub>2</sub> capture and storage system during the project, our project advanced the SOT for sustainably sourcing concentrated CO<sub>2</sub> for cultivating microalgae. Current sources include bottled and industrial waste CO<sub>2</sub> that are not sustainable for large-volume fuel applications. We developed and demonstrated a first-of-its-kind system for direct CO<sub>2</sub> capture from ambient air (410 ppm), a novel energy-efficient gas-liquid contactor for transferring low-concentration CO<sub>2</sub> into a liquid brine for storage, and a thermal extraction system for releasing the CO<sub>2</sub> on demand from storage with > 90% CO<sub>2</sub> on a laboratory scale and > 70% CO<sub>2</sub> in a much larger outdoor system. The system was operated for several extended periods within a harsh desert environment with +40°C temperatures, sustained +10 ultraviolet index, periodic intense +40-mph wind, dust, and rainstorms. The accompanying graphic shows the field implantation of the entire system.
- Detailed TEA, made possible through this award, identified the most critical parameters for optimizing the system, including a path to drastically improve the economics of CO<sub>2</sub> capture and storage using continuous active CO<sub>2</sub> transport (not batch cycles) through membranes with much lower capital and maintenance costs; this is being pursued through a follow-on award, DE-FOA-0001858 (Advanced Research Projects Agency-Energy). This much simpler design should alleviate some of the hardware and software challenges encountered in the BETO project.
- The TEA also highlighted the value of delivering captured CO<sub>2</sub> with near 100% efficiency, which was shown effectively using the membrane delivery technology during multiple month-long cultivation trials without performance degradation. This promising technology will be further evaluated for delivering industrial waste CO<sub>2</sub> as a part of award DE-FOA-0001908.

# SOFAST: STREAMLINED OPTIMIZATION OF FILAMENTOUS ARTHROSPIRA/SPIRULINA TRAITS

#### Lumen Bioscience, Inc.

#### **PROJECT DESCRIPTION**

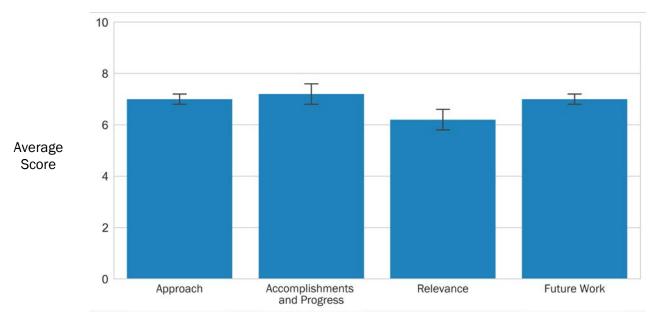
To enable the development of algae-based biofuels and bioproducts, this project is making fundamental improvements in the major areas of strain development, specifically tailored to an already highly productive and commercially deployed species *Arthrospira* (also commonly known as *Spirulina*), and aimed at achieving a doubling of the SOT of algal biomass productivity. *Arthrospira* species are attractive for commercial biofuel

| WBS:                      | 1.3.2.601           |
|---------------------------|---------------------|
| CID:                      | EE0008120           |
| Principal Investigator:   | Dr. Damian Carrieri |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,851,376         |
| Project Status:           | Ongoing             |
|                           |                     |

production because of their ability to grow in highly alkaline seawater as well as their relative ease of harvest; however, *Arthrospira* also suffer from notable deficiencies: the cells are sensitive to photodamage in bright sunlight, impeding growth, and they contain substantially less high-energy lipid than eukaryotic algae. This project leverages Lumen Bioscience's proprietary method of genetically engineering *Arthrospira* to build strains that are both more photodamage resistant and accumulate more lipids than unmodified *Arthrospira*. We have assembled functionally rich combinatorial overexpression libraries and used competitive selection coupled with pioneering methods in metabolic profiling at NREL and whole-genome sequencing to discover expression element combinations that have the best growth rates. We will continue these screens and characterizations and construct new strains using winning constructs. These newly made strains will be tested under indoor and outdoor growth conditions to demonstrate improved biomass productivity and lipid accumulation relative to their wild-type parent strains.

# Weighted Project Score: 6.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- This project leverages previously developed high-throughput strain characterization and selection techniques to improve biomass productivity of *Spirulina*. The team demonstrated progress on most milestones. Unfortunately, however, the project pivoted away from outdoor raceway trials to indoor simulated trials.
- This project appears to have strong technical and management approaches that are appropriate for the project objectives. The team was forthcoming about project challenges, executed mitigation plans, and had clear plans to get the project back on schedule. It is unclear if the current plans for outdoor testing would contribute to advancements in MYP goals.
- This is a novel approach to increase biomass and biofuel productivity on a strain that is not commonly used for lipid production; however, there was no true explanation as to how the team is going to validate at scale their improvements.
- The Streamlined Optimization of Filamentous *Arthrospira/Spirulina* Traits (SOFAST) project addresses both the development of tools for strain improvement and characterization as well as the use of those tools to improve an industrially relevant strain. Focusing on *Spirulina* as a target is logical and relevant given the long history of outdoor cultivation at scale. Key steps have been made toward the project goals around tool development. The use of competition experiments to identify top-performing strains under selective pressure is clever and likely to result in a highly efficient methodology. It is unfortunate that the validation of the strain performance will not be conducted in outdoor trials.
- The goal of this project is to produce engineered *Arthrospira platensis* strains with improved photosynthetic and cold-tolerance traits and increased lipid content. The team is taking an approach to transform libraries with various traits and compete these. The approach is innovative and potentially very high-throughput. The team would then sequence to identify constructs that imparted best fitness or most wax esters, then rebuild these constructs into *A. platensis* to produce optimized strains. Stacking of growth, tolerance, and wax production traits would then take place. The approach is very focused and sound. The competition experiments are ongoing and showing successful and unsuccessful genes that might confer appropriate stress resistance. Metabolic profiling using mass spectrometry near-infrared spectroscopy show ability to understand lipid and protein composition. The high-resolution mass spectrometry imaging capability for phenotyping and selection is deemed to be very innovative within this concept. Both indoor and outdoor cultivation studies are underway. The project is working on developing a robust strain of *A. platensis* that is resistant to predation and other stresses and can be easily harvested. If the productivity goals are achieved, the work could approach the FY 2022 productivity targets. The work is also developing new genetic tools to help increase robustness and fitness of strains. Therefore, the project is deemed to be well aligned with the BETO goals.
- Some weaknesses were noted by this reviewer in the development of wax ester production and association of this effort with overall goals of the program.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The project pivoted from outdoor raceway trials to outdoor flat-panel trials. Indoor simulations were always planned and remain in the project goals. We regret that this was unclear to some reviewers.
- Outdoor validation trials will indeed be completed.

# PREVENTION OF LOW-PRODUCTIVITY PERIODS IN LARGE-SCALE MICROALGAE CULTIVATION

#### **Global Algae Innovations, Inc.**

#### **PROJECT DESCRIPTION**

GAI is a leader in low-cost algae cultivation and has developed a high-productivity, crash-resistant cultivation system; however, even with this advanced cultivation system, periods of unexplained low productivity are observed. We will investigate the causes of low productivity and develop strategies to control microbial ecology and dissolved organic matter (DOM) released by microbes. These strategies will include tools to monitor the

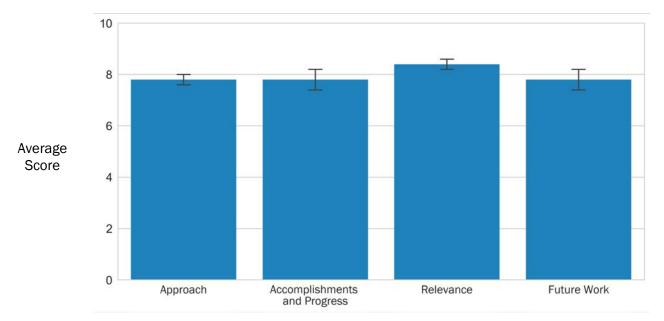
| WBS:                      | 1.3.2.630           |
|---------------------------|---------------------|
| CID:                      | EE0008121           |
| Principal Investigator:   | Dr. Aga Pinowska    |
| Period of<br>Performance: | 10/1/2017-6/30/2020 |
| Total DOE Funding:        | \$3,000,000         |
| Project Status:           | Ongoing             |
|                           |                     |

system ecology, methods to avert low-productivity conditions from microbes or DOM, and methods to promote microbes that improve productivity. We will collaborate with SNL to deploy a low-cost SpinDX detection system to monitor the cultivation pond ecology. The microbial and viral ecology of low- and high-productivity conditions will be analyzed and cataloged. Then target microorganisms will be cultivated to test their impacts as well as probiotic, antibiotic, and DOM remediation strategies.

The project team includes SNL, the University of California at San Diego Scripps Institution of Oceanography, and J. Craig Venter Institute.

# Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

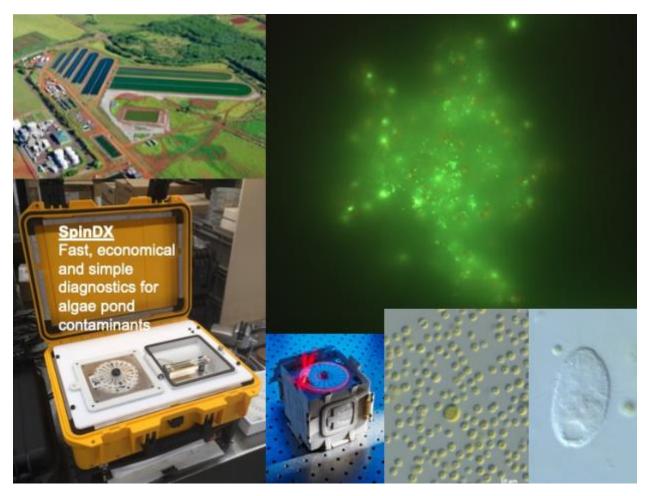


Photo courtesy of Global Algae Innovations, Inc.

## **OVERALL IMPRESSIONS**

- This project is developing an easy-to-use, rapid analytic instrument to ultimately prevent pond crashes and unexplained periods of low productivity.
- This project addresses an important challenge in large-scale production and has designed a wellmanaged study to try to understand periods of abnormally low productivity. The project includes basic research and tool development. The team has a sound technical and management approach and appears to be on track in accomplishing its initial objectives. Future work was described in detail and appears consistent with original plans.
- This is one of several projects using microbiota to increase biomass production. This project is strongly coupled to this specific site but could help establish a baseline for real-time large-scale contaminant occurrence. These data could be used by all other sites and start building solutions to mitigate these contamination occurrences.
- This project is a great example of the potential value of collaborations between academic laboratories and industrial partners. The team used large-scale cultivation systems to generate large, relevant data sets aimed toward the reduction of crop loss in the field. The microbial population data collected to date and demonstration of the utility of the Spin DX tool are key accomplishments. The project will benefit from

continued effort on management and integration of the microscopy, sequencing, and productivity data to ensure a smooth handoff and broad usability.

- The project's goal is to reduce periods of unexplained low pond productivity by identifying and controlling microbiota cultivated with target algae. The partnership includes a strong team from industry, academia, and national laboratories. The team aims to build a broad genomic database of key organisms associated with the water ecology of algal cultures and will identify key organisms and determine their effects on productivity along with treatment methods when necessary. This is an area that is not well understood in the literature, and this work has great potential for impact. The team will also use a SpinDX instrument to identify and quantify organisms in the field. The instrument is innovative and carries some risks in implementation, but there is little reason it cannot be successful in the field as long as samples are properly pretreated prior to analysis. Then the team will implement a broad-spectrum treatment of culture to reduce organic contaminants in cultures. The approach is deemed reasonable, and major challenges have been identified with appropriate mitigating steps. The project's progress is deemed reasonable at this stage. The project addresses key areas in understanding pond ecology and effects on productivity, which can have major contributions to sustainable production and meeting the goals of the BETO program in the development of highly productive strains and cultures that are resilient and robust. Future work is deemed reasonable and should lead to high-impact strategies for cultivation controls.
- A minor weakness was noted in describing/envisioning strategies for the treatment of pathogenic organisms.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their thoughtful comments and suggestions. We agree with the reviewers that the biggest challenge in using SpinDX for the identification and quantification of organisms contaminating algal ponds is sample preparation and pretreatment. We are focusing on developing the right approach for extraction of DNA and RNA for specific microorganism identification. We know that approaches are different depending on the target organism that will be detected: eukaryotes, bacteria, or viruses. Another reviewer concern was on developing approaches to treat pathogenic organisms. We already have a few treatments developed to mitigate problems caused by bacteria and ciliates. We have very little understanding on what organisms they target and how specific they are. This will be addressed in the next phase of this project. We also expect to develop new specific treatments when SpinDX is available and as sequencing data continues to be processed. At this point, one new treatment approach to mitigate bacteria problems was already proposed based on the results of first round of sampling and sequencing. We have many potential treatments ready to test.

# HIGH-THROUGHPUT DIRECTED EVOLUTION OF MARINE MICROALGAE AND PHOTOTROPHIC CONSORTIA FOR IMPROVED BIOMASS YIELDS

#### The Colorado School of Mines

#### **PROJECT DESCRIPTION**

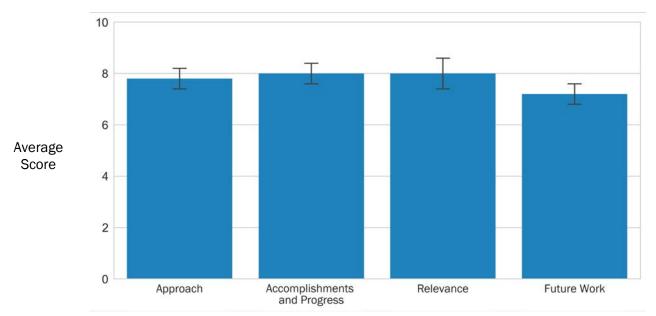
Directed evolution and targeted trait selection remain among the most powerful and successful tools available for attaining the process improvements necessary to enable commercial success in many biotechnology sectors. To develop robust and efficient algal biotechnological chassis, we propose using "solar-simulating" bioreactors to select strains evolved for improved growth rates and improved tolerances to high levels of light, pH, and oxidative stress;

| WBS:                      | 1.3.2.640            |
|---------------------------|----------------------|
| CID:                      | EE0008245            |
| Principal Investigator:   | Dr. Matthew Posewitz |
| Period of<br>Performance: | 9/30/2017-9/30/2020  |
| Total DOE Funding:        | \$2,459,178          |
| Project Status:           | Ongoing              |
|                           |                      |

and to identify photoautotrophic microbial consortia that are able to improve algal biomass yields. We will use deep sequencing (genome, transcriptome) in conjunction with comparative genomics approaches to probe organismal and consortia evolution and identify genomic alterations that enable increased biomass yields and adaptations to growth in outdoor open pond systems. Outdoor validation will be done in collaboration with GAI using their advanced open pond cultivation system that is shown to prevent contamination and attain a threefold productivity increase relative to standard raceways. Organism foci include a diatom routinely grown at GAI, rapidly growing cyanobacteria, as well as consortia of these organisms. We anticipate being able to exceed the targeted productivities for the spring and annual growth cycles. Despite the widespread use and proven track record of directed evolution in other bio-based applications, these tools have seen only limited use in the algal biofuel sector. This is primarily because of the cost, the engineering and human fiscal resource constraints imposed by these techniques, especially when attempting to simulate the extreme photon flux and sinusoidal nature of solar light and environmental temperature fluctuations. Additionally, currently available

# Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

commercial systems do not mimic outdoor growth well, have poor lighting systems that lack feedback measurements and adjustments, are not particularly robust, and/or are prohibitively expensive. We are using low-cost, modular, and scalable growth stations that mimic algal pond parameters of importance for outdoor growth. Importantly, these easily reach the highest photon intensities of sunlight and are capable of programmable temperature swings. We are using these "solar-simulating" bioreactors to select strains evolved for improved growth rates and improved tolerances to high levels of light, pH, and oxidative stress; and to identify photoautotrophic microbial consortia that can improve algal biomass yields. We will use deepsequencing metagenomics to probe organismal and consortia evolution and probe alterations that enable increased biomass yields. Data from experimental work will be used to inform sustainability assessment work with results from modeling work used to understand the impacts of the research. Currently, we have finished determining pH, oxygen, and temperature optima, and we are now leveraging this information to improve tolerances.



Photo courtesy of The Colorado School of Mines

#### OVERALL IMPRESSIONS

- This project attempts to apply directed evolution (a well-known and used technique in adjacent fields) to increase productivity of current strains further. The team has made significant progress to date.
- This competitive project appears to be managed well and is directly relevant to MYP goals and the BETO mission. The project is on track to meet its objectives, and the team included quantitative goals that it still believes are achievable.

- The "directed evolution" path is not presented in a step-by-step process, which makes it hard to understand how the target strain was "adapted." The presentation does not highlight how the phototrophic consortia will be maintained throughout the different laboratories and testing.
- The project team is strong because it includes academic and industry partners with a broad set of expertise. Several students were employed at the Colorado School of Mines to build the reactors, bringing creativity and student engagement to the project. Focusing on an existing industrial production strain, the team has developed a unique laboratory system to select for strain modifications under relevant environmental stresses. The method of strain improvement also enables rapid deployment of field-testing, avoiding any restrictions associated with strain importation or release of genetically modified strains, which could be advantageous. The field demonstration will be a critical step to evaluate the stability of the evolved strain in production and ensure that there are no unintended negative impacts on biomass quality.
- The team hopes to use directed evolution approaches as a tool to improve photoautotrophic microorganism biomass yields and select strains/consortia that attain 24 g/m²/day in the spring growing season in Kauai. The approach is to evolve a specific strain to have good growth characteristics under the typical high-O<sub>2</sub>, low-pH, and high-temperature conditions observed during culturing. The new evolved strains will be grown in environmental simulation bioreactors. They will also assemble and evaluate the productivities of consortia. Evolved strains will be cultivated outdoors, and TEA/LCA modeling will be performed. The approach is deemed to be appropriate and sound. The team represents a strong partnership between academia, industry, and national laboratories. The project is still starting and exercising major capabilities in growth characterization. The projects goals to reach productivities of 24 g/m²/day for the spring growing season in Hawaii would help the BETO program reach and possibly surpass its targets. Further, because the algal species selected are being subjected to growth at extreme salt, temperature, and pH environments, these cultures would likely be very resistant to predation, thus addressing goals in fitness and robustness of cultures. The team's efforts for future work are in-line with the project goals.
- No weaknesses are noted.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers and DOE BETO management for their insightful and constructive comments on our Productivity Enhanced Algae and Toolkits research project. We are encouraged that the review team acknowledges the power and potential usefulness of directed evolution strategies. We concur that these techniques have the potential to help realize MYP goals. We also agree with their assessment that maintenance of evolved strains might be challenging, which is why we established cryopreservation techniques and intend on maintaining selective pressures. We are currently evaluating the stability of our first-generation cell lines at multiple laboratories, and we are attaining the necessary regulatory approval to transfer strains to the GAI site. The evolutions are being conducted one parameter at a time and with all parameters applied simultaneously. Pressures between the two laboratories are similar and designed to mimic outdoor data from GAI. As noted, starting with an industrial strain in hand is encouraging, and careful mapping of pH, temperature, and O<sub>2</sub> optima is allowing quantitative comparisons between baseline and optimized strains. As suggested by the reviewers, if additional throughput is necessary, we could build and deploy smaller volume, higher throughput reactors. We also concur that important progress has been made since the initiation of the project and that the development of a more defined timeline of goals is appropriate.

# SUCCESS THROUGH SYNERGY: INCREASING CULTIVATION YIELD AND STABILITY WITH RATIONALLY DESIGNED CONSORTIA

#### New Mexico Consortium, Inc.

#### **PROJECT DESCRIPTION**

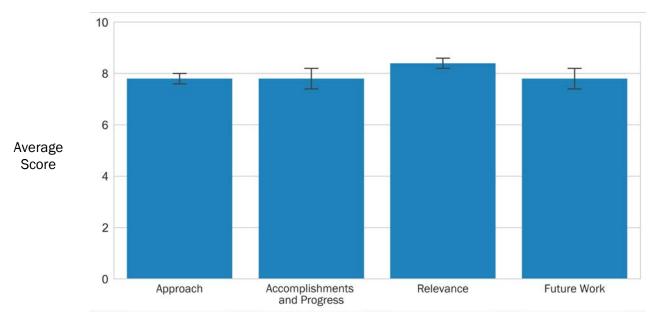
The commercialization of algal biofuels will not be realized until major technical and economic barriers are overcome. As outlined in BETO's update to the *National Algal Biofuels Technology Roadmap*, there is a need to improve culture productivity and stability as well as to better understand these metrics at commercial scales. In this project, we address these gaps. Specifically, we aim to increase productivity of open, outdoor *Nannochloropsis* 

| WBS:                      | 1.3.2.641           |
|---------------------------|---------------------|
| CID:                      | EE0008122           |
| Principal Investigator:   | Dr. Alina Corcoran  |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$2,486,149         |
| Project Status:           | Ongoing             |
|                           |                     |

cultures from 7 g/m<sup>2</sup>/day to 14 g/m<sup>2</sup>/day (doubling of fall SOT value) through a stepwise process to ecologically engineer consortia consisting of (1) multiple *Nannochloropsis* species and strains, (2) growth-promoting bacteria and individual *Nannochloropsis* strains, and (3) complex communities with multiple *Nannochloropsis* strains and bacterial taxa. Previous research focused on consortia has resulted in successes and failures. We argue that the failure to produce more productive and stable cultures has stemmed from two pitfalls: experimental approaches that employed haphazard inclusion of species into polycultures and technical limitations that prohibited screening of high numbers of consortium members. Our project addresses these limitations through rational design and high-throughput bacterial screening. The project, which started in February 2018 with verification, is currently 30% complete and on track with respect to budget. To date, we have met six milestones and have work in progress for an upcoming milestone. In our presentation, we analyzed an existing data set and generated additional data sets of strain tolerances to field medium, salinity,

# Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

temperature, and pests. From this analysis, we constructed nine consortia and are currently testing their performance compared to a baseline field strain through high-throughput screening and bioreactor trials. Data collected thus far show that certain consortia outperform the baseline strain under certain conditions. Second, we are overcoming the limitations of traditional bacterial screening by using a high-throughput tool (High-throughput Screening of Cell-to-cell Interactions [HiSCI]) to isolate and select specific bacterial partners that enhance the productivity and stability of cultures. To date, we have successfully modified the HiSCI system for *Nannochloropsis*, collected environmental samples for input material, and conducted three HiSCI runs. Three bacterial strains have been scaled from these efforts and are being tested in field-relevant conditions. We have also sequenced multiple *Nannochloropsis* strains, not only to develop and implement molecular tracking tools for this project but also to contribute to the repository of algal genomes for the scientific community. Finally, we discuss future work, including lab and field trials, as well as mitigation efforts to address potential challenges.

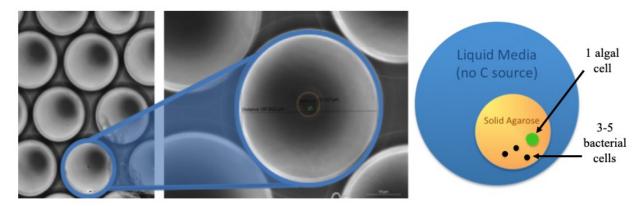


Photo courtesy of New Mexico Consortium, Inc.

#### OVERALL IMPRESSIONS

- The team is developing novel techniques to increase productivity and reduce crashes in open ponds. The work is significant and encouraging progress has been made to date.
- The team appears to have a strong technical approach for a project that is highly relevant to the BETO mission and MYP goals. Initial baseline accomplishments are on track, and strong project management will be required to complete an ambitious set of remaining objectives.
- The team is using a novel consortia-based polyculture approach to achieve higher production. This is a complex approach with high probability for false correlation.
- This approach to consortia development is based on targeted improvement to productivity while maintaining consistent biomass quality in-line with MYP targets. The use of strategic consortia designed to reduce productivity loss from abiotic and biotic stress has high potential. The inclusion of additional algal strains and sources of potentially beneficial bacteria should be considered for future work.
- The objective of this project is to rationally design intrageneric *Nannochloropsis* consortia and *Nannochloropsis*-bacteria consortia to increase productivity, stability, and yield of open, outdoor cultures, with the goal to reach a productivity target >14 g/m²/day with consistent biomass composition. The team is developing tools to rationally design consortia of algae within the same genus but different phenotypes. To do this, a molecular tracking system to distinguish consortium members is being developed using the ccsA amplicon sequence. Consortia are integrated in a high-throughput screening system using agarose beads. The use of this tool is viewed as very innovative and a simple and fast approach to screening consortia of multiple compositions. The team has met all the milestones to date.

The ability to synthesize and control polycultures and microbial consortia could be an excellent approach to increase biomass productivity and crop resilience. This would help meet major BETO goals in these categories for the Productivity Enhanced Algae and Toolkits 2020 targets. The approach is seen as innovative with a direct impact potential on BETO program efforts. The team is on task on all milestones and performance.

• Only one minor weakness/concern is noted for this project, which is related to the high-throughput screening potential for biases in culturing diverse organisms.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that our objectives are ambitious—and we believe they are attainable given our project management plan, which relies on traditional tools (e.g., statement of project objectives [SOPO], Gannt chart) as well as question-based and iterative/incremental approaches. The reviewers aptly asked that we consider (1) the inclusion of additional algal and bacterial strains, (2) potential biases in our high-throughput screening approach for bacterial identification and isolation, and (3) false correlations (in productivity improvements, we suspect) stemming from complexities in our approach.
- Although proposed in our SOPO as only a mitigation strategy, we are currently testing bacterial isolates that have been identified in the literature and/or by collaborators as having growth-promoting characteristics. We are also using non-*Nannochloropsis* algal taxa for the construction of intergeneric consortia; this activity was proposed during verification as a stretch goal of the project. With respect to biases, we agree with the reviewers that bacterial growth in the gel microdroplets (see image) might be different than growth in liquid cultures or raceway ponds. Yet, we also believe that our approach offers a chance of success that is worth this trade-off. Moreover, in the early stages of this project, we altered the scaling platform for captured bacteria from a chip-based platform to one in which microdroplets can grow with shaking in-field medium under fall cultivation conditions. In addition, built into our project plan is the isolation and scaling of captured bacteria for addition into liquid *Nannochloropsis* cultures. We are currently scaling one bacterium for algal-bacteria consortia testing within bioreactors to assess translatability to the field. With respect to the final criticism, we recognize that multiple ecological interactions can make interpretation of cause and effect difficult. Yet, we have a robust flask-to-field pipeline that should help minimize false correlations.

# DEVELOPING ADVANCED GENETIC AND SYNTHETIC BIOLOGY TOOLS FOR IMPROVED ALGAE PRODUCTIVITY

#### University of California, San Diego

#### **PROJECT DESCRIPTION**

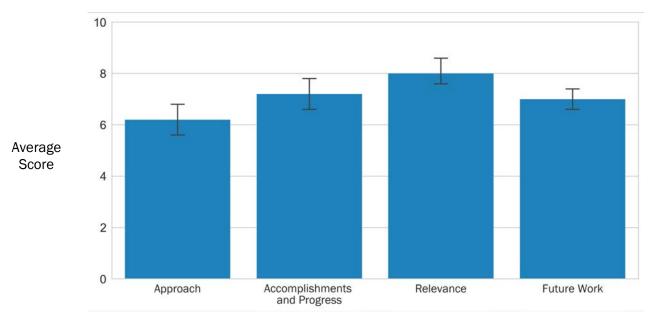
Under this proposal, we will develop genetic tools, highthroughput screening methods, and breeding strategies for green algae and cyanobacteria commercial host strains. We will develop transformation strategies and vectors, synthetic promoters and regulatory elements, and improved methods for nuclear gene editing and transgene expression for engineering of any algae. We will demonstrate the metabolic engineering capabilities of these

| WBS:                      | 1.3.2.650            |
|---------------------------|----------------------|
| CID:                      | EE0008246            |
| Principal Investigator:   | Dr. Stephen Mayfield |
| Period of<br>Performance: | 9/30/2017-9/30/2020  |
| Total DOE Funding:        | \$3,000,000          |
| Project Status:           | Ongoing              |
|                           |                      |

tools by engineering unique branched-chain wax esters into cyanobacteria and green algae for conversion into energy-dense jet fuels and renewable polymers. We will work with three key commercial partners—Triton Algae Innovations, Algenesis Materials, and GAI—to ensure that the tools and technologies developed are relevant to commercial algae production. For Triton, we will specifically develop robust nuclear genetic control systems that allow expression and secretion of recombinant proteins as high-value coproducts as well as develop breeding strategies to improve biomass productivity in their commercial strains. We will work with GAI to develop genetic tools and high-throughput technologies that will enable improved productivity in two of their commercial strains: a green alga and a cyanobacterium. We will develop these tools and technologies to be as universal as possible, allowing them to be adapted to any algae or cyanobacteria of commercial interest. Under previous support from DOE, we developed a suite of basic algae and cyanobacteria genetic tools that were made available to the entire algal community through the "Life Technologies" catalog, and we will continue to develop and distribute these new tools under a similar arrangement. As a proof of concept

# Weighted Project Score: 7.1

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

under the Productivity Enhanced Algae and Toolkits challenge, we will demonstrate the utility of these developed tools by engineering and selecting commercial strains with improved biomass, protein, and lipid composition. We will take these strains into pilot-scale outdoor production at our University of California, San Diego algal pilot facility, and obtain a U.S. Environmental Protection Agency TERA approval for any testing of genetically modified algae in outdoor cultivation, as we have previously done. We will characterize biomass productivity and lipid and protein accumulation using TEA/LCA to evaluate product and coproduct production in our facility. In collaboration with Algenesis Materials, we will evaluate both protein and lipid products for their potential to make bio-based petroleum replacements products, especially renewable polymers, and again use TEA/LCA to assess economic viability and environmental sustainability of these potential coproducts.

#### **OVERALL IMPRESSIONS**

- This project continues key learnings of past DOE projects with hopes of creating a process tool kit for improving the algal yield of high-value coproducts.
- This is a great project working on important genetic tools that will be needed to improve algal strains to produce diverse products as well as increase overall productivity to reduce the cost of production.
- This project successfully identified valuable coproduct opportunities that would immediately improve the economics of algal biomass production while contributing to the longer term MYP targets. Improved processes in the development of genetic tools such as promoter suites and breeding are highly valuable to the BETO portfolio of projects. The team is clearly connected with relevant industry partners for both input to cultivation parameters driving testing conditions and opportunities for coproduct development. The project will benefit from additional structure around the prioritization of future activities and connection to TEA assumptions.
- This project appears to be managed well, has a strong technical approach, and is on schedule to achieve project objectives. The project contributes directly to the BETO mission, MYP goals, and to commercial advancements. The team is encouraged to add quantitative targets to its scale-up and demonstration efforts.
- The goal of this project is to develop a process for making advanced genetic tools using genomics, synthetic biology, high-throughput screening methods, and breeding technologies. The project is very ambitious, and any one of the objectives set forth can be (and in some cases is) a whole project within the BETO program. The team is working on synthetic promoters for recombinant gene expression in *Chlamydomonas reinhardtii*, reported gene expression in cyanobacteria, and mating in *C. reinhardtii*. The team shows a pipeline that can optimize a strain in 17 weeks. The development of improved molecular biology tools, along with breeding of strains, will help advance the goals of the BETO program by providing the tools necessary to create, breed, and adapt strains with the necessary traits to grow with high productivity and be resilient to environmental pressures. This project is just beginning, and future work will continue developing the genetic tool capabilities.
- The main weakness observed is related to the need for a comprehensive plan to move toward all the objectives delineated and providing focus for the project.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# A COMPREHENSIVE STRATEGY FOR STABLE, HIGH-PRODUCTIVITY CULTIVATION OF MICROALGAE WITH CONTROLLABLE BIOMASS COMPOSITION

#### The University of Toledo

#### **PROJECT DESCRIPTION**

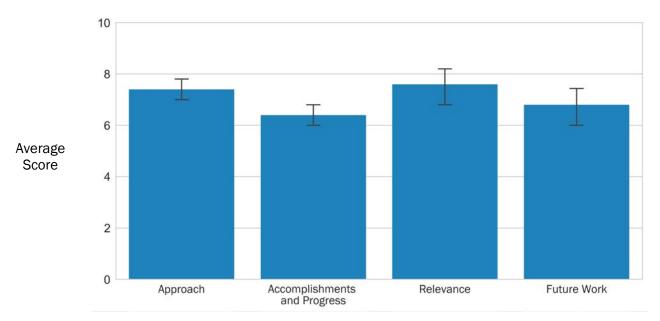
For algal biofuels to replace fossil fuels, it is imperative that cultivation systems are not constrained by (1) proximate availability of flue gas or other highconcentration  $CO_2$  sources and (2) the energy and infrastructure burden to deliver  $CO_2$  long distances. A recent study by Quinn and coworkers estimated that microalgae cultivation systems that are constrained by the availability of flue gases (in addition to low-slope barren

| WBS:                      | 1.3.2.651             |
|---------------------------|-----------------------|
| CID:                      | EE0008247             |
| Principal Investigator:   | Dr. Sridhar Viamajala |
| Period of<br>Performance: | 9/30/2017-7/31/2020   |
| Total DOE Funding:        | \$2,397,698           |
| Project Status:           | Ongoing               |

lands and favorable climates) could achieve less than 10% of DOE's 2030 advanced fuel targets. We propose cultivation of microalgae in high-salinity and alkalinity media (pH greater than 10, alkalinity greater than 100 milliequivalents, salinity ~30 g/L) to achieve high biomass productivity and culture stability. Our cultivation media comprise high concentrations of dissolved inorganic carbon (DIC) (greater than 60 mM) at pH higher than 10. As alkaliphilic cultures grow, bicarbonate ( $HCO_3^-$ ) is taken up by the algae, CO<sub>2</sub> is abstracted and fixed, and hydroxide (OH<sup>-</sup>) is released. In parallel, because of the high pH of the medium, gaseous CO<sub>2</sub> is dissolving into the culture medium at a rapid rate, even from ambient air. The resulting high alkalinity in the growth medium ensures that enough  $HCO_3^-$  remains available in the solution for continued carbon fixation. At night, when photosynthesis is absent, the bicarbonate depleted from the solution during the day is replenished via transfer of CO<sub>2</sub> from the atmosphere. Our strategy is to use this high-pH and high-alkalinity culturing

## Weighted Project Score: 7.0

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

strategy to achieve high-productivity cultivation of strain SLA-04 without any inputs of concentrated CO<sub>2</sub>. Additional productivity improvements are envisioned through the development of molecular tool kits, including metabolic modeling combined with targeted genome editing.

#### OVERALL IMPRESSIONS

- This is a novel application and development of molecular biology tool kit to prevent pond crashes and decouple algal farm locations from (expensive) CO<sub>2</sub> sources and delivery mechanisms. It leverages past DOE projects to demonstrate improved biomass productivities at a reduced cost in outdoor ponds by the conclusion of this project.
- Developing approaches to reduce dependence on CO<sub>2</sub> availability is highly valuable to reduce the cost of algal biomass production. The project team, led by The University of Toledo, has a long history in working together and appears to have the required resources to drive this initiative forward. Because this project is just beginning, there is an opportunity to ensure that the outdoor cultivation experiments are tightly connected to the tool development and economic analysis. It is critical that the biology impact is considered when refining models for CO<sub>2</sub> exchange with the pond media. Overall, the project would benefit from additional clarity and connection of biology to the experimental design and model assumptions.
- This presentation and project are well thought out. There is a possibility that the team might want to do too much, especially when they enter the later genomic editing deliverables. Their efforts do not seem to focus a on the biofuel production stages or open, large pond deployment. The multiseason experiments focusing on productivity and algal community dynamics should highlight the positives and negatives associated with this growth strategy.
- This project addresses an important challenge of large-scale algal production: the cost of CO<sub>2</sub> acquisition, distribution, and delivery. The goals, objectives, and management approach appear appropriate for the project. The project is on track, and early results are promising. The team is encouraged to make sure that the mixing and growth conditions tested will be representative of large-scale production.
- The goal of this project is to develop cultivation approaches that use high-pH and high-alkalinity media (1) for high rates of atmospheric CO<sub>2</sub> capture and (2) to provide nonlimiting DIC concentrations for growth. The main outcome is a high-biomass and biofuel-precursor productivities in outdoor open ponds using atmospheric CO<sub>2</sub> alone. The team plans to lay out and test the chemical and engineering principles associated with CO<sub>2</sub> transfer into alkaline media. They will use a *Chlorella* isolate for their evaluations. The team plans to develop a metabolic network model and genome editing approaches to improve the carbon uptake and tolerance of the selected strain. The project is just beginning and showing progress toward its main tasks. It is noted that the selected *Chlorella* strain shows productivities of 22 g/m<sup>2</sup>/day to 32 g/m<sup>2</sup>/day in high-alkalinity media. The development of high-productivity cultures that can grow on atmospheric CO<sub>2</sub> inputs would have major impacts on the implementation and success of BETO efforts. This project is deemed highly impactful for the overall program efforts. Because the project is just beginning, future work will incorporate all the main objectives and tasks for the project.
- No major weaknesses are noted for the project's approach and outcomes.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their overall positive comments on the project and for recognizing the "highly impactful" merit of our high-pH/high-alkalinity approach for decreasing/eliminating the cost of CO<sub>2</sub> acquisition, supply, and delivery. Per reviewer suggestions, we plan to integrate the biology tool kits more closely with the cultivation experiments as we progress through the project. Further, we will use first-principles mathematical modeling of the mass transfer process and correlate model predictions with experimental data to estimate mass transfer fluxes in commercial-scale systems and quantify the effects of mixing on the CO<sub>2</sub> mass transfer rates.

# MICROBIOME ENGINEERING OF *DESMODESMUS* TO ALLEVIATE CARBON LIMITATION

#### Lawrence Livermore National Laboratory

#### **PROJECT DESCRIPTION**

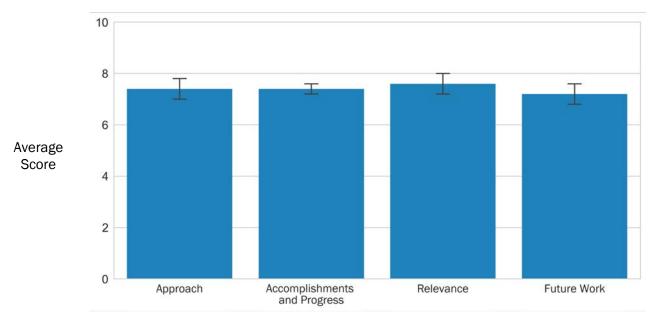
Roughly half of the carbon photosynthetically fixed by microalgae is lost through extracellular exudation of DOM. In high-biomass-density ponds, algal cells are also CO<sub>2</sub>-limited and stressed from overproduction of O<sub>2</sub> from photosynthesis. In summer conditions, high light and temperature stress further decrease algal photosynthetic efficiency. To reach the goal of 26 g/m<sup>2</sup>/day ash-free dry weight produced during summer months, and using

| WBS:                      | 1.3.2.652           |
|---------------------------|---------------------|
| CID:                      | NL0033320           |
| Principal Investigator:   | Dr. Xavier Mayali   |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,539,149         |
| Project Status:           | Ongoing             |
|                           |                     |

*Desmodesmus* strain C046 as a model system, our research aims to ecologically engineer the algal microbiome to enrich for bacteria that efficiently remineralize DOM to  $CO_2$  and simultaneously remove  $O_2$ . Our approach is to examine the microscale interaction between surface-attached bacteria and the *Desmodesmus* cells and use high-throughput sorting and screening with microfluidic incubation chambers developed by our industrial partner General Automation Lab Technologies. Using a combination of assays for DOM, microbial community analysis and algal growth quantification, we identify individual microbiome components with desired characteristics, such as high respiration rates and efficient DOM removal. In addition to alleviating  $CO_2$  limitation and  $O_2$  toxicity, the outcome of this synthetic ecological engineering approach will decrease algal pond DOM at harvest, which is a wasted resource, a supply of organic pollution if released into the environment, and which enables colonizing and possibly detrimental microorganisms to more easily invade the pond community. Our work includes scaling microbiome effects on algal growth from microwell to 1,000-L scale and the development of tool kits to be made available to the research community, including (1) a high-

# Weighted Project Score: 7.4

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

throughput assay approach for screening the effect of tens of thousands of distinct microbiomes on algal growth and (2) a medium-throughput assay for screening hundreds of microbiomes for high respiration and recycling of DOM.

#### OVERALL IMPRESSIONS

- This promising early-stage AOP project appears to be supported by a strong technical and management approach. Early results are consistent with project goals, and the team is well-equipped to complete its bench-scale objectives. Outdoor demonstration of the technology might be challenging given the additional ecological complexity, but the team is commended for including these larger scale tests in its objectives.
- This project strives to improve the productivity and robustness of algal strains by identifying microbiome consortia particularly well suited for different stressful environments—early results are encouraging.
- The positive synergetic relationship between algal cells and bacteria is not a new concept; many other groups have attempted to harness this relationship with somewhat minimal results. This project has the potential to achieve better results because they are using novel instrumentation for their initial high-throughput phases as well as isotope tracing for their later grow phases. This is a research area with great opportunity that could be a major driver for the improvement of productivity at scale. There might be some issues with running these experiments at scale, and the push to the field could be difficult.
- There is tremendous opportunity in engineering a beneficial microbiome to improve algal productivity. This project focuses on a naturally occurring consortia of *Desmodesmus* and associated bacteria. The demonstration of reduced DOM and increased productivity under temperature and light stress is a strong indication of the potential of this approach. There are several key steps for this concept to be applicable at the industrial scale. Of note, the biomass composition will need to be evaluated to ensure there is no negative impact of the presence of the microbial community. Overall, it is exciting to see this type of project within BETO's portfolio.
- The project's aim is to use a high-throughput microfluidic screening system to identify mutualistic bacteria with high respiration metabolism and protective pigmentation that lead to increased *Desmodesmus* growth under summer conditions and test at different lab and outdoor scales. The goal is to target 26 g/m<sup>2</sup>/day biomass production under high-light and high-temperature stress (1,000-L scale). The approach will use microbial community analysis along with high-throughput cultivation in microwells and phenotyping of single cells using nanoscale secondary ion mass spectrometry for phenotyping. The approach is deemed to be reasonable. The team has characterized the microbiome associated and aggregated with different isolates of *Desmodesmus* showing differences in communities and growth characteristics. Xenic cultures in the microwell systems have higher cell yields. The project is just beginning and therefore has limited results to date. Controlling the bacterial microbiome in algal cultures provides an opportunity to enhance productivity. If successful, the project can directly impact the goal targets for the BETO program. Future work will focus on the main tasks delineated in the project.
- The main weakness noted was in providing a better explanation/justification on the use of isotope tracing for this project.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# DIRECT PHOTOSYNTHETIC PRODUCTION OF BIODIESEL BY GROWTH-DECOUPLED CYANOBACTERIA

#### Arizona State University

#### **PROJECT DESCRIPTION**

The breakthrough catalyzed by this project is a direct production of excreted, drop-in, ready biofuel (methyl laurate or ethyl laurate) by cyanobacteria using CO<sub>2</sub>, water, and light as the main inputs and not wasting carbon and energy by limiting the amount of biomass produced. The main advantages over current biofuel products are (m)ethyl laurate's immediate application as biodiesel and its limited solubility in water, thus reducing the availability to

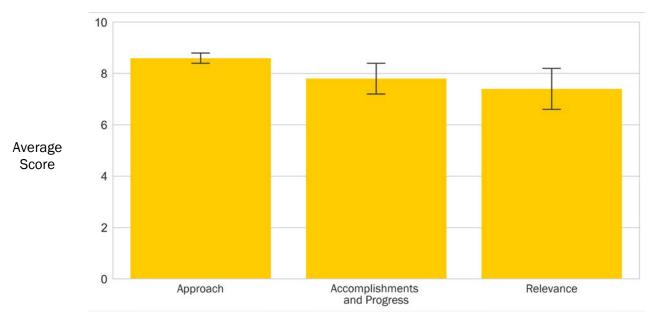
| WBS:                      | 1.3.2.910           |
|---------------------------|---------------------|
| CID:                      | EE0007561           |
| Principal Investigator:   | Dr. Wim Vermaas     |
| Period of<br>Performance: | 9/1/2016-12/31/2018 |
| Total DOE Funding:        | \$1,818,000         |
| Project Status:           | Sunsetting          |
|                           |                     |

heterotrophs in the culture and increasing the ease of harvesting. The productivity of (m)ethyl laurate is increased by (1) boosting metabolic flux through the fatty acid biosynthesis pathway to (m)ethyl laurate and (2) reducing the production of extracellular polymeric substances such as exopolysaccharides. A further research aim is to uncouple growth of the culture (biomass production) from production of the biofuel, thus increasing (m)ethyl laurate yield and productivity while reducing the production of biomass. The resulting combination is disruptive to current biofuel production because of the type of biofuel produced and the reduction in exopolysaccharides, whereas decoupling cell growth and fuel production might enable the organism to put even more resources into biofuel.

This approach provides a "one-stop-shop" cyanobacterial platform that generates liquid transportation fuel from  $CO_2$  and water with sunlight as the energy input. As established biodiesel molecules, methyl and ethyl laurate are suitable for direct use as a diesel replacement. Moreover, lauroyl esters have many additional



Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 ${f I}$  One standard deviation of reviewers' scores

applications. The ester moiety, meanwhile, provides a "protective cap" to the fatty acid molecule, reducing product degradation by heterotrophic scavengers, a key consideration for large-scale PBR systems. The product is readily harvested because of its poor solubility in aqueous media. This simplicity streamlines the biofuel production process and improves overall economic viability.

The concept builds on the team's prior success in efficient photosynthetic production and scale-up of laurate by a modified strain of the cyanobacterium *Synechocystis sp.* PCC 6803; this strain contains a thioesterase from the plant *Umbellularia californica*, which releases the fatty acid laurate when native fatty acid biosynthesis reaches the C12 stage. This platform strain is further engineered to improve laurate production and to convert laurate to (m)ethyl laurate. Conversion of laurate to methyl laurate is done by a S-adenosyl methionine-dependent enzyme, and conversion to ethyl laurate proceeds via lauryl-CoA and ethanol coproduction; the latter is done using constructs provided by Algenol. Inducible gene circuits are engineered to control the expression of decoupling mechanisms to arrest cell growth without harming viability and metabolic activity. Genetic changes to reduce the level of exopolysaccharides help to further push fixed carbon toward biofuel production and to reduce the level of nutrients available to heterotrophs.

Although ethyl laurate production was unstable, the majority of laurate was efficiently converted to methyl laurate by appropriately modified cyanobacteria, and the methyl laurate was excreted from the cell and captured in a biocompatible organic solvent, which greatly aids in harvesting. This provides an efficient method to produce and excrete biodiesel using a cyanobacterial culture, CO<sub>2</sub>, and light.

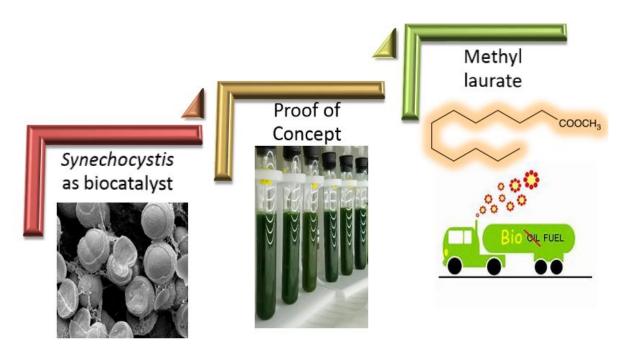


Photo courtesy of Arizona State University

#### **OVERALL IMPRESSIONS**

• This innovative project was able to accomplish its bench-level objectives after successfully navigating a pivot in target products. The team was managed well, and if the approach could be scaled up successfully, it could make a strong contribution to MYP goals. It was unclear if scale-up efforts were able to replicate the bench-level accomplishments.

- This project employs molecular biology tools to engineer the photosynthetic algae to directly excrete the biofuel, significantly limiting the downstream processing involved. This project successfully accomplished the goal, and the preliminary TEA is promising.
- The production of novel compounds from algae as a coproduct or precursor to biofuel is critical for economic viability. This extremely unique approach to the production of methyl laurate provides a demonstration of feasibility. The secreted coproduct can be relatively easily separated from the algal culture for a continuous production system. This is a great example of a stretch project providing potentially disruptive approaches to increase the value of algal production systems.
- The team appears to have been successful in engineering a strain that can produce methyl laurate. Questions remain about how this could be used for production, but this is a good first step toward a viable production system. Methyl laurate is an easily labile substrate for many marine alkane-degrading organisms. It is possible that if this were excreted extracellularly at scale in open air ponds, a large bacterial bloom would be observed, resulting in consumption of the product. This is a concern that should be addressed in operational designs if methyl laurate production is ever taken to scale.
- The main objective of the project was to develop cyanobacteria that excrete photosynthetically produced biodiesel with increased carbon flux into this pathway. The team took the approach of engineering *Synechocystis cyanobacterium* for fatty acid synthesis and overexpression. They developed a stable methyl laurate producing strain. They attempted to decouple growth and laurate production and reduce exopolysaccharide production. Then the team demonstrated production in a 55-L PBR system and perform a TEA. The technology is deemed very innovative. The team met several obstacles and developed strategies around these. Some weaknesses were noted in the association with the separation and collection of the methyl laurate and the modeling efforts.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thorough evaluation of the project and their overall very positive take on the progress.
- We appreciate the comment that methyl laurate might be consumed by specific marine organisms. The compound appeared stable under our experimental conditions, including when bacterial contamination was introduced; however, we realize that there could be culture conditions where methyl laurate is less stable than desired in open pond conditions. If this proves to be an issue, then covered ponds might be considered.
- The value of methyl laurate is on the order of \$1,000 per metric ton. A major consideration for the growing laurate and methyl laurate market is that cyanobacteria produced methyl laurate is significantly more sustainable than current production mechanisms, which involve palm oil plantations on recently converted tropical rain forest land. We agree that the production split between biomass and methyl laurate production is not yet firmly established and that TEA analyses done in this project are preliminary, without a thorough analysis of required downstream infrastructure; however, these preliminary results show that in principle the approach is promising.
- In the presentation, we did not sufficiently stress that an organic overlay of the culture (e.g., dodecane), functioning to harvest produced methyl laurate, did not negatively affect the culture in any way. Separation of the aqueous and organic layers typically is straightforward, but sometimes an emulsified interface will form that complicates clean separation of the phases. This is one issue we ran into at the 55-L scale, together with the loss of much of the organic overlay (along with the product) as a result of aerosolization and capture into the aerosol-quenching bleach solution that is required for larger scale cultures of transgenic cyanobacteria. This will need to be investigated further if commercialization is contemplated.

# A NOVEL PLATFORM FOR ALGAL BIOMASS PRODUCTION USING CELLULOSIC MIXTROPHY

#### Arizona State University

#### **PROJECT DESCRIPTION**

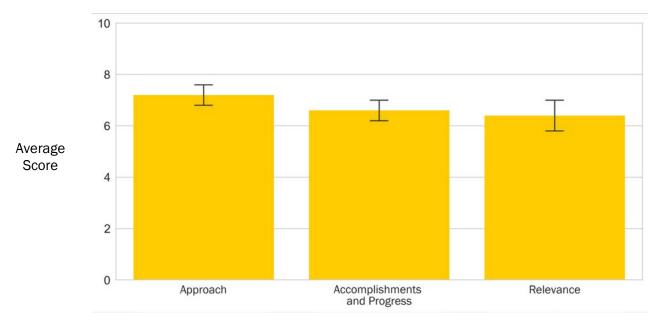
Algal feedstock production platforms specifically designed for scale-up on land with limited water resources remain an important gap in the DOE BETO algal R&D portfolio. As a result, abundant flat land in the southwestern United States plays little or no role in current DOE resource assessments, yet this region offers significant potential for algal biofuels that would not compete with food production if the water barrier could be addressed. The BETO

| WBS:                      | 1.3.2.920           |
|---------------------------|---------------------|
| CID:                      | EE0007562           |
| Principal Investigator:   | Dr. Peter Lammers   |
| Period of<br>Performance: | 10/1/2016-9/30/2018 |
| Total DOE Funding:        | \$1,689,791         |
| Project Status:           | Sunsetting          |
|                           |                     |

portfolio has focused on open pond cultivation systems, but these systems have struggled with stability and productivity in outdoor scale-up trials. The goal of the proposed research is to close these gaps in the BETO portfolio. To this end, we will grow thermostable, acidophilic algae mixotrophically in PBRs to improve biomass productivity and reduce water consumption by reducing evaporation and eliminating cooling requirements. We will determine if the expected order-of-magnitude improvement in productivity outweighs the added costs of mixotrophic cultivation.

## Weighted Project Score: 6.7

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 $\square$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- This novel project on carbon metabolism appeared to be managed well and accomplished many of its objectives. The project included an extensive list of publications in preparation or in print. It is unclear if the approach has relevance to biofuel production scenarios because it seems to require a unique bioreactor and a high-value coproduct to support the TEA.
- The team's goal was to create a system suitable for arid regions of the country by using cellulosic sugars as a feedstock and closed PBR systems to reduce water consumption. Iterative modeling with the TEA team provided useful experimental direction.
- The project team has taken a unique approach to the challenge of water limitation in arid regions where algal production might otherwise be highly successful. In addition, the team has an industrial partner with a focus on a valuable coproduct that will drive the economics of the system. The resulting TEA from this project has created a focus for the project team toward improved cultivation systems. There is also an opportunity in projects of this nature to assess the strain choice and further explore the assays for assessing mixotrophy potential of the culture.
- This is an interesting model, but it is not clear if the approach address BETO's goal of reducing fuel costs or generating biomass for fuel purposes. This system does not appear to be a coproduct as much as a system designed solely to generate high-value products.
- The objective of this project was to demonstrate mixotrophic cultivation on cellulosic sugars from acidpretreated cellulose hydrolysate by the alga *Galdiera sulphuraria* and produce a phycocyanin coproduct. The approach is deemed innovative and unique to the BETO portfolio. The project was successful in demonstrating biomass productivities over 1 g/L/day on corn stover hydrolysate, with yields of 07–1.1 g biomass/g sugars. These high productivities and yields can be beneficial to the overall economics of the process. The team showed that mixotrophic conditions provide an opportunity to produce high yields of biomass with high contents of polysaccharides. Further, the team showed the ability to optimize the system for high productivity of phycocianin. The TEA showed the need for reduced PBR costs and production of a high-value product. Thus, the project addresses major goals of the BETO program in crop resilience and productivity.
- The main weakness for the project is providing supporting information from the TEA/LCA showing that this pathway to fuels would be more beneficial than a direct pathway that converts the stover into a biofuel.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# ALGAL FEEDSTOCKS LOGISTICS AND HANDLING

## Idaho National Laboratory

#### PROJECT DESCRIPTION

This project focuses on understanding the post-harvest physiology of algal biomass to enable the development of process technologies that preserve, and even improve, the quality of algal biomass prior to downstream conversion. Post-harvest physiology spans the time frame between harvest and conversion, which can range from minutes to months. This research project will provide solutions to feedstock supply chain and logistics challenges that occur between algal biomass production and conversion, meanwhile reducing the risk of feedstock loss. The two objectives of this project are to (1) solve the problem of seasonal variation in algal biomass production by developing a long-term storage approach that can reliably

| WBS:                      | 1.3.3.100          |
|---------------------------|--------------------|
| CID:                      | NL0032357          |
| Principal Investigator:   | Ms. Lynn Wendt     |
| Period of<br>Performance: | 4/1/2015-9/30/2019 |
| Total DOE Funding:        | \$2,360,000        |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$800,000          |
| DOE Funding FY18:         | \$760,000          |
| DOE Funding FY19:         | \$800,000          |
| Project Status:           | Ongoing            |
|                           |                    |

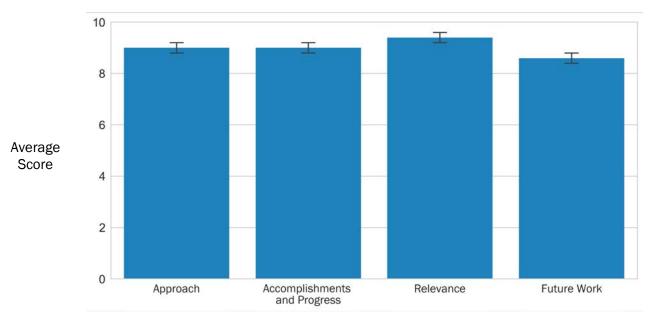
stabilize algal biomass while reducing energy input in a cost-competitive manner compared to the current state of the art and (2) increase conversion throughput by reducing ash content in periphytic biomass originating from an algal turf scrubber (ATS).

We have shown that seasonal variation can be mitigated through the development of a wet anaerobic storage process for algal biomass. This effort has used lab-scale experimentation, process optimization,

characterization of stored materials, and TEA to achieve algal biomass stability in a cost-competitive manner. Algal biomass, 20% solids blended with lignocellulosic biomass and stored using existing practices for silage production, was accomplished at the 20-L scale for 3 months with 3% dry matter loss. Continuous, bench-scale

## Weighted Project Score: 9.0

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $\square$  One standard deviation of reviewers' scores

HTL tests of the stored material conducted at PNNL suggest no change in biocrude yield as a result of storage. We also demonstrated a stabilization approach for algal biomass at 20% solids that results in 10% total loss in dry matter over 6 months, and this approach reduces costs compared to drying followed by dry storage. This project also provides continued support to the BETO's annual SOT algal production effort by assessing the post-harvest stability of algae harvested from seasonal cultivation trials in outdoor test beds.

Physical and chemical ash-removal approaches conducted to date have revealed multiple pathways for ash reduction in biomass harvested from the ATS floways. Despite high biomass productivities and water remediation opportunities for ATS systems, their adoption as biofuel feedstock production platforms is limited because of high ash content, which is consistently 60 wt %–65 wt % for this biomass. Elemental ash analysis revealed that biomass from ATS systems sourced from seawater contain ~20% sodium and chloride, which are easily removed by water extraction. Water extractions reduced ash by 28%–40%, although overall ash content was 40 wt %–50 wt % and is considered too high for many conversion approaches, including HTL. Alkaline treatment was successful at removing silica, which can constitute 50% of the ash because of large contributions from diatoms, such that final ash contents ranged from 20–40%.

In summary, this research is providing solutions to feedstock supply chain and logistics challenges that occur between algal biomass production and conversion, meanwhile reducing the risk of feedstock loss. This effort supports multiple MYP barriers (e.g., storage systems, quality) and contributes to the goals of increasing biomass value through coproduct formation and ultimately for producing \$2.50/gal biofuels.



Photo courtesy of Idaho National Laboratory

#### OVERALL IMPRESSIONS

• The incorporation of algae into existing bioenergy feedstock streams is a clever and actionable approach. The project update was exceptional with clear communications of the value drivers, challenges, accomplishments, and critical next steps. The opportunity to improve the economics of biofuel production through combining feedstock sources has been shown through this innovative and well-run project. I look forward to seeing the future development of this exciting work.

- The relevance of the project was clearly linked to MYP goals, such as biomass storage challenges and preservation of biomass quality. The team is guided by strong technical and management approaches. An extensive publication list is an indication that the team is committed to project results being used to advance the SOT for bioenergy applications. Project results have been incorporated into BETO's SOT and resulted in improved future fuel selling prices.
- This research focuses on the vital, but often overlooked, aspect of logistics (between biomass harvesting and downstream processing). Promising progress to date related to maintaining quality of biomass during storage. Task 2, ash reduction, will be incredibly valuable across the industry if successful.
- Wet storage of algal biomass is a novel concept that needs to be further explained. This project has made great progress in addressing many questions, but it is lacking additional results from large-scale harvests. The team's collaboration with AzCATI should be expanded to include multiple strains grown in different seasons to see if there is a variability. The data already show significant variability from different strains, and further evaluation of seasons and how growing conditions affect the storage will be also important.
- The team will use feedstock logistics operations to develop process technologies that preserve and even improve the quality of algal biomass prior to downstream conversion. The key outcomes are (1) a process that both preserves harvested microalgal biomass during a 6-month period to manage seasonal production variation and enables a biorefinery to run year-round with a consistent feedstock supply and (2) a process to improve the quality of biomass derived from an ATS through ash reduction that could be applicable to multiple high-ash algal species. In feedstock stabilization, the team is blending the algal feedstock with terrestrial feedstock under anaerobic conditions and stabilization with lactic acid to understand fundamentals in preservation process. They are also working on ash composition analysis and removal from algae coming from scrubbers through several methods. This is overall a well-conceived and unique project that can have great impact on the industry. The team has shown algal preservation for 6 months for all components, with only minor changes in carbohydrates, under the blending with corn stover. No change in performance is seen in the HTL of the blended material that was stored. The team also found that adding lactic acid decreased storage losses from 44% to 6%, but this is not economically feasible. The ash characterization studies are being performed in water from an estuary that contains up to 75% ash. The team is working on systematic removal of ash by alkaline washes and determining removals and effects on remaining algae. The team is working on ash accumulation studies in an ATS floway in California. Progress has been steady, and the project has great potential for impact. The TEA shows that successful wet storage contributes to a decrease in the MFSP of the SOT. The relevance and direct impact of these efforts are deemed to be very high for the BETO program. Future work is deemed reasonable and appropriate.
- No weaknesses are noted.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for the positive feedback. We agree that addressing biomass availability and quality in the feedstock logistic supply chain is important in advancing the commercialization of algalbased biofuels. We will continue to seek a fundamental understanding of algal post-harvest physiology in support of BETO MYP goals of reducing costs of algae-based biofuel production. This project has been collaborating with AzCATI since Spring 2018 on assessing the storage stability and ash content of multiple strains grown outdoors from each season, and we will continue this effort to understand strain-to-strain variability, seasonal variability, and the fundamental aspects of preservation through wet storage with a goal to make wet stabilization approaches universally applicable. Ash mitigation in outdoor systems is a growing concern for the algal industry. We will expand our work to include algal biomass cultivated in raceways and in wastewater effluent to develop solutions that result in reduced ash content in a variety of sources of algal biomass.

# ALGAE TEST BED PUBLIC-PRIVATE PARTNERSHIP (ATP3) – A RAFT PARTNERSHIP

#### Arizona State University

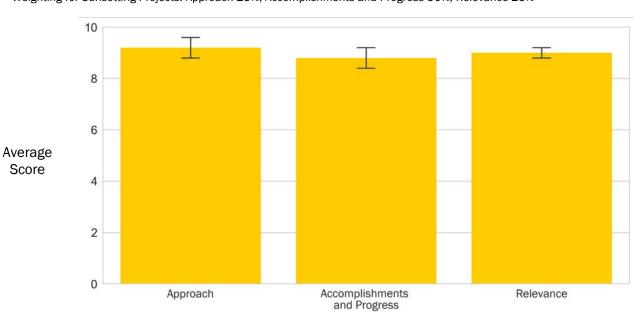
#### **PROJECT DESCRIPTION**

The ATP3 is a multi-institutional effort funded by DOE to establish a network of operating test beds that bring together world-class scientists, engineers, and business executives with the goal to increase stakeholder access to high-quality facilities by making available an unparalleled array of outdoor cultivation, downstream equipment, and laboratory facilities to the algal R&D community. ATP3 used the same powerful combination of facilities and

| WBS:                      | 1.3.5.100           |
|---------------------------|---------------------|
| CID:                      | EE0005996           |
| Principal Investigator:   | Dr. John McGowen    |
| Period of<br>Performance: | 1/31/2013-9/30/2018 |
| Total DOE Funding:        | \$14,999,658        |
| Project Status:           | Sunsetting          |
|                           |                     |

technical expertise to support the TEA/LCA and resource modeling and analysis activities, helping to close critical knowledge gaps and inform robust analyses of the SOT for algal-based biofuels and bioproducts. ATP3 included test bed facilities at AzCATI and augmented by university and commercial facilities in Hawaii (Cellana), California (California Polytechnic State University, San Luis Obispo), Georgia (Georgia Institute of Technology), and Florida (Florida Algae), in addition to partners at the NREL, SNL, Valicor Renewables, University of Texas at Austin, and Commercial Algae Management, Harmon Consulting, Evodos and Litree.

ATP3 aimed to make significant advancements in the algal biofuel arena by promoting opportunities through an open collaborative test bed network. Our regional test beds were equipped to develop and evaluate value propositions in support of multiple algal market value chains. We successfully served clients across a range of applications and needs from water testing and species identification, productivity, and analytic measurements from biomass grown in novel PBRs and ponds, biomass supply from gram to multiple kilogram quantities,



#### Weighted Project Score: 8.9

Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

identification of bioactive molecules that promote animal health and associated scale-up processes, and equipment testing, in particular novel PBRs and dewatering equipment. Our network offered access to such desirable features as open and closed, small to large pilot cultivation systems; access to natural saltwater, wastewater, and CO<sub>2</sub> streams; and integrated harvesting unit operations. During the program, ATP3 engaged more than 50 clients from academia, national laboratories, and industry; included international deliveries of hundreds of kilograms of algal biomass to partners; conducted 15 educational and training workshops; and completed more than 80 client projects generating additional revenue in support of the overall test bed network.

ATP3 used our facilities to perform coordinated long-term cultivation trials producing robust, meaningful data sets from this regional network determining the effects of seasonal and environmental conditions. These data are critically important to support the modeling community and guide R&D toward the transformative goal of cost-competitive algal biofuels and bioproducts by 2030. ATP3 implemented an experimental framework, termed "unified field studies" which were conducted across six distinct geographic regions using standardized mini-raceway ponds, standardized protocols, and data acquisition and tracking methodology. In addition, we leveraged specific site capabilities, including PBRs, access to wastewater and CO<sub>2</sub>, larger pilot-scale raceway ponds, and dewatering equipment to conduct targeted cultivation trials termed "advanced field studies." From September 2013 through December 2018, more than 95 individual experiments were conducted across the network, with an average duration of at least 50 days. These experiments included standardized, validated methods with an emphasis on continuous improvement, more than 15 strains used in outdoor cultivation experiments with the majority of multiseason data coming from 5 strains with an average run time of more than 40 days. ATP3-generated productivity data continue to be the primary data sets supplied to the DOE-sponsored SOT metrics for 2015, 2016, 2017, and 2018 and under the DISCOVR for 2019 and beyond.

- The ATP3 project successfully implemented a multilocation algal field trial network using standardized protocols and cultivation practices. This type of field testing is instrumental to the advancement of the industry by providing sites to host outdoor experiments and continue to refine the TEA accuracy. The team has done an extraordinary job of collaborating across the industry by providing an important service and quality data as well as education opportunities. The continued support of programs like this and expansion of field-testing locations would be highly valuable to the continued development of algal biofuel production.
- Large consortia focusing their efforts on year-round large-scale deployment of top three algal strains at three outdoor test bed locations. All data accumulated during the 3 years is available to the public. Their efforts and results will become the next baseline for future projects just as other large consortia projects have done before the RAFT and ATP3.
- ATP3 is a large project addressing a key goal for the BETO program by establishing and operating a test bed capability to facilitate innovation and growth of the algal biofuel and bioproduct R&D and industrial community. To meet this goal, the ATP3 team formed a national partnership/network with entities that could provide a diverse set of capabilities across the United States. As part of the process, the team made the facilities available to a broad range of investigators from academia, national laboratories, and industry. Further, the team provided access to much of the cultivation data collected during various large-scale experiments to the community through appropriate web portals. The list of accomplishments by the ATP3 team is impressive, covering supply of biomass (>1,000 kg), equipment testing, analytic methods testing and validation, culture maintenance, scale-up of cultures (including setting up initial stages of GMO trials), along with education and training workshops. The test bed capability was developed by the BETO program in response to a stakeholder outcry for capabilities to supply biomass, standardize cultivation practices, provide facilities for testing and evaluation, and concerted development of training and outreach. The ATP3 partnership clearly addressed these needs and provided the algal community and the BETO program with an excellent capability. The capability has evolved to become

an integral component of the BETO program and engages stakeholders broadly. Further, the ATP3 project addressed key needs in workforce development and technology dissemination. Very few weaknesses were noted. The ATP3 partnership and the BETO program are commended for this excellent success.

- This ambitious project has served a critical role in generating publicly available data in outdoor conditions at a variety of scales. Outputs include an impressive list of peer-reviewed publications and numerous workshops, training sessions, and other forms of stakeholder engagement. The project has played a central role in supplying SOT data and continues to be closely aligned with BETO priorities and MYP goals. The team and assets also serve as an important collaborator on many other BETO-funded projects.
- ATP3 has contributed—and continues to contribute—a significant wealth of knowledge and baseline data to the algal industry. It is proven to be a great resource for researchers to trial new concepts.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- ATP3 thanks the reviewers for the comment. Our commitment to facilitating stakeholder access to facilities and expertise was core to our formation and through this program.
- ATP3 conducted harmonized, highly coordinated cultivation trails across five sites with three commercially relevant strains for more than 2 years, and we leveraged additional experimentation for another 3 years and another five commercially relevant strains. We agree there is a continued and important place for large, well-run consortia projects, and we were honored to participate and contribute to the BETO AAS portfolio.

# **REGIONAL ALGAL FEEDSTOCK TESTBED PARTNERSHIP**

## **University of Arizona**

#### **PROJECT DESCRIPTION**

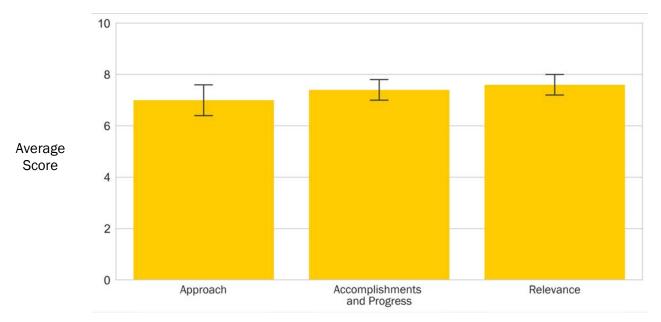
The RAFT project completed detailed characterization of 12 potential production strains and extensively tested the three best strains in long-term seasonal cultivation trials. During these trials, the team completed 272 cultivation experiments at three outdoor test bed locations during 3 years, testing seasonal effects as well as various harvest, crop protection, and strain rotation strategies. The team developed a sensor to continuously monitor cell density

| WBS:                      | 1.3.5.111          |
|---------------------------|--------------------|
| CID:                      | EE0006269          |
| Principal Investigator:   | Dr. Kim Ogden      |
| Period of<br>Performance: | 9/1/2013-5/31/2018 |
| Total DOE Funding:        | \$8,000,001        |
| Project Status:           | Sunsetting         |
|                           |                    |

and submitted a patent application. The team also developed and validated models for predicting strain performance, determining biomass productivity, and evaluating cultivation system design and operational strategies in large-scale production scenarios. In addition, the project established a detailed database for long-term cultivation trials with discrete data from the test bed cultivation experiments. The database will be maintained by the University of Arizona (https://raft.arizona.edu/cultivation-data/) for public access and continued academic evaluations. The RAFT project also produced numerous presentations, peer-reviewed publications, patents, theses, and dissertations.



Weighting for Sunsetting Projects: Approach-25%; Accomplishments and Progress-50%; Relevance-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- This project included a balanced set of tasks spanning strain optimization, scale-up, field-testing, and modeling. The team appeared to be managed well and was able to accomplish its project objectives. Results had clear relevance to the BETO mission, MYP goals, and the algal industry. Data generated in outdoor growth trials are publicly available, and the project resulted in an extensive publication list.
- The RAFT project has supported the development of an outdoor open pond algal productivity data set for use by the public. Facilities to test cultivation practices and new strains are critical to the development of the algal biofuel program. The team has taken the first step in building a database of production data collected across the U.S. Southwest. The continued funding of work for this purpose is critical to ensure resources of this nature are available to researchers working toward the achievement of MYP targets.
- This is a large consortia focusing their efforts on year-round, large-scale deployment of the top three algal strains at three outdoor test bed locations. All data accumulated during the 3 years are available to the public. The team's efforts and results will become the next baseline for future projects, just as other large consortia projects have done before RAFT and the ATP3.
- RAFT has captured and disseminated a large amount of knowledge regarding long-term algal cultivation to the broader research community. Data and key learnings are available on the website and in the final report.
- The RAFT project goals included setting up long-term cultivation processes that would provide cultivation data to understand and promote algal biomass production. This would include algal biomass production and support the BETO goals toward cost-competitive algal biofuels by 2022. To achieve these goals, the four partners put together a data management plan and information management that would support and provide data on the long-term cultivation of two strains during two seasons, the growth and productivity of three strains as a function of abiotic parameters, two strains cultivated in impaired waters and nutrient recycle, along with cultivation of two strains in three different regions. The team showed the ability to perform multiple productivity runs across the partnership sites, some showing excellent productivities. The RAFT team selected three primary strains to work with, which came from a previous program. These were cultivated during various seasons using a number of cultivation strategies, including polycultures, municipal wastewaters, saline well waters, etc. To do this, the team evolved a number of best practices in characterization and laboratory analysis, strain maintenance, scale-up, outdoor cultivation, control strategies, and molecular diagnostic tools. The RAFT final report will be a great asset for the program and a resource to the community. The team's efforts resulted in 34 publications, 37 presentations, and three patents. The RAFT program created a successful strategy to obtain cultivation data on algal biomass production. This is a major effort, which, if performed on a continuous and well-characterized basis, could feed very relevant information to growth and assessment tools critical to the program. Further, the project was able to incorporate the use of a sizable number of doctoral, Bachelor of Science, and high-school students, along with postdoctoral researchers. This inclusion will help evolve the algal workforce of the future.
- Several weaknesses were noted, primarily in the development of external efforts and the diversity of strains and length of cultivation processes.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# ALGAL BIOFUELS TECHNO-ECONOMIC ANALYSIS

## National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

The objective of NREL's algal biofuel TEA project is to provide process modeling and analysis to support algal program activities using TEA models to relate key process parameters with overall economics for cultivation, processing, and conversion of algal biomass to fuels and coproducts. By quantifying economic implications of key process metrics, TEA models highlight the technical requirements to achieve future program cost goals as well as enable a means to track progress toward these goals.

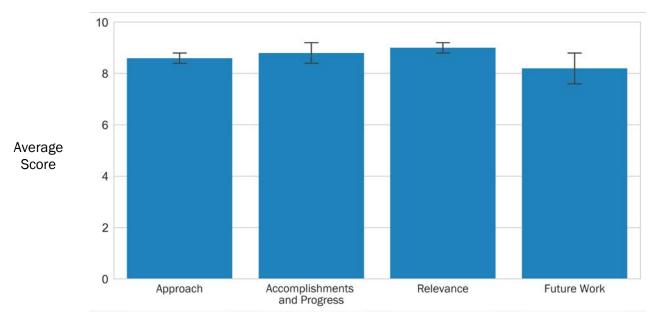
This project is highly relevant to BETO in that the project produces critical cost data tied to funded research at NREL and other collaborators, with the analyses subsequently

| WBS:                      | 1.3.5.200           |
|---------------------------|---------------------|
| CID:                      | NL0021975           |
| Principal Investigator:   | Mr. Ryan Davis      |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$1,300,000         |
| DOE Funding FY16:         | \$300,000           |
| DOE Funding FY17:         | \$300,000           |
| DOE Funding FY18:         | \$350,000           |
| DOE Funding FY19:         | \$350,000           |
| Project Status:           | Ongoing             |
|                           |                     |

exercised by BETO to guide program plans, FOA priorities, and other strategies to direct bottom-up research toward achieving cost targets that are set from the top down. This includes costs for both algal biomass production (dollars per ton) and downstream conversion to fuels (dollars per gallons gasoline equivalent), most notably to support BETO's fuel cost targets to less than \$2.5/GGE by 2030. Moreover, our work strives to address the large disparity in public claims regarding cost potential for algal biofuels by establishing rigorous, peer-reviewed cost models based on multiple input sources. This project also interfaces closely with other BETO-funded efforts, such as the DISCOVR consortium and algal test-bed partners to align TEA models with current data and future planning priorities.

# Weighted Project Score: 8.7

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

The algal TEA project has made significant achievements since the 2017 peer review, including (1) coordination of a recently published *Harmonization Report* update (joint with PNNL and ANL) quantifying opportunities for national-scale algal biomass biofuel production enabled by carbon capture and the inclusion of high-value coproducts, (2) highlighting potential paths to achieving future \$2.5/GGE fuel cost goals based on multifuel/product biorefinery concepts under NREL's combined algal processing (CAP) pathway, and (3) benchmarking progress toward those goals through SOT updates based on the latest experimental data for both algal cultivation and CAP conversion.

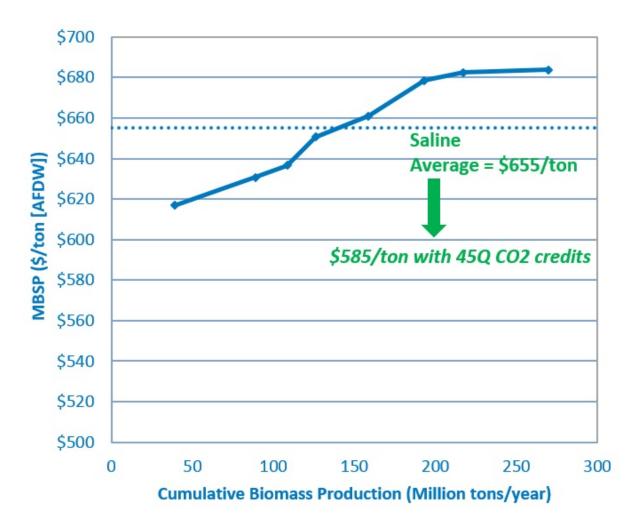


Photo courtesy of National Renewable Energy Laboratory

- Since 2010, this project has contributed much insight to algal productivity and commercialization. CO<sub>2</sub> sourcing from carbon capture in the new model is interesting because it decouples sites from certain areas. A negative is that TEA modeling is highly relevant only if the approaches are relative to the field. Siloing all growth information with one grower in one location is problematic.
- This project appears to be managed well, is meeting milestones, and continues to provide a valuable service to the community. The SOT modeling is a core tool for BETO and tracking progress toward MYP goals. The project is commended for making the underlying Excel model available to the public.

- This project directly relates to and collaborates with many other AAS projects. These TEAs provide valuable insight into identifying crucial factors across the entire algal platform that result in high-value coproducts that have the potential to reduce the gallons gasoline equivalent to achieve MYP targets.
- The current version of the TEA provides a comprehensive model for the drivers of algal fuel production. Especially of note is the inclusion of extraction and a broad diversity of coproducts. The project team continues to build on their experience strengthening the value of the TEA data to drive the prioritization of R&D activities. There is a now a great opportunity to explore the interactions between cost and value drivers as well as refine areas such as the impact of crop protection in cultivation. It will be great to see further development of the tool as stakeholders begin to use the model and provide feedback.
- The aims of this project are to provide TEA to support algal program activities. This includes the creation of process/TEA models for cultivation, processing, and conversion of algal biomass to fuels and coproducts (CAP conversion), relating key process parameters with overall economics. The approach is rigorous and builds checks to ensure credibility of models. The team has delivered several products since the last review. This project provides direction, focus, and support for industry and BETO by providing bottom-up TEA to show R&D needs for achieving top-down BETO cost goals. This project will guide R&D toward economic viability and the eventual adoption of algal biofuels/products into the U.S. market. In the future, the project will put together a number of assessments in algal cultivation on wastewater (Q1 FY 2019, complete); biomass growth versus quality modeling; FY 2019 CAP design report update; SOT benchmarking for biomass production plus CAP conversion; and TEA support for the DISCOVR Consortium.
- No weaknesses are noted.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive feedback in recognizing the utility of this project for BETO and the algal community. We hope to further develop and refine the newly published algal farm TEA tool to maximize its utility based on feedback from stakeholders. Moving forward, we also plan to continue expanding on recent efforts to further explore cost-versus-value trade-offs around algal cultivation practices, biomass growth rates, and compositional quality as applicable for conversion to fuels and value-added products.
- Regarding the comment about focusing on growth in only one location, for the SOT data sourcing this was done out of necessity given that only one location (AzCATI) has been available to furnish year-round outdoor cultivation data for informing inputs to annual SOT updates. Beyond SOT efforts, however, the algal farm TEA models have considered a large range of possible locations, e.g., as presented in the recent 2017 *Harmonization Update*, which evaluated TEA and resource potential for more than 500 plausible algal farm locations spread across the contiguous United States.

# ALGAE TECHNOLOGY EDUCATIONAL CONSORTIUM

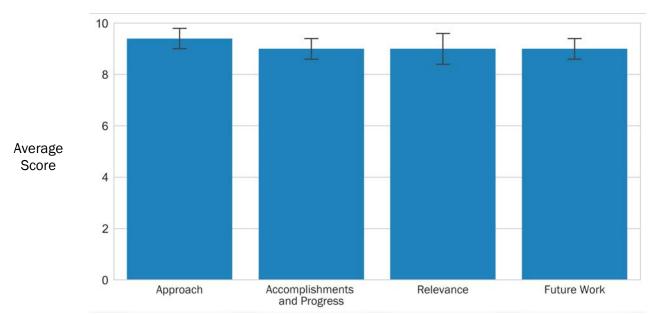
## National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

The ATEC project is a collaboration of academic and commercial algal experts that created two separate community college degrees in algal farming and biotechnology, providing an educational platform resulting in the next generation of algal professionals. Additionally, ATEC has assembled an IAB comprising senior management from leading U.S. algal companies to ensure that the ATEC skill set meets industry needs. Future efforts include formalizing relationships with more community colleges; online courses; institutionalization of the intensive, in-person laboratory courses; distribution of the Algae Cultivation Extension short-course learning modules; distribution and analysis of the second-

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generation algal-based jobs survey, targeting the biotechnology and wastewater treatment industries; and curriculum and learning outcome assessment by an external educational assessment team and the ATEC IAB. ATEC continues to engage all stakeholders and pursues collaborative relationships with algal companies, academics, and community colleges as this program grows.



#### Weighted Project Score: 9.1

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

 $\square$  One standard deviation of reviewers' scores



Photo courtesy of National Renewable Energy Laboratory

- ATEC is garnering interest for and building algal industry-related community college curricula for a variety of skills and interest to support the industry by creating a skilled workforce. The team successfully met the original intention, goals, and objective of this project.
- This project is both workforce development and a forward-facing approach to support the integration of algal biomass in the bioeconomy. The program has been very successful in terms of the reach, expansion, and feedback of program participants. This type of outreach is also valuable to spur interest in the sciences at large to ensure a strong future for algal biofuel development.
- This is a great project with a well thought-out plan to get students and teachers more interested in algae.
- The focus of this project was to improve workforce development for the nascent algal industry through K–12 and community college education. The team presented an impressive list of accomplishments, spanning Massive Open Online Courses (MOOCs); K–12 science, technology, engineering, and math materials and coursework; and community college engagement. The team presented impressive enrollment in all programs and discussed successful outcomes from early participants, such as job offers, increased salaries, and college acceptances.
- The objective of this project is to develop and implement collaborative educational programs ranging from K-12 to community college degrees and extension short courses. The approach includes online education modules, extension training, and programs in community colleges. Each area includes courses and training programs. The community college effort, in particular, sets a program that is reviewed by an IAB and independent educational assessment team. In addition, the team is setting up micro and macro algal extension short courses targeting personnel already involved in the aquaculture industry. The approach is thorough and well thought out. The team has set up collaborations with nine community college. It is notable that the online algal MOOC has received more than 3,500 students, with 17% reporting increases in pay. Further, each approach has gained acceptance in the community and is being promoted actively.

The program clearly supports BETO's efforts in helping create the workforce for the future of algae. The industry stakeholders are implementing and using the programs to educate and recruit employees. The team plans to continue the expansion of the ATEC courses to additional community colleges and have targets to reach K–12 students. The team anticipates completion of the algal biotechnology MOOC and an increased number of students taking the online modules. They will also market the extension training short courses. The team is setting up an external certification and endorsement program for college curricula. They plan to expand the curriculum into more specialized areas and expand their collaborative network. Future activities are deemed very appropriate.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# HYDROTHERMAL LIQUEFACTION MODEL DEVELOPMENT

## **Pacific Northwest National Laboratory**

#### **PROJECT DESCRIPTION**

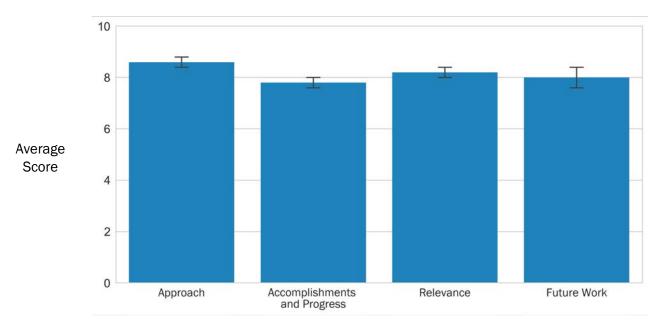
This project provides technical, economic, and sustainability analysis for algal conversion via HTL and upgrading to hydrocarbon fuels and chemicals to direct research toward high-impact results. HTL is a biomass conversion process that uses time, temperature, and pressure to produce a biocrude product that can be hydrotreated and distilled into hydrocarbon transportation fuels. A target conceptual biorefinery model was developed with researcher input and compared against benchmark models that incorporate currently achieved research results. This (1) identifies barriers, cost-reduction strategies, sustainability impacts; (2) helps to set technical and costs targets; and (3) tracks research progress.

| WBS:                      | 1.3.5.202           |
|---------------------------|---------------------|
| CID:                      | NL0025839           |
| Principal Investigator:   | Ms. Sue Jones       |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$800,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$600,000           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

A key outcome is the support for meeting the out-year conversion-only cost goals. The annual SOT is prepared reporting the modeled costs for that year and the associated research used in the modeling. Another outcome is the coordinated harmonized analysis between the PNNL work to estimate farm siting and scale; NREL analysis providing costs for cultivation, harvest, and dewatering this project; and ANL for sustainability considerations. Current and future work will focus on developing new conversion cost-reduction strategies to inform a revision to the original target case published in 2014. This will involve considering alternative HTL reactor and heat exchange configurations, valorization of aqueous phase carbon, and enhanced biocrude upgrading.

# Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $\square$  One standard deviation of reviewers' scores

Data availability is a common challenge for all analysis projects. This is mitigated by frequent, close interactions with researchers to exchange information and review sustainable cost-reduction strategies. Collaboration with analysts at ANL, INL, and NREL enhance project effectiveness. Frequent communications with BETO technology leads ensure impactful outcomes. Disseminating results for use by stakeholders is achieved through publications and presentations.

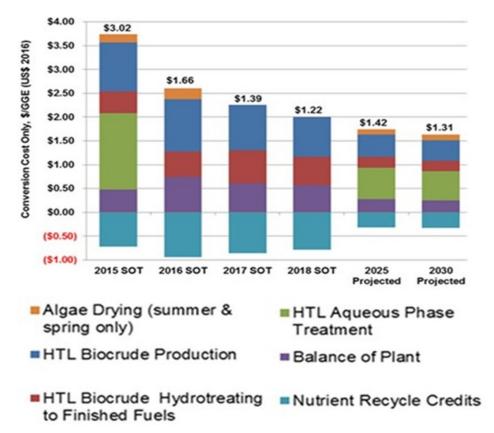


Photo courtesy of Pacific Northwest National Laboratory

- This project appears to be managed well and is on track to meet stated objectives. The project has clear relevance to the algal industry and BETO's mission. The team is encouraged to remain focused on HTL when collaborating on related modeling efforts.
- This project applies broadly across the AAS portfolio and provides valuable guidance to directing research dollars to the biggest opportunities for improvement. As experimental data continues to be generated, it will be vital that this type of analysis continues to be performed in an iterative way.
- The group would like to incorporate a lot of data from other programs, which are essential for a robust model. Working closely with the researchers helps to strongly enforce or assist in identifying future research opportunities.
- The HTL model development team has successfully partnered with key stakeholders, making great progress toward the project goals. The inclusion of statistical tests of confidence is a strength of the accomplishments to date. The project will benefit from further inclusion of value drivers, such as the interaction of nutrient recycle and the impact on biomass quality. Overall, the support toward establishing the SOT with the inclusion of multiple scenarios will be highly valuable to achieving BETO's program goals.

- The project develops process and cost models for the HTL pathway that inform the annual SOT assessments. Thus, the project has a direct impact on the economic analysis published in the BETO MYP. The team takes a rigorous analysis approach using process models in AspenPlus and cost models in Excel. The team follows technology development for the HTL R&D (R&D) portfolios and uses datadriven approaches for their models and analysis. Therefore, the project relies on the quality of the data provided by the R&D portfolio in this area. This is seen as an excellent approach to understanding the progress in R&D based on quantitative assessments of the technology, which can provide the BETO program and R&D investigators with an analysis of the impacts of technology development and gaps in research. Since the last review, the team has published an Algae Farm Cost Model and worked on the SOT model for HTL conversion using three pathways. The team has also developed a predictive algal HTL model based on biomass composition and Monte Carlo uncertainty analysis. This project directly supports the algal processing pathway toward meeting the 2030 BETO performance goal. The work develops experimentally based modeled production costs indicating high-impact research areas for conversion. The models help advance the current knowledge on the SOT for HTL processes and provide a view to gaps and areas that need further analysis and development. The team plans to work on the HTL FY 2019 SOT assessment and HTL biocrude upgrading.
- No major weaknesses are noted.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We sincerely thank the reviewers for their time and efforts in providing critical evaluation and valuable feedback.
- We plan to incorporate experimental learnings to enhance predictive modeling and uncertainty analysis, identify cost drivers, and consider alternative processing options (such as multistage HTL) that lead to improved economic viability.
- We agree that leveraging the learnings and methods by researchers outside of PNNL is important. To that end, although we based our predictive model on a consistent set of continuous experiments conducted at PNNL, we used calculation methodology found in the literature and compared our results to published HTL models (which were based on batch HTL processing at a variety of conditions).
- The PBR cost model was a preliminary estimate to consider whether there might be an advantage over open ponds. Because of the limitation of real field data viability and the large variability in data from different sources, we concluded that more data are needed. A sensitivity study for key parameters based on expert suggestions and the literature search was included.
- We agree that ash content is important for the cost analysis and that different feedstock can have different ash contents. Our algal HTL model is on a dry ash-free mass basis and thus avoids the different ash content impacts on plant scale. This is consistent with the algal feedstock flow rate information provided by NREL, which is also at a dry ash-free basis. For HTL, much of the feed ash is soluble and ends up in the aqueous phase.
- Nutrient recycling testing work is ongoing, and in the future we will have more data available for improving our cost analysis regarding the nutrient recycling credits. For ongoing work, algal cultivation, harvest, and dewatering inputs are provided by NREL from their open pond model. We do not use the PBR cost model for annual SOT assessments and reporting to BETO.
- In our ongoing and future work, we are considering coproducts from HTL aqueous in single-stage and multistage HTL to offset the high cost for algal production.

# **MICROALGAE ANALYSIS**

## **Pacific Northwest National Laboratory**

#### **PROJECT DESCRIPTION**

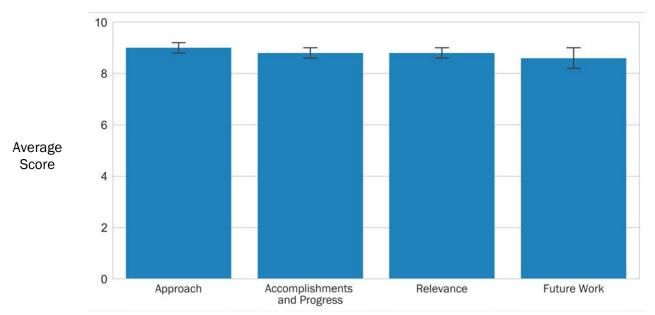
Fundamental questions must be considered for the realization of algal biofuels, including where production can occur; how much nutrient, land, and water resource are required; how much energy is produced; where ideal production sites are located; as well as trade-offs inherent to algal enterprises. The Biomass Assessment Tool (BAT) is a biophysics-based analysis platform for BETO and industry research activities to achieve high-impact objectives. The BAT provided the first highspatiotemporal, national assessment of potential open pond algal biomass production and water demand. Results from this study were referenced in a 2012 Presidential Energy Policy speech.

| WBS:                      | 1.3.5.203           |
|---------------------------|---------------------|
| CID:                      | NL0022302           |
| Principal Investigator:   | Dr. Mark Wigmosta   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$2,550,389         |
| DOE Funding FY16:         | \$800,389           |
| DOE Funding FY17:         | \$600,000           |
| DOE Funding FY18:         | \$600,000           |
| DOE Funding FY19:         | \$550,000           |
| Project Status:           | Ongoing             |
|                           |                     |

Accounting for "climatic conditions, fresh water, inland and coastal saline water, and wastewater resources, sources of CO<sub>2</sub>, and land prices" in a "national assessment of land requirements for algal cultivation" is recognized by the National Research Council as a need for informing how algal biofuels could be produced economically in the United States (NRC 2012). The BAT, developed and advanced in this project, using high-resolution spatiotemporal data and models (i.e., 30-m x 30-m topography, soils, and land cover—43.3 billion locations on the landscape; hourly meteorological data; and biomass growth simulations), is used to address these questions. Multiple criteria must be considered, and the highest biomass production site might not be the "best" site because of infrastructure, resource, or economic constraints. The BAT is uniquely suited to this task

# Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

by considering suitable lands; hourly meteorology; fresh saline alternative water demand and supply; strainparameterized biomass growth modeling in an open pond or PBR; waste CO<sub>2</sub> colocation and transport; electrical transmission lines; gas pipelines; road, rail, and barge transportation networks; known and quantified nutrient demand and available supply; and refinery infrastructure.

Results from this study are used to inform BETO's annual SOT and have resulted in 19 peer-reviewed publications of direct benefit to industry to evaluate optimal site locations, strains, and operations.

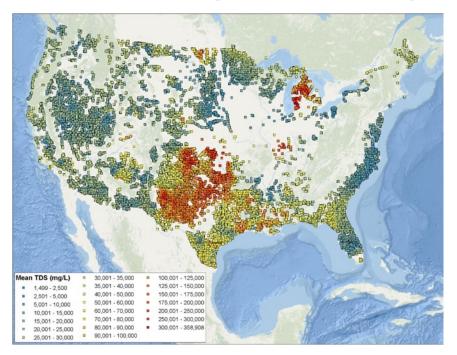


Photo courtesy of Pacific Northwest National Laboratory

- The project is considering multiple important criteria that fall outside some other models currently being developed but that have great impact on deployment and environmental sensitivities, such as water demand, biomass growth, water supply, and CO<sub>2</sub> colocation. Detailed input of groundwater availability in addition to the reduction of water stress is a big step in the right direction. Incorporating actual groundwater salinity data and depth to salinity groundwater is a great tool for any future algal farm.
- The project appears to be managed well and is on track to meet its stated objectives. The team is commended for incorporating uncertainty in its modeling efforts. Challenges and limitations were acknowledged, and the team is committed to remaining relevant to the algal industry as well as BETO's mission.
- The BAT is an incredibly useful analysis tool relevant across the AAS portfolio. The tool strives to simplify the complexity associated with considering more than 15 factors that directly impact the cost of converting algae to biofuels. The locations that result in the highest biomass productions might not actually be feasible for achieving the BETO gallons gasoline equivalent goals given the other infrastructure and resource demands to grow, cultivate, and process algae.
- The use of modeling to optimize algal productivity by exploring both geographic placement and cultivation practice is critical to achieving the BETO MYP targets. As the available data set to feed the model continues to grow and becomes more relevant to commercial production, this project team is well

positioned to incorporate these data and further refine the accuracy and utility of the tool. The team has set ambitious publication targets for the remainder of the project. Upon completion, the papers should be valuable to guide prioritization of future work in algal biomass production. There is an opportunity to explore advances in satellite technology in other fields to further enhance these modeling tools.

- The project aims to provide a national assessment of where algae production can occur, along with nutrient, land, and resource requirements. They have taken an approach that reviews the full U.S. landscape with superimposed geo-specific climate as well as resource supply and demand to map appropriate production strains through cultivation, conversion, and downstream logistics. The project addresses key barriers in biomass availability, cost, sustainable production, and resource management. The approach is to be sound and robust. Progress continues to be steady, with significant publications in the field. The team provides assessment tools for BETO that help link national resources to potential industry efforts in the cultivation and processing of algae. The project underpins national resources with key national and industry goals. This is seen as a vital part of the BETO algal program and is of great interest to stakeholders. Future work will assess sustainable collaborative BETO targets for FY 2020.
- There are no major weaknesses noted for this effort.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- For all aspects of the BAT, we develop components and a level of detail as BETO, MYP goals, and the algal research community requires. A systematic process is used to provide additional detail as the needs and data support increases. We agree that satellite imaging is a vital resource; our team has more than 20 years of experience using multimodal imaging and analytics in various domains, including land use/land cover, ground-truthing, and water resource assessments. Additional imaging applications will be investigated.
- We agree that highest productivity biomass locations might not be economically feasible because of required infrastructure. We addressed this in a collaborative study with Sapphire Energy and continue to address various aspects of this (2017 Algae Harmonization Study). We continue to evaluate PBRs and examine operational strategies to improve year-round biomass yield, along with alternative sources for water and nutrients, including colocation with wastewater treatment facilities and CO<sub>2</sub> emitters.
- Brackish/saline groundwater resources (>2.5 practical salinity unit) have the potential to reduce freshwater demand while providing a largely noncompetitive year-round supply, but they come with variable geochemistry and increased cost to acquire and manage. We used more than 500,000 brackish/saline groundwater well records to characterize depth, salinity, pH, and 18 nonorganic chemical constituents. Currently, depth and salinity data are used in strain-specific open pond productivity and blowdown calculations to quantify groundwater pumping demand/cost and volume of brine on a site-specific basis; costs for various brine disposal pathways are being investigated.
- We feel it is important to acknowledge challenges and limitations in our approach and capture of uncertainty in our results. Our evolving approach allows an end user to examine, with direct consideration of uncertainty, the likelihood that a particular action will achieve the desired result (e.g., MYP target) or which alternative shows the most promise.

# DEVELOPMENT OF ALGAL BIOMASS YIELD IMPROVEMENTS IN AN INTEGRATED PROCESS

#### **Global Algae Innovations, Inc.**

#### **PROJECT DESCRIPTION**

This project will build on the success of phase one of the GAI Algae Biomass Yield project to accelerate the commercialization of algal biofuels through the development of an integrated, economic, photosynthetic, open raceway system to produce algal oil. Two parallel pathways to a biofuel will be investigated. In the algal crude oil pathway, the dewatered algal biomass slurry is used as a feed to HTL to produce an algal crude oil and

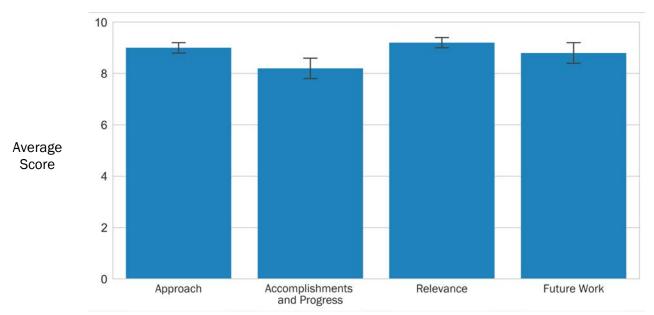
| WBS:                      | 1.3.5.211           |
|---------------------------|---------------------|
| CID:                      | EE0007689           |
| Principal Investigator:   | Dr. David Hazlebeck |
| Period of<br>Performance: | 10/1/2016-6/30/2019 |
| Total DOE Funding:        | \$6,250,000         |
| Project Status:           | Ongoing             |
|                           |                     |

recycle aqueous stream. In the algal lipid oil pathway, the algal biomass slurry is dried and the oil is extracted to produce an algal lipid oil biofuel intermediate and a high-protein algal meal coproduct. Upgrading to drop-in fuels has been demonstrated for the biofuel intermediate in both pathways. Because the algal lipid oil pathway requires lipid accumulation, the productivity is generally less than the algal crude oil pathway, but the required productivity for economic algal biofuel production is also less because the product value is greater. Thus, we have separate biofuel intermediate productivity targets for each pathway. Our phase two targets for these two pathways are:

- 5,000 gallons per acre per year at a projected minimum lipid oil selling price of \$1.60/gal
- 8,000 gallons per acre per year at a projected minimum lipid oil selling price of \$4.10/gal.

## Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 ${f I}$  One standard deviation of reviewers' scores

The project team provides expertise across the full breadth of strain development, advanced algal cultivation, open raceway contamination control, CO<sub>2</sub> supply, harvesting, dewatering, extraction, HTL, TEA, and LCA. The approach is to combine best-in-class cultivation and preprocessing technologies with some of the world's leading strain development laboratories. The strain development task is bolstered by expertise from the Hildebrand laboratory at Scripps Institution of Oceanography and the Mayfield laboratory at the University of California, San Diego. TSD Management Associates provides expertise in CO<sub>2</sub> supply, algal harvesting and dewatering, and algal drying and extraction. Texas A&M University provides algal harvesting and extraction expertise. PNNL brings HTL technology, and GE Water and Power brings membranes technology. NREL rounds out the team with extensive expertise in algal TEA/LCA.

Our phase one project resulted in tremendous productivity and preprocessing improvements in an integrated, large-scale, low-cost cultivation and preprocessing process that has moved algal technology closer to economic viability for biofuels than ever before. Phase two combines these advances with better strains through teaming with world-class algal strain developers, additional open pond cultivation innovations, and a new drying and extraction unit operation to facilitate the development of a commercial algal biofuel industry.

- The commercial ambitions of the lead participant in this team bring focus and relevance to the project objectives. TEAs are used to inform project priorities, and the project scope is aligned with the BETO mission and MYP goals. The team presented a strong technical and management approach, and most tasks are either complete or in the final stages of completion. The project was able to make several advances across the value chain and demonstrated these accomplishments in an integrated industrial environment.
- This holistic, integrated project is nearly complete and achieved all the original goals (in some cases, exceeded significantly) because of strong project management implementation. The Zobi harvester<sup>®</sup>, patent pending, is commercially available.
- The development of the harvester is a significant contribution of this work and directly focuses on reducing the cost of algal biofuel production. The team has employed several methods to improve strains and cultivation practices while developing laboratory and research pond systems designed to reflect commercial outdoor conditions. There is an opportunity to further explore the lack of translation of traits during field deployment that is critical to stability. Overall, this project is a huge success and exemplifies the opportunity in industry and academic collaborations.
- This is an interesting project with great results on non-GMO strain improvement tools. The two main tasks are completely disjointed, with the preprocessing energy task being essentially an introduction to the trademarked instrument.
- The goal of the project is to develop improved strains and cultivation methods to increase the algal biofuel intermediate yield by at least 70% and to develop a new drying and extraction technology to reduce the energy for downstream processing by at least 50% to work in an integrated outdoor system that reduces the projected minimum selling price of algal biomass by 20%. The approach benefitted from a rigorous technology assessment using cost models. The team used strain improvement by directed evolution, developed advanced cultivation methods, and evolved biomass harvesting and processing technologies to reduce costs and increase efficiencies. This is a very strong team that can appropriately take laboratory improvements into field-scaled cultivation quickly. In the strain improvement category, the team showed the ability to develop new strains with two to three times higher lipid and protein contents than wild type. Two strains were shown to have excellent temperature tolerance and high productivity of up to 29 g/m<sup>2</sup>/day with good lipid content of approximately 36%, which brings the overall projected productivity very close to the targets at 3,500 gallons per acre per year. Further, improvements in the Zobi harvester and processing systems showed an ability to reduce energy

requirements by 97%. These reductions are substantial improvements in the SOT. The project directly supports BETO goals in increasing yields of biofuel intermediate and reducing the energy requirements for processing algal biomass. The project advances the SOT significantly in all categories it is working on. The Zobi harvester technology is being made available as a commercial product.

• Few weaknesses were noted for this project because it is still developing successfully. The main goal should be to take the strains into scaled cultivation to verify modeled productivities.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The two main tasks have separate objectives, although they were integrated in that the strains and cultivation technology from the first task were used to generate the feedstock for the second task. The preprocessing energy task included both harvesting and extraction/drying. The extraction/drying included the development of multiple new unit operations that were combined in a novel way to obtain an additional 85% energy reduction in energy use relative to the reduction already attained in phase one of the Algae Biomass Yield project. The harvesting energy savings were based on the development and demonstration of the Zobi harvester technology, which is patent pending and being produced as a commercial product.

# INTEGRATED LOW-COST AND HIGH-YIELD MICROALGAL BIOFUEL INTERMEDIATES PRODUCTION

#### MicroBio Engineering, Inc.

#### **PROJECT DESCRIPTION**

Improving algal biomass productivity and composition is required to meet BETO's MYP goals of 3,700 gal of biofuel intermediate per acre-year by 2020. This project will increase the baseline yields of wild-type algal cultures by integrating several innovative processes, including:

• Improving algal strains for increased biomass productivity and/or storage of oils or carbohydrates

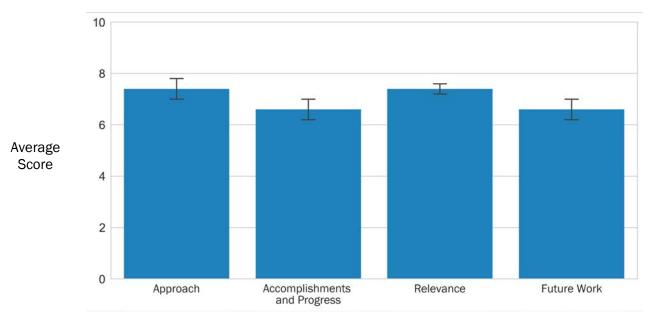
| WBS:                      | 1.3.5.243           |
|---------------------------|---------------------|
| CID:                      | EE0007691           |
| Principal Investigator:   | Dr. John Benemann   |
| Period of<br>Performance: | 10/1/2016-9/30/2020 |
| Total DOE Funding:        | \$5,000,000         |
| Project Status:           | Ongoing             |
|                           |                     |

- Increasing biomass productivity in open ponds by incorporating mixotrophic processes
- Producing biofuel intermediate by biomass extraction, fermentations, and anaerobic digestion.

Project collaborators with MicroBio Engineering Inc. (MBE) include California Polytechnic State University (Cal Poly) on strain improvements, outdoor cultivation, fermentations to ethanol and anaerobic digestion; SNL (Livermore) on genomic characterization of improved strains and protein fermentations; and Heliae Development LLC on mixotrophic cultivation of microalgae. Initial experiments by the MBE-Cal Poly team included screening 15 pure culture strains from culture collections and three native isolates in the lab for productivity and ease of handling. The eight most promising strains were further tested in outdoor wastewater ponds for productivity and culture robustness, defined as relative resistance to diseases, predation, and

## Weighted Project Score: 7.0

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

competition from weed species. Three strains from the species *Scenedesmus* obliquus (DOE 0152z), *Desmodesmus armatus* (Utex B 2533), and *Tribonema sp.* (a new isolate) were identified as promising for further study and improvement. Biomass from *Scenedesmus* obliquus (DOE 0152z) and *Tribonema sp.* were used in protein and carbohydrate fermentations, respectively; and residuals from the carbohydrate fermentations were digested anaerobically to produce methane. In phase three of this project, baseline productivity, robustness, and composition (proteins, oils, and carbohydrates) of the wild-type will be compared to the improved strains outdoors.



Photo courtesy of MicroBio Engineering, Inc.

- This ambitious project addresses a wide range of MYP goals, including as productivity, long-term cultivation, nutrient recycle, and whole biomass conversion. The team appears to be managed well, with a strong technical approach guiding project activities. The team is making strong progress on many of its original objectives. The team is encouraged to consider challenges encountered and TEA results to help prioritize future work.
- This project's integrated approach combines strain improvement, mixotrophic cultivation, and lipid extraction/fermentation downstream processing to achieve BETO's 2020 targets. If successful, it will provide more diversity to the AAS portfolio.
- The path to achieving improved algal productivity with reduced cost will require highly integrated approaches such as the one being followed in this project. The use of commercially relevant strains and focus on wastewater for cultivation is a strength for this work. It will be a significant challenge to pull together the many components of the project to achieve the goal of understanding integrated low-cost and high-yield production. This will be especially true as the improved strains enter outdoor testing. Overall, there is tremendous opportunity in this project that will be realized with strong project management support.

- This is a great project that is working to optimize several areas at once to reduce the cost of biomass production. Although all the areas the group is working on are important, there is ambiguity in how the tasks are approached and how the tasks interact with each other. The scope might be too broad for many tasks to be used to their full potential, such as the goal that states that optimization of strains will be done through non-GMO approaches, but there is a specific task that is using GMO approaches. Outdoor cultivation is getting great data on polyculture, which a novel approach to this project only, but the fermentation and HTL tasks are not using the polycultures that are being used in the field. Focusing on the tasks that are unique to this project would make the most impact on the industry.
- The goal of this project is to develop technologies that enable mature modeled annual average algal yields of 3,700 gallons per acre per year of biofuel intermediate by developing a non-GMO approach to produce strains with increased productivity for total biomass, or individually for proteins, carbohydrates, or lipids; and to demonstrate the long-term strain productivity and robustness in outdoor ponds on wastewater. The project will also leverage mixotrophy in algal cultivation to improve productivity and convert algal biomass to biofuel intermediate through fermentations of carbohydrates to ethanol and proteins to fusel alcohols and anaerobic digestion of the biomass residuals to biogas. This will be verified through TEA and LCA. This is a strong team led by industry with support from academia and national laboratories. The approach is sound and appropriate. Further, the team is progressing the goals of the project and providing appropriate quantitation through TEA/LCA modeling.
- Some weaknesses are noted in the approach to intermediates because multiple pathways are being taken for various fractions of the biomass that could interfere with each other.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the positive feedback and recognition of the multifaceted nature of the project. Revisions have been made to streamline the overall work plan following the go-no-go project review. The TEA/LCA is being updated with a sensitivity analysis performed to provide a focus for future research efforts.
- The project has an integrated approach and includes multiple processes. Our project management is focused on keeping the integrative aspects on track for a successful project.
- Project management is a significant effort in this multifaceted project; monthly conference calls and routine in-person meetings and site visits have been employed to coordinate efforts between project partners. Further, task-specific (including strain improvement, pond cultivation, carbohydrate fermentation, and anaerobic digestion) meetings are held weekly to integrate workflow. Material for the peer review was based on results acquired up to the go-no-go project review, based on which the workflow was streamlined to focus on increased productivity for total biomass, which would also improve the productivity of specific biomolecules.
- Strain improvement through genetic engineering is not part of the current project; however, results from this project could be used to inform GMO approaches in the future. In this project, improved strains developed through a non-GMO directed evolution approach are tested in the laboratory and then moved outdoors for trials in open ponds. The focus of this project is on the improvement and validation of defined strains; therefore, the native polyculture serves as a control for productivity comparisons. Further, we used the polyculture as a resource for novel strains. For example, the *Tribonema* strain currently being used in the fermentation and anaerobic digestion effort was isolated from the native polyculture.
- The initial phases of this project focused on identifying suitable strains for improvement and testing approaches for improving the productivity of specific biomolecules. At the conclusion of these trials and following the go-no-go project review, the workflow was streamlined to focus on increased productivity

for total biomass, which is necessary for the economic viability of large-scale biofuel production and would also improve the overall productivity of specific biomolecules. For example, rapid growth also leads to high protein content; therefore, the incorporation of selective pressure for enhanced faster growth and productivity is synergistic with improvements in protein content, a biofuel intermediate that can be fermented to produce fusel alcohols (as part of the SNL work).

# PRODUCTION OF BIOCRUDE IN AN ADVANCED PHOTOBIOREACTOR-BASED BIOREFINERY

#### Algenol Biotech, LLC

#### **PROJECT DESCRIPTION**

Algenol Biotech, NREL, Georgia Institute of Technology, and Reliance Industries have formed a team to advance the state of the art in algal production and downstream processing with the end goal a sustainable, economically viable biofuel intermediate (biocrude) product. The project includes examination of high-value coproduct production as a market entry strategy and to enhance the economics of a biorefinery for biofuel intermediate production. The

| WBS:                      | 1.3.5.260            |
|---------------------------|----------------------|
| CID:                      | EE0007690            |
| Principal Investigator:   | Dr. Paul Roessler    |
| Period of<br>Performance: | 10/1/2016-12/31/2019 |
| Total DOE Funding:        | \$4,239,755          |
| Project Status:           | Ongoing              |
|                           |                      |

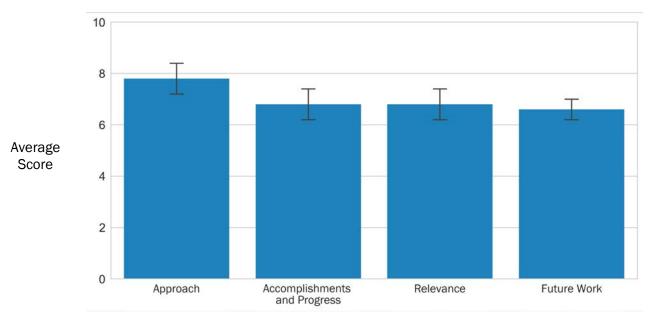
project targets innovations in biology, operations, and engineering. It builds on the experience gained at Algenol in its DOE-funded project for an integrated biorefinery for ethanol production.

The goals of the project are: biofuel intermediate productivity greater than 4,000 gallons per acre per year of biofuel intermediate on an annualized basis; energy-efficient innovations in biomass harvesting, dewatering, and HTL, resulting in an energy expenditure less than 10% of the biofuel intermediate energy content and a carbon footprint reduction of more than 60% compared to fossil alternatives; and a comprehensive TEA that identifies limiting factors for commercial viability of a PBR-based biofuel product.

The project is on track to achieve the overall goals. Strain development efforts have resulted in the identification of a strain (AB1166) that, relative to existing strain AB1, exhibits a 10%–15% increase in productivity and also results in cultures with greater than 50% reduction in viscosity at low shear rates that

# Weighted Project Score: 7.0

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

improve harvesting efficiency; these results represent the achievement of key phase two milestones. Progress has also been made in altering the biochemical composition of algal biomass to improve the yield and quality of biofuel intermediate produced via HTL. These strain enhancements plus improved outdoor cultivation practices, including semicontinuous operation, have increased areal productivity by nearly 80% over the established baseline productivity; this result greatly exceeded the 30% improvement metric required to achieve a "go" decision to enter phase three of the project. The annualized biomass productivity achieved (26.8 g/m<sup>2</sup>/day ash-free dry mas), coupled with HTL conversion yields realized thus far (36% biofuel intermediate), results in 3,900 gallons per acre per year of biofuel intermediate, exceeding the FY 2020 BETO goal of 3,700 gallons per acre per year of biofuel intermediate.

Significant progress has also been demonstrated in PBR and large-scale production system design, operability, and cost reduction. A 24,000-L production module of interlinked PBRs was constructed and successfully operated. The productivities obtained convincingly demonstrated the scalability of laboratory measurements to large-scale outdoor operations covering a culture volume range of 2 mL to more than 20,000 L. The system was used to cultivate *Arthrospira platensis (Spirulina*), an industrially relevant cyanobacterium and source for phycocyanin, an approved blue food colorant that Algenol is developing as a risk-reduction strategy for future biofuel projects and as a potential business opportunity. A key project milestone to develop phycocyanin extraction and purification technologies was achieved ahead of schedule, and product samples have received positive feedback from potential customers.

The production and downstream operations data generated in this project are being used to conduct and refine TEA and LCA to provide research guidance to reduce the costs and environmental footprint of algal biofuel and coproduct manufacturing plants. These assessments will enable detailed comparisons of PBR versus open pond production systems.

The progress in this Algae Biomass Yield Phase Two project addresses many barriers identified for the AAS R&D program and are directly relevant to achieving the established BETO goals associated with large-scale biofuel production and cost reduction.



Photo courtesy of Algenol Biotech, LLC

- The project appears to be managed well with an appropriate technical approach for project objectives. The project contributes to the BETO mission and MYP goals. Tasks include demonstration at meaningful scales in an industrial environment, and the team indicated that future coproduct development work will de-emphasize very niche products in favor of those with larger markets and moderate cost targets.
- Algenol is leading a fully integrated project to optimize algal strains, PBR configuration, downstream processing, and coproduct extraction to improve the economics of PBRs. The team shows strong project management coordination for such an ambitious project.

- The production of biocrude in an advanced PBR-based biorefinery project leverages significant commercial experience and enables access to experimentation at the industrial scale. The team has identified a very interesting strain with high tolerance to temperature that might have broad utility in algal biomass production. The project has established clear target goals with coproduct targets that will improve the economics of the process. The market opportunity for the coproduct and impact on potential for fuel production should be continually assessed to maintain commercial relevance.
- Focusing on the validation of results will add tremendous value to the project because currently there is much ambiguity on how the data are being generated and how their improvements are being measured.
- The goal of the project is to develop highly productive algal strains, a cost-effective PBR-based production system, enhanced cultivation practices, energy-efficient downstream processes, and a coproduct strategy that will advance the technology needed for economic, large-scale algal biofuel production. The approach taken includes strain development, cultivation engineering, downstream processing, and plant integration. A phycocianin coproduct intermediate supports the economic viability. This is a strong industry-led team with national laboratory and academic participation.
- A few weaknesses were noted that are associated with support of the modeling efforts with year-round cultivation at scale of one or two of the most productive strains.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Regarding the selection of phycocyanin as a coproduct, we fully recognize that the limited, albeit growing market would be saturated with a large-scale biofuel facility. As stated in the original proposal, phycocyanin production represents a market entry strategy. We expect the favorable economics of phycocyanin production to facilitate project financing for an initial, small-scale biofuel facility, which could be enlarged as the technology for biofuel production advances. Mid-volume, mid-value coproducts are also being evaluated at Algenol and will be incorporated as a scenario in our TEA modeling.
- With respect to the desire for further validation of results, productivity modeling, and general aspects of system performance, we would like to point out that the Algenol productivity model takes into account actual weather station data (light and temperature) and photosynthetic parameters derived from laboratory and small-scale outdoor experiments (quantum yield, photosaturation, light acclimation, respiration).
- Our outdoor growth data for *Arthrospira* is essentially year-round (at scales up to 24,000 L) and confirms the modeling results. By the end of the project, we will have data for *Cyanobacterium* from several seasons of the year and expect additional validation of our modeling approach. Further validation comes from year-round productivity data from past work with ethanol-producing *Cyanobacterium sp.* AB1. In addition, we have excellent agreement with PNNL with respect to laboratory performance parameters for AB1, the strain we provided to PNNL for inclusion in their DISCOVR project. The final project report will include extensive information on the development and validation of the productivity model, including indoor and outdoor testing at various scales and at several sites around the world (e.g., India, Arizona, Florida).

# REWIRING ALGAL CARBON ENERGETICS FOR RENEWABLES (RACER)

## National Renewable Energy Laboratory

## **PROJECT DESCRIPTION**

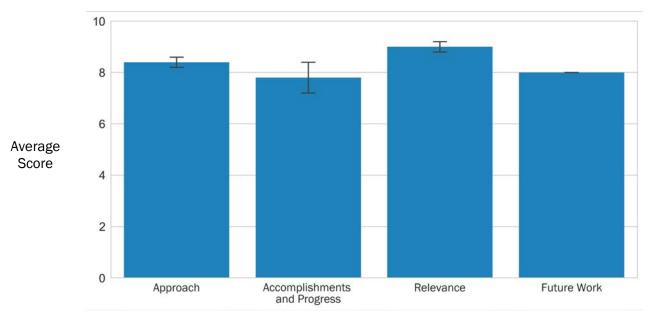
Critically needed improvements in biomass and biofuel intermediate productivity can be made by addressing fundamental inefficiencies in algal carbon conversion efficiency to biofuel feedstocks, cultivation performance, as well as the conversion to fuel intermediates. Algal photosynthesis is, at best, able to convert incident light energy to biomass at a carbon conversion efficiency of approximately 5%–7%, whereas downstream conversion to

| 1.3.5.270           |
|---------------------|
| NL0032697           |
| Dr. Lieve Laurens   |
| 8/1/2017-12/31/2020 |
| \$5,000,000         |
| Ongoing             |
|                     |

fuel intermediates in the current design process falls 15%–-25% short of its maximum potential because of inefficiencies along the pathway. There is room for improvement to achieve much higher biomass and biofuel intermediate yields through manipulating the basic biological processes of photosynthesis and carbon sink metabolism in the cells and integrating the upstream cell biology with downstream conversion process improvements. This presentation covers recent progress in the RACER project consortium and focuses on a means to address these carbon conversion inefficiencies in a pathway from algal biomass to a trifecta of fuel intermediates, ethanol, lipids, and green biocrude in a coordinated and integrated manner. The goal of this work is to engineer a single, commercially relevant algal species *Desmodesmus armatus* (SE 00107) to demonstrate both areal biomass productivity improvements of 64% relative to a conservative baseline of biomass productivity with an overall doubling of the fuel intermediate yields. The new algal biorefinery paradigm embodied in the RACER approach opens opportunities for algal engineering beyond efforts typically targeted solely at lipid content or improved light harvesting efficiency. We present progress on parallel

# Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

approaches toward improved (1) photosynthetic carbon conversion efficiency through the elimination of wasteful diversion of energy during photosynthesis and increasing carbon flux through carbon assimilation by increasing the transitory carbon storage in the cells; (2) outdoor operation and nutrient management strategies; and (3) fundamental operational efficiency of downstream conversion and extraction in a CAP approach to fuel and high-value product intermediates.

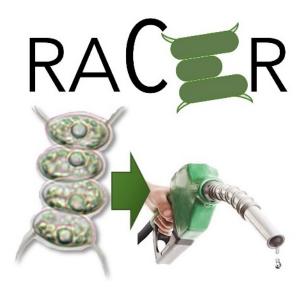


Photo courtesy of National Renewable Energy Laboratory

- The RACER project aims to improve the productivity and biomass composition of a commercially relevant algal strain directly aligning with the MYP target goals. The team has overcome several challenges around the production of the transformants as well as production of biomass. The learnings from this project are likely as valuable as achieving the targeted goals. A clear strategy for 2020 including risk mitigation steps has been established by the team.
- This ambitious project clearly addresses BETO priorities and MYP goals. The team has been able to stay largely on track despite reductions in project budget. Accomplishments were explained in detail and matched original objectives. The team is encouraged to incorporate TEA in the prioritization of future tasks.
- This ambitious project attempts to integrate and coordinate strain engineering, cultivation operations, and conversion engineering of a robust, industrially relevant algal strain. Significant progress has been made to date, including contributing to the FY 2018 SOT less than halfway through the project.
- This is a good strategy to boost production. The multifaceted approach using multiple targets for improvement increases the chances for hitting strain enhancements. The timeline and goals to accomplish are well thought out and achievable within the period set forth. The project is yielding good results, but long-term yields are potentially being stunted because assumptions are being made for the amount of time that the culture might be induced for lipid accumulation at production scale.
- The team will improve the overall carbon-to-fuel intermediate productivity for a biorefinery using *Dromogomphus armatus* as a production species to reach at least 3,900 gallons per acre per year. This will be done through improvements in photosynthetic carbon conversion efficiency through random

mutagenesis and targeted engineering; cultivation management advances through the implementation of informed permutations of operations and nutrient management; and tailoring and optimizing conversion processes to extractable lipids, carbohydrate-derived fuel intermediates, and HTL biocrude from protein residue. This strain shows good productivity in year-round cultivations. The Sapphire project has made available the strain along with genome and transformation and mutagenesis protocols. The project tasks are specific and well defined. The transformation of D. armatus showing cNAT resistance and mCherry reported has been demonstrated by the team. The team has shown successes with overexpression transformants and has identified additional genes to effect photosynthetic apparatus. Mutagenesis has yielded one mutant with a 50% increase in lipid and no reduction in growth rate. The project's summer cultivation productivity has been included in the BETO FY 2018 cultivation SOT. The team has also demonstrated good efficiencies in fermentation and has engineered Zymomonas mobilis to metabolize mannose to 2,3-Butanediol. The team has demonstrated an extraction of lipids with a cosolvent and more than 30% yield on HTL of protein-rich stillage. They are working on the TEA/LCA of the integrated process. Progress to date is deemed reasonable. This is an end-to-end project aiming for carbon conversion efficiency improvements by coordinating photosynthesis and carbon sink engineering as the basis of biomass accumulation and biofuel production. The project is well aligned with BETO's AAS Program and likely to contribute significantly to additional improvements in the SOT. The project will continue to work on the major tasks and address milestones and has go-no-go decision points.

• No weaknesses are noted.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their complimentary feedback on this project. Several comments by the reviewers were reiterated, and we appreciate the opportunity to respond to some of the main questions, in particular on the integration of TEA in our decision-making process. When we planned this project, we included the TEA group to help prioritize different tasks. By targeting biomass productivity in the main tasks of this project, we directly address the primary factor driving the biomass selling price and, by extension, fuel selling price, one of the metrics called for in the Algae Biomass Yield Phase 2 FOA announcement. Further, the respective fraction yield improvements in the CAP (fermentation of soluble sugars, extractable lipids, and protein to HTL crude) that we are targeting in the conversion task were calculated to have a significant impact on the projected biofuel yield and price. We are continuously communicating progress with the TEA team, and a comprehensive analysis of the quantitative improvements achieved in the first phase of this project will be presented to the interim verification team.
- We want to clarify our experimental and cultivation approaches in that this work does not include a dedicated lipid induction phase during the outdoor cultivation experiments. The targeted metabolic engineering tools that are in the process of being developed will focus on genetic targets impacting central carbon assimilation and carbohydrate storage. It is thus much more likely that carbohydrates will accumulate prior to lipids, which will function more as overflow storage of metabolic energy. The outdoor cultivation approach on nutrient and pond operational management will include different permutations on the harvesting strategy, e.g., keeping the cultures at high cell density but low depth will increase light stress with the potential to rapidly shift the composition and maximize biomass productivity, both of which would be highly beneficial in the overall integrated process operations.

# PRODUCING ALGAE FOR COPRODUCTS AND ENERGY (PACE)

## **Colorado School of Mines**

#### PROJECT DESCRIPTION

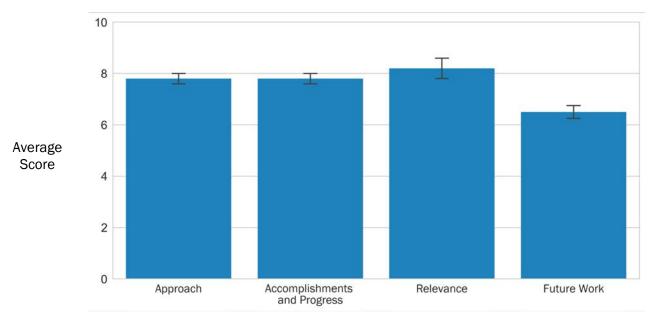
Producing Algae for Coproducts and Energy (PACE) is a consortium of academic, industrial, and national laboratory partners that is addressing major technological challenges that remain for the sustainable and economic production of algal biofuels at scale. Beginning with the best technologies developed through the National Alliance for Advanced Biofuels and Bioproducts (NAABB) consortium, our overall objectives are (1) to reduce the

| WBS:                      | 1.3.5.300            |
|---------------------------|----------------------|
| CID:                      | EE0007089            |
| Principal Investigator:   | Dr. Matthew Posewitz |
| Period of<br>Performance: | 10/1/2015-3/31/2019  |
| Total DOE Funding:        | \$9,000,000          |
| Project Status:           | Ongoing              |
|                           |                      |

cost of fuel produced from algae; (2) to enhance the stability and performance of integrated algal biofuel production systems at scale; and (3) to enhance the energy return on investment for algal biofuel production while reducing CO<sub>2</sub> emissions, water consumption, and demands for fertilizer supplements. Specifically, we are targeting improved biomass yields, the production of value-added coproducts, and the optimization of process integration. Reliance Industries is our primary cost-share partner, enabling access to their large and integrated algal biofuel facility in Gagva, India. Targeted goals include 25 g/m<sup>2</sup>/day algal biomass yields, the production of coproducts (guar gum and phenylethanol), an energy return on investment of three, and a carbon index of 55 grams CO<sub>2</sub> per megajoule. At the Gagva facility, yields of approximately 20 g/m<sup>2</sup> can be achieved and integrated with harvesting and processing to algal biocrude. Liter quantities of photoautotrophic algal biocrude are readily being produced, and a suite of processing approaches are being investigated for conversion to fuels and engine testing. The NAABB identified the green alga *Chlorella sorokiniana* as a promising algal biofuel candidate. The PACE consortium has developed a suite of genetic manipulation tools to enable *C. sorokiniana* strain engineering. Overexpression of sucrose nonfermenting (SNF)-related kinase

## Weighted Project Score: 7.6

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

(SNRK) in C. sorokiniana resulted in lines with elevated rates of photosynthetic activity and higher levels of starch accumulation relative to wild-type control cells in solar-simulating environmental PBRs. A TERA was submitted and approved by the Environmental Protection Agency. Testing of this promising engineered strain for improved biomass phenotypes at the AzCATI is anticipated in 2019. Putative genes for the generation of the coproducts guar gum and phenylethanol were transformed into C. sorokiniana, and phenotypes are being analyzed. Multiple lines produced phenylethanol, and process conditions are being optimized to maximize yield. Strains expressing phosphite oxidoredutase and Pyrroline-5-carboxylate synthase (P5CS, a key enzyme controlling proline levels) were successfully attained, and phenotypes show potential applications in crop protection. The PACE consortium is also investigating marine species of Nannochloropsis that have established genetic tools. Constructs overexpressing a suite of carbonic anhydrases, bicarbonate transporters, and Calvin-Benson cycle enzymes were successfully generated, and biomass phenotyping is underway. In sum, multiple hypotheses are being tested to engineer biomass improvements. Kilogram quantities of algal biomass are being generated and used to optimize the processing of biomass to fuels, including two-stage hydrothermal processing to recover carbohydrates. Additionally, a suite of promising coprocessing and blending approaches are being investigated to generate transportation fuels. Last, an end-to-end PACE Aspen model for fully integrated TEA and LCA was developed.

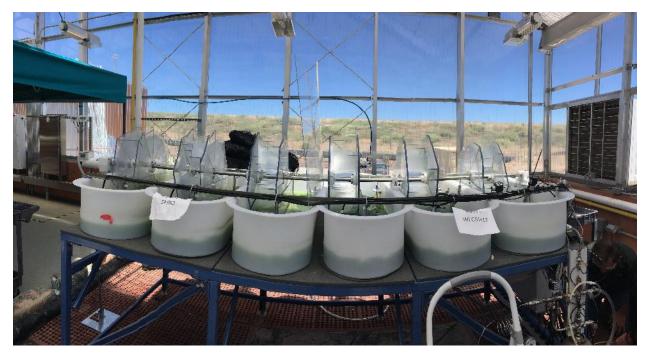


Photo courtesy of Colorado School of Mines

- This broad partnership includes academic, federal laboratories, and industry working together to address a set of barriers that is clearly aligned with BETO priorities and MYP goals. The team has been able to accomplish a wide range of its planned tasks, including strain improvement and demonstration in an outdoor industrial environment. An ambitious set of activities remains prior to project completion, and the group believes a no-cost extension can be used to accomplish all tasks.
- Despite encountering many roadblocks, the PACE project has now delivered on multiple fronts toward the MYP targets. The access to extracted oil from a large-scale facility is a great asset to this program. Several high-potential modified strains have been developed to improve productivity, enhance crop protection, and produce potentially valuable coproducts toward economic targets of algal biofuel

production. The team now aims to stack these traits and run field trials to validate the observed laboratory performance. Given the progress made to date, I expect that the team can deliver on the significant challenges ahead.

- The project has made good progress in the genetic modification field, yielding much higher growth rates and carbohydrate production. Focus on validation of results will add tremendous value to the project.
- This ambitious project set out to investigate multiple aspects along the process flow (genetic engineering, cultivation, harvesting, and downstream processing) to increase algal biomass production to more than 25 g/m<sup>2</sup>/day while reducing costs by more than two times. Significant results have been demonstrated (and the remainder are planned to be completed by the end of the extension), whereas other objectives have been de-emphasized because of time and resource constraints (which is not entirely surprising given the enormous scope of this project).
- The main goal of the PACE project is to improve areal biomass productivities and enable the production of high-value coproducts using strain engineering. Further, PACE will integrate the cultivation and processing steps and demonstrate a reduction in the overall cost of algal-derived biofuel. The project set several objectives and metrics to determine progress and success factors. This is a large effort, under the TABB FOA, with a very strong partnership including academia, national laboratories, and industry. The management team demonstrated good practices for regular meetings and reporting. The team efforts addressed technical challenged in genetic transformation, gene stacking, producing biofuels and valuable products simultaneously, crop protection, and efficient harvesting. The success indicators for the project are clearly delineated and measurable. The effort is very well defined, and the team is deemed as very strong, involving key players in all areas of performance.
- Several areas deemed as possible weaknesses in the approach and future efforts are noted. The team is encouraged to develop focused strategies that can determine potential failures and develop mitigations, if necessary.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

We thank the program reviewers and DOE for their time and constructive advice regarding the PACE project. As noted by the reviewers, the national laboratory, academic and industrial partners on the research team have made significant progress in several challenging areas and MYP goals. Specifically, several successful strain engineering targets were achieved, and these strains are enabling the consortium to test strategies aimed at biomass yield improvements, coproduct production, and enhancing culture stability. Additionally, promising and novel culturing, processing, and fuel conversion strategies are being developed. Comprehensive TEA/LCA demonstrate that we are now approaching several of the project's programmatic economic targets. As noted by the reviewers, trait stacking and outdoor testing/validation of engineered strains remain a significant challenge. The SNRK expression line has been approved for outdoor growth at AzCATI, and these trials are currently being planned and initiated. Trait-stacking efforts are ongoing with a focus on P5CS/SNRK. A primary objective in the summer trials is to attain outdoor growth data for SNRK grown at AzCATI and determine whether enhanced biomass yields are attained from this transgenic line. These areas are among the primary foci of the no-cost-extension period, and we are confident that we will be able to insert multiple genes into C. sorokiniana (trait stacking) and test an engineered strain in the AzCATI outdoor test bed. In sum, many programmatic goals have been attained, and the no-cost-extension period should enable the completion of most of our remaining objectives.

# MARINE ALGAE INDUSTRIALIZATION CONSORTIUM (MAGIC): COMBINING BIOFUELS AND HIGH-VALUE BIOPRODUCTS TO MEET RFS

#### **Duke University**

#### **PROJECT DESCRIPTION**

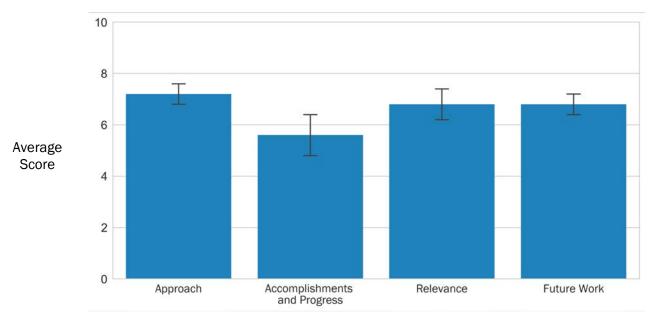
The objective of this project is to demonstrate, using a multiproduct commercialization path, an algal biofuel at commercial scale with a positive energy return that achieves the Renewable Fuel Standard, (RFS), and sells at a price of less than \$5/GGE. The approach is founded on our achievements to date in algal biofuel and coproduct development, and it is aimed at increasing the overall algal product value (and thereby decreasing the net cost of algal hisfaul). This project is driven hyperbolic product and the product of the

| WBS:                      | 1.3.5.310           |
|---------------------------|---------------------|
| CID:                      | EE0007091           |
| Principal Investigator:   | Dr. Zackary Johnson |
| Period of<br>Performance: | 10/1/2015-8/31/2019 |
| Total DOE Funding:        | \$5,240,313         |
| Project Status:           | Ongoing             |
|                           |                     |

biofuel). This project is driven by product specifications in four markets, including (1) drop-in fuels, the foundational product; (2) a salmon feed ingredient equivalent to fishmeal in protein content and biochemically superior to soy and other protein meals; (3) a poultry feed ingredient that is superior to commonly used soymeal in protein content and contains other important micronutrients; and (4) a dairy food replacement for human food, equivalent in protein content to soy, rice, and other plant-based replacement products but superior in the content of essential fatty acids and micronutrients. All three coproducts approximately scale with fuel and thus are viable solutions on the commercial scale. To demonstrate product value for each product, we will (1) define product specifications and commercialization opportunities in collaboration with commercial partners; (2) match product specifications for these products as closely as possible to marine algal strains from our highly characterized collection of hundreds of strains; (3) cultivate selected strains at the bench scale to

# Weighted Project Score: 6.6

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 ${f I}$  One standard deviation of reviewers' scores

provide a comprehensive assessment of their performance against product specifications; (4) cultivate, harvest, and process approximately 10 strains in quantities of approximately 50 kg per strain, providing ample material for product development trials; and (5) continuously evaluate commercialization potential by using economic and LCA iteratively as a design tool at each stage to guide product development. Results from this project will have a substantial impact on the environmental and economic benefits of algal biofuels. The proposed bioproducts, to the extent they replace current feed and energy crops, would also confer a significant increase in benefits with regard to recognized greenhouse gas emissions by virtue of the positive effect of indirect land use change brought about by the 50-fold land-use intensification achieved by algal production. Core members of this consortium—who have during the past 10 years taken the initial leading steps in product development and demonstration with substantial industry and government support—are joined by members with specific commercial interests in the development of biofuels, aqua feeds, poultry feeds, and human foods. The combined abilities and experience of this proposed consortium position it for success and will broadly benefit the U.S. algal industry, from growers of algae, to developers of harvesting and extraction tools, to end users of bioproducts.

### OVERALL IMPRESSIONS

- This project identified a broad set of goals that were directly related to the BETO mission and MYP goals. Many tasks remain prior to project completion, and the group plans to use a no-cost extension and several mitigation steps to complete the work. The team is encouraged to report quantitative productivity and coproduct targets (value and specifications) to enhance the relevance and future value of their work to the broader algal community.
- The project seems to have a thorough process for validation. An assessment of the barrier to enter certain markets and the cost required to meet certain product specification is lacking detail.
- This project is identifying, demonstrating, and validating high-value coproduct production by investigating optimizations along the entire process chain (from strain selection, to cultivation, to end-use applications). Preliminary results are encouraging, but significant gaps will require more trials and market research of the intended end use to build a meaningful TEA/LCA model.
- The MAGIC team has worked through many challenges associated with a complex project spanning geographies and objectives. The construction and operation of the research ponds at Duke University is a highlight of the work to date. The ability to produce both animal feed and fuels from algal biomass significantly improves the economics and near-term commercialization opportunity. The team has identified promising strains with the potential of improving animal feed quality and has now initiated the feeding trials. The results of this work will be critical to understanding the value and economic potential of this approach.
- The main goals of the MAGIC consortium are to increase the valuation of lipid-extracted algae by testing across algal strains and coproduct types. Specifically, the team will develop 10 strains to meet product requirements, produce 30 kg–50 kg of 10 strains for algal feedstock for biofuels and feed ingredients, assess product efficacy and value, and analyze the potential of commercial-scale facilities. The team comprises academic and commercial partners. The team developed a method for ranking strains according to key variables, e.g., growth rate, sinking index, along with ash, lipid, and protein content. Ten top strains were selected from a large culture collection for scaled cultivation. The team delivered more than 120 kg of biomass of four strains. Product characterization and assessment were performed for three strains; two of these strains had poor recovery. An Xcel-based formulator was used to develop optimal feed compositions for further testing and analysis. TEA/LCA were performed on the strains. The results showed large variabilities in the final values.
- Several weaknesses were noted, mostly associated with the lack of optimization of processes, which causes large variations in TEA/LCA analyses.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipient choose not to respond to the reviewers' overall impressions of their project.

# CONVERSION RESEARCH AND DEVELOPMENT

The T

PROGRAM AREA

# INTRODUCTION

### CONVERSION R&D SUPPORT OF OFFICE STRATEGIC GOALS

The strategic goal of the Conversion Research and Development (R&D) program is to develop efficient and economical biological and chemical technologies to convert biomass feedstocks into energy-dense liquid transportation fuels, such as renewable gasoline, diesel, and jet fuel, as well as bioproducts, chemical intermediates, and biopower. To achieve this goal, a variety of conversion technologies are being explored that can be combined into pathways from feedstocks to products, including gasoline, diesel, jet fuels, biochemicals, biopower, and other enabling bioproducts.

While Conversion R&D is managed as a single platform, the large number of projects funded by this area could not fit in a single session over the course of a week. Projects were grouped into seven smaller sessions in order to better target reviewers with specific expertise, and to allow the full review to take place in the time allotted. The seven sessions were as follows:

- Agile BioFoundry
- Biochemical Conversion
- Carbon Dioxide Utilization
- Catalytic Upgrading
- Lignin Utilization
- Performance Advantaged Bioproducts and Separations
- Waste-to-Energy.

To the extent possible, projects were grouped with those utilizing similar technologies, though the Bioenergy Technologies Office (BETO) recognizes that many projects contain elements that could fit into multiple sessions. Each project was only reviewed in one session.

### CONVERSION R&D SUPPORT OF OFFICE PERFORMANCE GOALS

The overall goal of Conversion R&D is to develop technologies that enable a reduction in the estimated modeled mature technology processing cost of converting algae, lignocellulosic biomass, or waste resources to hydrocarbon fuels and bioproducts, while maximizing the renewable carbon in the desired products. The ultimate aim for all processes is an increase in both carbon and energy efficiency relative to the theoretical maximum. To benchmark technical progress against the barriers to overcome, BETO conducts techno-economic analyses and life cycle assessments of a few representative pathways that link conversion technologies from feedstock to end product. These analyses result in the following Conversion R&D performance goals:

- By 2021, complete the research necessary to verify in 2022 a mature modeled minimum fuel selling price (MFSP) of \$3/gasoline gallon equivalent (GGE) or less for a complete technology pathway to hydrocarbon biofuel and, where appropriate, a coproduct, with a minimum 50% reduction in emissions relative to petroleum-derived fuel.
- By 2029, complete the research necessary to verify integrated systems research at engineering scale for hydrocarbon biofuel technologies at a mature modeled MFSP of \$2.50/GGE using economically advantaged feedstocks to produce renewable fuels and coproducts.

### CONVERSION R&D APPROACH FOR OVERCOMING CHALLENGES

Conversion R&D has identified the following challenges and barriers across the supply chain as key hurdles to achieving the goals outlined above. Some challenges are shared across other platforms.

### Pathway-Specific Barriers

- Defining metrics around feedstock quality
- Efficient preprocessing and pretreatment
- Process development for conversion of lignin
- Advanced bioprocess development
- Improving catalyst lifetime
- Increasing the yield from catalytic processes
- Decreasing the time and cost to develop novel industrially relevant catalysts
- Gas fermentation development
- Development of processes capable of processing high-moisture feedstocks in addition to conventional anaerobic digestion
- Identification and evaluation of potential bioproducts
- Developing methods for bioproduct production.

### **Enabling Research Barriers**

- Decreasing development time for industrially relevant microorganisms
- Current reactors not designed to handle harsh conditions inherent to converting biomass feedstocks
- Multiscale computational framework toward accelerating technology development
- Selective separations of organic species
- Selective separations of inorganic contaminants.

The Conversion R&D approach for overcoming these conversion challenges and barriers is being addressed by a combination of specific, pathway-focused projects with industry, universities, and at individual U.S. Department of Energy national laboratories, and by bioenergy consortia that combine the unique capabilities of several national laboratories in collaboration with industry via technical advisory groups and joint projects.

# AGILE BIOFOUNDRY CONSORTIUM

TECHNOLOGY AREA

R

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# INTRODUCTION

The Agile BioFoundry Consortium (ABF) Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 10 projects were reviewed in the ABF session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$52,040,000 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 6.1% of the BETO portfolio reviewed during the 2019 Project Peer Review. During the Project Peer Review, the principal investigator (PI) for each project was given 10–50 minutes (depending primarily on the funding level and priority with respect to near-term goals) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the ABF, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. Jay Fitzgerald as the ABF Technology Area Review Lead, with contractor support from Mr. Clayton Rohman (Allegheny Science & Technology). In this capacity, Dr. Fitzgerald was responsible for all aspects of review planning and implementation.

# **ABF OVERVIEW**

Currently, the industrial biotechnology sector often scales up processes on a case-by-case basis, without tools that can be extrapolated to multiple host organisms, pathways, and applications. The ABF develops and integrates tools, technologies, software, and instrumentation across the DOE national laboratory system for the robust and predictive engineering of biological systems to improve efficiencies in the conversion of biomass to fuels and products. The ABF creates new pathways and organisms engineered to produce biofuels and renewable chemicals from domestic, non-food lignocellulosic biomass. Central to this effort is development of robust host organisms and new microbiology techniques, in conjunction with databases and machine-learning methods, which enable automated design of bioprocesses with predictable performance and scaling, as well as significantly increased conversion efficiency. These efforts are incorporated into a Design-Build-Test-Learn (DBTL) methodology to enable faster, more efficient bioproduct development cycles.

The ABF is a virtual consortium organized around six tasks: Design-Build-Test-Learn, Integrated Analysis, Host Onboarding, Process Development and Scale-Up, Industry Engagement, and Management. To demonstrate the effectiveness of the ABF, strategic target-host pairs with relevance to the bioeconomy are pursued by the consortium in addition to ten industry-led partner projects. The ABF also uses its expertise in host development to contribute to BETO's State of Technology for Biochemical Conversion, in collaboration with the Biological Upgrading of Sugars and Targeted Microbial Development projects.

The ABF session review panel reviewed the six tasks of the ABF, as well as overall direction, management, and industry engagement and partnerships.

# **ABF REVIEW PANEL**

The following external experts served as reviewers for the ABF Technology Area during the 2019 Project Peer Review:

| Name            | Affiliation                                |
|-----------------|--|
| Ben Gordon*     | Broad Foundry                              |
| Matthew Tobin   | Matthew B. Tobin Consulting                |
| Farzaneh Rezaei | Pivot Bio                                  |
| Chris Rao       | University of Illinois at Urbana–Champaign |
| Steve Van Dien  | Persephone Biome, Inc.                     |

\*Lead Reviewer

# TECHNOLOGY AREA SCORE RESULTS

| Average Weighte   | d Scores | s by Pro | ject            |     |     |
|---|----------|----------|-----------------|-----|-----|
| ABF Consortium (2.5.3.104f): ABF - Integrated Analysis                        |          |          |                 |     | 9.1 |
|   |          |          |                 |     |     |
| ABF Consortium (2.5.3.104h): ABF - Process Integration<br>and Scale-up        |          | 1        | 1               |     | 8.8 |
| ABF Consortium (2.5.3.104a): ABF - Overview                                   |          |          |                 |     | 8.8 |
| ABF Consortium (2.5.3.104i): ABF - Industry Engagement                        |          |          |                 |     |     |
| and Outreach  |          |          |                 | 8   | 8.6 |
| ABF Consortium (2.5.3.104e): ABF - Design-Build-Test-<br>Learn Infrastructure |          |          |                 | 8   | .5  |
| ABF Consortium (2.5.3.104c): ABF - Rhodosporidium                             |          |          |                 | 8.3 | 2   |
| toruloides  |          |          |                 | 0.0 |     |
| ABF Consortium (2.5.3.104j): ABF - Directed Funding<br>Opportunity Management |          |          |                 | 8.2 |     |
| ABF Consortium (2.5.3.104d): ABF - Aspergillus<br>pseudoterreus               |          |          |                 | 8.1 |     |
|   |          |          |                 |     | Ī   |
| ABF Consortium (2.5.3.104b): ABF - Pseudomonas putida                         |          |          |                 | 7.8 |     |
| ABF Consortium (2.5.3.104g): ABF - Host Onboarding                            |          |          |                 | 7.5 |     |
|   | 0        | 2        | <b> </b><br>4 6 | 5   | 8   |



# ABF REVIEW PANEL SUMMARY REPORT

### Prepared by the Agile BioFoundry Review Panel

The ABF aims to reduce the time and cost of commercialization of bioproduction of advanced biofuels and renewable high-volume chemicals through the development of integrated capabilities across the national laboratories. In the peer review, the ABF team presented its approach to this challenge, which comprises three overlapping thrusts: foundational technology development, proof-of-principle projects, and industry engagement.

Technology development is organized around so-called DBTL engineering cycles. It includes innovative work concerning individual technology DBTL components, such as new methods for collecting and analyzing omics data. It also includes efforts toward program-wide technology integration. Importantly, this portfolio of components extends beyond core DBTL technologies to include upstream techno-economic analysis (TEA) and life cycle assessment (LCA), as well as downstream process integration and scale-up.

Proof-of-principle efforts are focused on a number of testbeds, which are structured as microbial production hosts that have been paired with specific chemical targets via TEA/LCA. Three different host-target efforts were presented, and all reported substantial progress enabled by the DBTL integration efforts.

ABF's third thrust aims to ensure the commercial relevance of ABF efforts. To do this, the team has undertaken a multifaceted program for industry engagement that includes collaboration, novel funding, intellectual property (IP) mechanisms, formal surveys, and direct guidance via an industrial advisory board. The review panel evaluated ABF activities both individually and in aggregate. This report summarizes the panel's key impressions of the aggregate effort.

### IMPACT

The ABF appears to be on course to fill a critical need not currently addressed by industry or academia facilitating the growth of the bioeconomy by lowering technical and economic barriers to commercialization of bioproduction, particularly from DOE-relevant feedstocks. As detailed in the sections that follow, individual technical efforts will advance diverse development opportunities by expanding the menu of options for converting feedstocks into commercially viable offerings. For example, by investing in general-purpose infrastructure that can streamline the multistep processes of bringing a new organism online, engineering it to produce molecules at commercially-relevant levels, and piloting scale-up, ABF efforts have the potential to provide an unparalleled mechanism for industrial entities to leverage the national laboratories to de-risk their own internal research and development (R&D). The potential of this impact may be especially high for nascent tech entities. The ABF aims to enable a path to access tools that are not otherwise available without substantial capital investment and/or specialized in-house expertise.

Recognizing that their technology development efforts will only have substantial impact once they are leveraged by industry, the ABF has placed considerable focus on engagement mechanisms. As evidenced by the response to directed funding opportunities (DFOs) and funding opportunity announcements (FOAs), demand and awareness from industry is already strong, and continues to grow. The panel was also particularly supportive of efforts to ensure impact by enforcing TEA/LCA-based prioritization of host-target pairs.

### INNOVATION

The ABF is demonstrating impressive innovation in three different spheres: (1) within the core DBTL technologies, (2) in areas extending beyond DBTL, and (3) in technology integration and program management. The demonstrations of core DBTL technologies that were highlighted in peer review were centered around three different target-host pairs, for which the team demonstrated the power of applying iterative rounds of strain construction, screening, metabolic modeling and machine learning, multiomics analysis, and fermentation development. The panel found it noteworthy that the team leveraged its flexibility

by deploying DBTL at different scales on a case-by-case basis. It applied "mini"-DBTL for fewer than a dozen strains, and "full" DBTL when needed for experiments requiring on the order of a hundred strains. In addition, by applying quantitative metabolic and kinetic models, and by combining them with omics data, the team identified nonobvious genetic targets for knockout and overexpression. Some of these have been experimentally validated, but more validation is required (and is reportedly planned). The ABF team also presented highlights of DBTL innovations, which included design and data management software systems, DNA sequencing, new technologies for generating sequence variation, omics, and machine learning. Over the course of the project period, the team also demonstrated improvements in overall DBTL times, though much more improvement is still needed.

The panel also recognized important innovations in areas beyond the DBTL core. The new host onboarding program focuses on de-risking the processes of selecting and adapting new microorganisms for production. This fills an important gap in the field by streamlining access to non-model organisms, and it therefore has the potential to generate significant value and to expand the pool of industrially-relevant hosts and host-target pairs. With respect to process integration and scale-up, novel "round-robin" testing across different facilities validates processes in new ways, and also prepares the team for tech transfer. On the more bureaucratic side, the team has innovated important means to encourage and streamline industry engagement through FOA, DFO, and cooperative research and development agreement (CRADA) mechanisms. As an example, the panel was encouraged by the team's experimentation with a uniform CRADA. This effort was conceived in response to extensive delays that arose from contract negotiations, and it aims to increase contracting efficiency by establishing terms up front via a public disclosure. If it is effective, then it will serve as a model for other efforts.

Finally, the review panel also favorably reviewed the management plan, which innovates by combining collaboration best practices and a dedicated project manager with new domain-specific technologies (e.g., the Design Implementation Validation Automation [DIVA] software platform). The ABF team uses this combination to manage communication and coordination of complex projects involving multiple laboratories, companies, and technologies. In the 2017 Peer Review, reviewers expressed concern that geographic distance would impede integration, but this has apparently not been the case so far.

### **SYNERGIES**

Perhaps uniquely within the BETO portfolio, the ABF is explicitly predicated on cultivating synergies across the national labs. The effort is predicated on the assumption that careful coordination of a portfolio of diverse technologies can bring about a paradigm shift in biotechnology R&D. In this light, perhaps the very most significant achievement of the current performance period is the project's operational status—the ABF platform is up and running! More than a dozen DBTL and mini-DBTL cycles have already been completed, validating the ability of the consortium to leverage synergies across the program. To its credit, the team has also started to incorporate TEA/LCA, host onboarding, and process integration into development cycles; more emphasis in these areas would further benefit the program.

The panel also noted a few synergies with other technology areas within the BETO portfolio. For example, a handful of projects in the Biochemical Conversion Technology Area are already leveraging the ABF to differing degrees. While these engagements should continue to be nurtured, the panel also recommends that the team explore the potential for synergy across several other technology areas, such as algal systems, carbon dioxide, and lignin utilization. Engagement with projects in these technology areas could also serve to provide metrics regarding technology impact, and information flowing back from these activities into the ABF could also provide helpful direction. For example, new technology developments regarding feedstocks, deconstruction technologies, CO<sub>2</sub> recovery strategies, or coproduct processes may change the math regarding target downselection.

### FOCUS

The panel was satisfied with the focuses across DBTL, integration, and industry engagement. We note, however, that a comprehensive review of all individual component technical thrusts of DBTL itself was not provided in the peer review due to time constraints. Similarly, the explicit technical connections between individual research project goals and the overarching program-level goal of 10-time improvement in efficiency were not presented. As a result, the panel's assessment of the ABF DBTL focus is limited to the testbeds and highlights that were provided. In these, the panel feels that the ABF is appropriately focused on improving the speed and power of DBTL cycles. That said, the panel also recommends that even more emphasis be placed on TEA, LCA, process integration, and scale-up. The panel recognizes that the program has already placed significant prioritization in these areas, but as they are critical for enabling and de-risking R&D efforts, additional measures should be taken to ensure that they keep pace with all of the emergent technologies in the portfolio.

The review panel also provided feedback on the ABF's prioritization of nonobvious "learn." They agree with the ABF team that the ultimate value of the platform will rest on its ability to provide actionable insights via DBTL efforts. However, it is not yet clear whether novel artificial intelligence and machine-learning algorithms are necessary to achieve this goal. For example, it may be the case that the unique data-generation capabilities of the ABF may produce information rich enough for simple, off-the-shelf, learning algorithms to be sufficient. As such, novel methods will need to demonstrate added value in comparison to standard, well-established methods.

Finally, the panel was very supportive of the ABF's focus on industry engagement. The team's diversified and innovative efforts are on target for an enterprise of this type, and through its interactions it has developed a unique expertise in regarding trends and opportunities. The panel recommends that the team find ways to disseminate this knowledge (e.g., via publication).

### TECHNOLOGY DEVELOPMENT PIPELINE

In general, the panel felt that the technologies pursued were very appropriate for the current stage of technology. The panel did note that the current testbed projects may be too early stage to realize (and test) the full potential of ABF's DBTL approach. In order to better validate and showcase the entire workflow, from TEA though DBTL to process development and scale-up, the panel recommends adding projects that are more mature (e.g., that are already 20%–50% of the way towards commercial goals). In this way, elements of the ABF workflow can be exercised without being hampered, for example, by bottlenecks in the development of genetic tools for new non-model organisms. These projects could be industry engagement projects, or projects linked to other technology areas within BETO. Feedback from such projects would provide valuable feedback to guide ABF future technology prioritization.

### RECOMMENDATIONS

First, the panel recommends placing an even greater emphasis on production-oriented research; specifically, TEA/LCA and process development. The work products from these thrusts were very well received, but there is a critical need for even more innovation from both. Similarly, where possible, projects should transition from sugars to feedstocks as early as possible. Some of this is happening already. The recommendation in the previous section regarding application of ABF workflow to more mature projects also falls into this category.

Second, the panel has made a number of technology-specific recommendations in the individual project reviews. Overall, these recommendations provide guidance to ensure both that the areas of technical weakness are appropriately remedied, and that outcomes are appropriately benchmarked. As an example area of weakness, the panel noted that although DBTL cycle times are improving over time, they are still slow. One emergent bottleneck was "Test," indicating an area that ABF should focus efforts to increase efficiency. Similarly, regarding benchmarking, the panel noted that novelty in "Learn" algorithms may not be a firm requirement for ABF success as described above. At the program level, there needs to be clearer, direct

connections made between project-level aims and milestones and the overall 10-times efficiency improvement goal.

Third, as the ABF matures, the panel felt strongly that its program management, governance structures, and business model will also need to mature. First, as mentioned above, concerns from the 2017 Peer Review regarding distributed operations have so far been successfully addressed via a number of mechanisms to facilitate collaboration. In the present review, however, the panel is concerned that these mechanisms will not scale as ABF's purview and portfolio of projects grows. It will therefore become important to institute tools and additional layers of technical project management and coordination, both in terms of personnel and in terms of additional formal mechanisms for technical tracking and communication that, for example, may go beyond DIVA and the Office of Energy Efficiency and Renewable Energy annual operating plan (AOP) system. Regarding governance, the industry advisory board (IAB) would be strengthened and its perspective expanded by adding companies outside of bioconversion and representing more of the country. Moreover, in order to ensure ongoing appropriate focus within the portfolio of foundational ABF technologies, the panel recommends instituting two additional governance structures complementary to the IAB: a scientific advisory board composed of external experts in academia in artificial intelligence, genetics, TEA, etc. to provide a mechanism for deep portfolio review of technical directions at a level of detail not compatible with the biannual peer review process, and a biosecurity advisory board to aid in the evaluation of dual-use technologies and other potential risks. The intention here is to help the leadership avoid allowing the shape of the portfolio to be determined by inertia rather than by careful, strategic assessment and reassessment. Finally, as the ABF transitions into a national resource, it should continue its ongoing work to develop a clear business model that includes long-term sustenance, IP strategy, and additional mechanisms to streamline engagement with third parties.

# ABF PROGRAMMATIC RESPONSE

### **OVERVIEW**

The program would like to thank the reviewers for their time and thoughtful comments throughout the review process. The program responses to reviewer recommendations are found in the following section.

### Recommendation 1: Focus on mature projects.

The Panel recommends placing greater focus on production-oriented research using TEA/LCA tools and real feedstocks as soon as possible within a project. We agree that utilizing TEA/LCA tools to prioritize targets will be key to achieving industrial relevance. The budget for TEA/LCA activities has been doubled moving into FY 2020 to increase the scope of activities, as well as to keep up with the additional new target and host demonstration projects being undertaken. Part of the selection process for new demonstration projects will involve an initial assessment of TEA/LCA, and R&D will continue to be guided by the findings of TEA/LCA sensitivity analyses. Metrics have been selected for target-host pair demonstrations that are >50% of the way toward commercial goals, and selection criteria will be developed to emphasize projects that are 20%–50% of the way toward commercial goals in projects from competitive solicitations. The ABF will continue to use deacetylated, mechanically refined, enzymatically hydrolyzed corn stover provided to each ABF R&D project as a standard, real-world feedstock. Starting in FY 2020, this material will also be pre-filtered and clarified for ease of use both internal to the ABF and for partner projects.

### Recommendation 2: Reduce DBTL cycle time.

The panel observed that cycle times for DBTL were improving over time but were quite high, particularly for "Test." In addition, the panel felt that more direct connections needed to be made between individual projects

and higher-level goals as the project matures. We agree that a focus on cycle time will be critical to the success of the ABF. Several milestones have been set for early FY 2020 to create a better definition of cycle time and to characterize cycle time for all ABF unit operations individually. New "Test" capacity is being brought online in the form of BioLector and ambr systems as well as DNA sequencing capacity, gas chromatography/mass spectrometry and high-performance liquid chromatography capacity, and proteomics capacity. In addition, we are creating a new set of milestones to address connectivity of individual projects to the overall ABF DBTL efficiency improvement goals. We will be using project management tools, such as Gantt charts and connectivity maps, to help ensure that dependencies are addressed clearly.

### **Recommendation 3: Management during growth.**

The panel noted that as the ABF matures and creates more partnerships, program management and governance structures must also mature. We agree with the panel that more external projects will require additional resource management on the part of the ABF. We are exploring the option of recruiting a coordinator for external projects who would be responsible for ensuring that equipment and personnel resources are properly managed to meet external obligations as well as increase internal capabilities. The panel also recommended that a scientific advisory board be formed to ensure that the technical direction of the ABF is being guided by the latest developments in the fields of synthetic biology, machine learning, and biomanufacturing. We agree that an external advisory group in addition to the IAB aimed more at scientific direction would have value and we are exploring options, such as adding additional scientific experts to the existing IAB, in this space.

# ABF – OVERVIEW

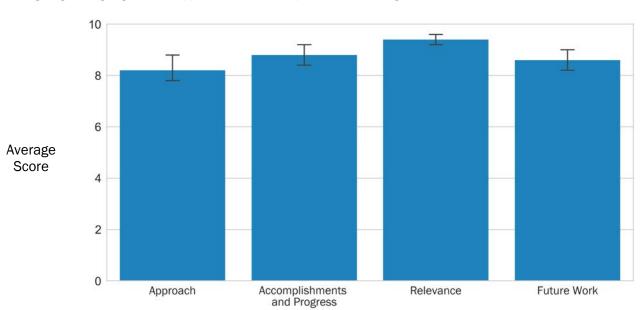
### Agile BioFoundry Consortium

### **PROJECT DESCRIPTION**

The overarching goal of DOE's Agile BioFoundry Consortium (ABF) is to enable biorefineries to achieve 50% reductions in time to bioprocess scale-up (as compared to the current average of around 10 years) by establishing a distributed biofoundry that produces synthetic biology. Towards achieving this goal, the ABF has brought together domain expertise and infrastructure that is distributed across eight U.S. national labs: Lawrence Berkeley National Laboratory, Sandia National Laboratories, Pacific Northwest National Laboratory, National Renewable Energy Laboratory, Argonne National Laboratory, Oak Ridge National Laboratory, Los Alamos National Laboratory, and Idaho National Laboratory. This

| WBS:                      | 2.5.3.104a          |
|---------------------------|---------------------|
| CID:                      | NL0030036a          |
| Principal Investigator:   | Dr. Nathan Hillson  |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$4,400,000         |
| DOE Funding FY16:         | \$300,000           |
| DOE Funding FY17:         | \$1,300,000         |
| DOE Funding FY18:         | \$1,700,000         |
| DOE Funding FY19:         | \$1,100,000         |
| Project Status:           | Ongoing             |
|                           |                     |

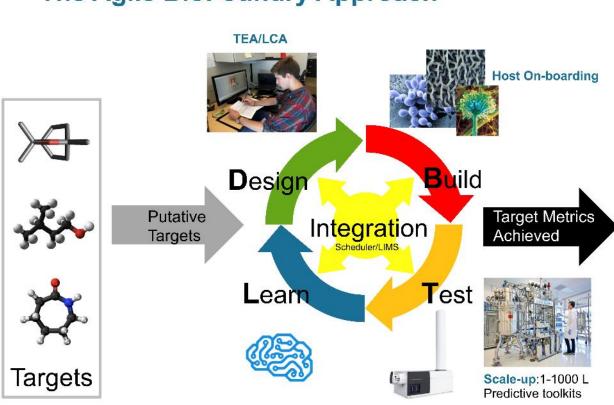
talk provided an overview of the ABF by setting the stage for the subsequent ABF presentations and provided some R&D highlights, including work with industry, from the first 2.5 years of the ABF's operations.



### Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 $\square$  One standard deviation of reviewers' scores



# The Agile BioFoundry Approach

Photo courtesy of Agile Biofoundry Consortium

### OVERALL IMPRESSIONS

- The overall goal of the ABF is to reduce the time and cost of commercialization through the development of a distributed foundry. The foundry is built around the DBTL paradigm. The team is focusing on the Learn component, which is the most challenging step in this process. They are placing particular emphasis on nonintuitive Learn predictions, which really amounts to showing that the Learn step provides concrete value. Overall, the vision is very compelling. Scale-up and TEA provide the main differentiators from other efforts along with the distributed nature of the foundry. Reasonable milestones are provided though they are somewhat vague. More concrete milestones would strengthen the project. Also, it is not clear how the the team will achieve their stated efficiency goals. Will it be through improved process knowledge, eliminating bottlenecks, better operational management, or simply increasing capacity?
- The ABF is well situated to lower technical and economic barriers faced by industry in developing new bioproducts, attempting to increase speed, and decrease risk. It is an optimal platform for integrating and accessing the potential of the national laboratories, synergizing strengths across sites with the right work, being done by the right lab, with the right team. There appears to be significant progress in national laboratory integration from previous reviews. Critically, the ABF is focused on alignment with industrial needs and realities—a must-have for its relevance and to achieve BETO objectives.
- The ABF was created to develop an infrastructure enabling a rapid DBTL cycle that can achieve a 50% reduction in project development time. The concept is to develop host-target pairs that can be leveraged

by industry to go the rest of the way to commercialization. Functional groups are set up to operate like an industry program. There is a very formal project management structure for tracking tasks and milestones, including a 50% time project manager. The team has met most of the milestones so far, and the accomplishments will be covered in the individual presentations. There has been good industry engagement, and this will be streamlined in the future. Technical aspects of the future work is well defined, though there is some ambiguity around how to measure improvement in DBTL cycle time. TEA work has been good so far for preliminary analysis of the host/target pairs, but will require more emphasis as the projects move forward.

• This is a well organized and clear project despite complexity of the project in regards to having multiple teams across the United States involved. As with the previous ABF project, the PIs are encouraged to expand on how their approach will help reduce development cycle by 10 times as this does not seem to be clear in any of the ABF projects.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The ABF overview presentation included substantially simplified milestone language. For example, slide 36 listed a FY 2019 Q2 milestone as "Deep Learning nonintuitive predictions." However, the actual language for this particular milestone is "Deep Learning from multiomics data sets for one or more Crop 1 or Crop 2 targets leads to a set of actionable genetic and/or process modifications (each individually or in combination predicted to increase titer, rate, or yield by 20% or more) to be implemented and evaluated for FY 2019 go-no-go decision." As such, the actual milestones are more concrete than the simplified versions presented to the reviewers. Regarding the achievement of our stated (10 times) efficiency improvement goals, as the reviewer notes, efficiency is a product of multiple factors, and as such, there are multiple facets through which efficiency could be improved. Whereas in the presentation we did discuss several of these facets (e.g., number of cycles required to obtain a given level of performance, strains/designs needed per cycle, personnel/instrumentation resources used per cycle, cycle time), the reviewer is correct in that we did not specify precisely through which facet(s) the efficiency goals would be achieved. We have been pursuing an all-of-the-above strategy, including, for example, emphasis on the Learn component, to not only reduce the number of cycles and strains required per cycle, but also to enhance operations toward reducing resource requirements and cycle times. For the ABF's second three-year AOP cycle, we will quantitatively evaluate efficiency improvements and analyze which facet(s) prove to be the best opportunities for further efficiency gains.
- The reviewer is correct in stating that there has been ambiguity in how we measure improvements to the DBTL cycle time. For our presentation during peer review, we had qualitative but not quantitative definitions of what constitutes a full DBTL (vs. mini-DBTL) cycle. For example, that DBTL requires a minimum set of unit operations, but what that minimum set is had not yet been specified. As such, without a concrete definition, it had not yet been possible to unambiguously measure DBTL cycle time (and as a consequence, improvements thereof). For the ABF's second three-year AOP cycle, we will have the concrete DBTL specification in place, and we will work towards increasingly and automatically capturing cycle time metrics in our workflow-supporting software infrastructure (e.g., DIVA), which will facilitate and standardize how cycle times (and their improvements) are measured. For the ABF's second three-year AOP cycle, we will place increasing emphasis on TEA and LCA as the project moves forward.
- A minor correction to the reviewer's comment. One outcome of the ABF will be to increase engineering cycle efficiency, not the cycle (time) exclusively. See above regarding the multifaceted approach to increasing efficiency.

# ABF – PSEUDOMONAS PUTIDA

### Agile BioFoundry Consortium

### **PROJECT DESCRIPTION**

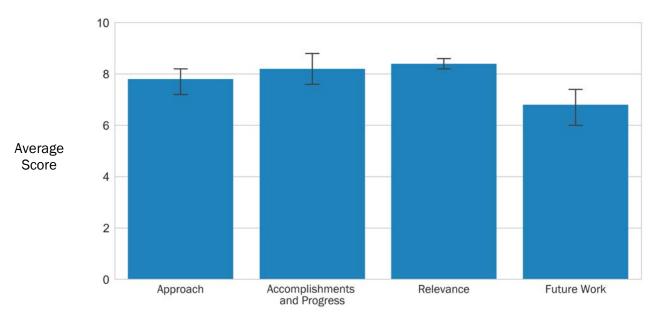
The goal of the target-host pairings in the ABF is to employ the DBTL cycle to engineer promising microbial hosts to produce target molecules of interest to the bioeconomy. This will aid in the establishment of the distributed foundry, highlight key bottlenecks in the DBTL process, and enable the accomplishment of critical milestones toward the foundry concept. *Pseudomonas putida* KT2440 has been selected as one of three hosts in the ABF because it is a readily engineered, Gram-negative, fast-growing bacterium that is well known to exhibit high toxicity tolerance to many established microbial inhibitors found in biomass-derived streams and for which reasonable genetic tools exist. Moreover, from a product

| WBS:                      | 2.5.3.104b          |
|---------------------------|---------------------|
| CID:                      | NL0030036b          |
| Principal Investigator:   | Dr. Gregg Beckham   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$10,300,000        |
| DOE Funding FY16:         | \$500,000           |
| DOE Funding FY17:         | \$3,800,000         |
| DOE Funding FY18:         | \$3,600,000         |
| DOE Funding FY19:         | \$2,400,000         |
| Project Status:           | Ongoing             |
|                           |                     |

perspective, it has both robust aromatic-catabolic pathways (relevant to producing shikimate-derived products) and naturally produces polyhydroxyalkanoates (PHAs) under nutrient-limiting conditions. For Target 1 of the ABF, *cis,cis*-muconic acid (and other C6 diacids in the same pathway) was selected as the primary target, which can be converted into adipic acid and terephthalic acid, as well as used as a functional replacement platform chemical. For Target 2 of the ABF with *P. putida*, branched-chain PHAs were selected as the primary target compounds, which can be used as a biodegradable and inherently recyclable packaging material.

### Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

The approach in this task in the ABF closely mirrors that of the other target-host pairings, bringing a multilaboratory team together to implement various aspects of the DBTL cycle and to promote tool development, with the aim of both demonstrating target molecule production and optimizing their titer, rate, and yield. One key focus in this task is to enhance the Learn functionality so that it will be able to effectively analyze key data from Design-Build-Test and make nonintuitive predictions that can be used to improve titer, yate, and/or yield of these crop molecules. The technical accomplishments to date in this task include the development of robust, baseline strains that are able to produce *cis,cis*-muconic acid, which resulted from the ABF pilot project. The strains were examined in the first DBTL cycle with multiomics Test, and nonintuitive predictions from Learn were used to engineer further improvements in strain performance. New DBTL cycles in this vein include "Learn-friendly" Test experiments that are ongoing now to more comprehensively characterize sugar utilization in this strain. In several mini-DBTL cycles, the project has employed DBTL cycles to accomplish direct adipic acid production in P. puitda, expanded the strain to be able to rapidly consume xylose and arabinose (in the presence of glucose), and developed multiple in vivo and in vitro biosensors for detecting key intermediates and products (to accelerate the DBTL cycle). Overall, these efforts have shown that the ABF concept works, and, most importantly, have identified areas where improvements can be made to increase process efficiency and decrease cycle time, both metrics that will enable the ABF to reach its primary goal of stimulating the bioeconomy by reducing time and cost for deployment of bioproducts into the market.



Photo courtesy of Agile Biofoundry Consortium

### **OVERALL IMPRESSIONS**

- As a testbed for the ABF effort, this team reports an impressive number of *P. putida* developments and innovations. Through a combination of different kinds of DBTL and mini-DBTL cycles, they have enhanced production of two target compounds, improved sugar utilization in the host, and made inroads into taking greater advantage of omics data, machine learning, and biosensors to further enhance development and to expand into new target compounds. It will be important to evaluate the impact of these latter efforts as they are completed during the next phase of the performance period.
- This subproject is focused on producing C6 diacids and branched-chained PHA in *Pseudomonas putida* to demonstrate the ABF framework. The team is mostly focused on improving rates based on TEA. Overall, the team is making good progress, in particular with regards to generating data sets for the Learn step. All of the proposed projects are commercially promising. The biosensor work is also very promising.
- With less than a year remaining in this project, future work seems ambitious. Prioritizing tasks and research to support key outcomes is needed.
- Development of a nontraditional and industrially important bacterial host in *P. putida* is of high interest, and this project has a good start, especially regarding muconic acid production. The use of a TEA to focus rate is a good sign that TEAs are being employed to make project decisions. The project appears to have discovered some nonintuitive predictions, a highly important validation from omics-driven Test-Learn.
- *Pseudomonas putida* is being developed as a host, with the model products being C6 diacids and branched-chain polyhydroxyalkanoates. Actual hydrolysate is being used to evalate performance. The overall objectives are to develop a robust bacterial host while demonstrating improvements to the DBTL cycle time and generating data sets to be used in modeling and learning. The team has demonstrated that the DBTL cycle can be applied iteratively to overcome bottlenecks and make improvements. Omics and computational work led to specific targets. However, improvement so far seems to be a result of improved sugar uptake alone, rather than any pathway enhancements. It may be that enzyme engineering is needed to improve pathway flux. In addition, the DBTL cycle is also quite slow. There are inherent limitations in the speed of conducting genetic manipulations and other tasks, but more workflow management could streamline progress.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewer for the positive feedback. We completely agree that we need to evaluate the impact of the tool development as part of the DBTL cycle and overall ABF concept, and we are actively doing that now. We note, for example, that the biosensor work has already led directly to improved muconate strains, so investment in those tools are generating improvements and accelerated DBTL progress.
- We agree that the future work is indeed ambitious, but we have an aggressive timeline and a large team working in close coordination to be able to be successful in our objectives.
- We thank the reviewer for the positive feedback, and we agree that the initial DBTL cycle timelines were very long. This was the case mostly because we were setting up the tools, workflows, etc. We anticipate that the timelines will be reduced significantly in future DBTL cycles.

# ABF – RHODOSPORIDIUM TORULOIDES

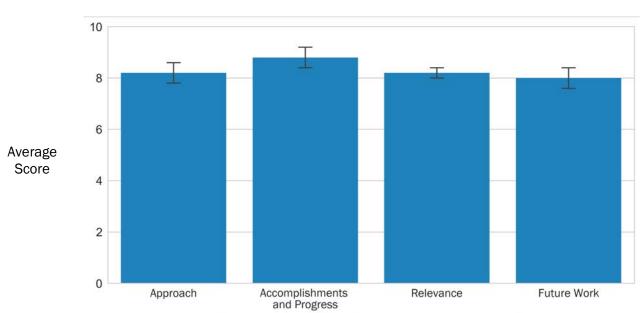
### Agile BioFoundry Consortium

### **PROJECT DESCRIPTION**

The goal of the target-host pairings in the ABF is to employ the DBTL cycle to engineer promising microbial hosts to produce target molecules of interest to the bioeconomy. This will aid in the establishment of the distributed foundry, highlight key bottlenecks in the DBTL process, and enable the accomplishment of critical milestones toward the foundry concept. *Rhodosporidium toruloides* IFO0880 has been selected as one of three hosts in the ABF because it is a readily engineered, fast-growing basidiomycete yeast that is able to grow on lignocellulosederived hexose and pentose sugars as well as ligninderived aromatics. It is also carotenogenic and oleaginous, indicating that it has high flux through two biosynthetic

| WBS:                      | 2.5.3.104c          |
|---------------------------|---------------------|
| CID:                      | NL0030036c          |
| Principal Investigator:   | Dr. John Gladden    |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$4,620,000         |
| DOE Funding FY16:         | \$20,000            |
| DOE Funding FY17:         | \$1,100,000         |
| DOE Funding FY18:         | \$1,600,000         |
| DOE Funding FY19:         | \$1,900,000         |
| Project Status:           | Ongoing             |
|                           |                     |

pathways that can be leveraged to produce a myriad of biofuels and bioproducts. For Target 1 of the ABF, four terpenes were selected (cincole, bisabolene, farnesene, and kaurene), each with applications as biofuels or bioproducts (e.g., adhesives, polymers, etc.). For Target 2 of the ABF, fatty alcohols were selected as the primary target compounds, which have many applications, such as lubricants and detergents.



### Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${f I}$  One standard deviation of reviewers' scores

The approach in this task in the ABF closely mirrors that of the other target-host pairings, bringing a multilaboratory team together to implement various aspects of the DBTL cycle and to promote tool development, with the aim of both demonstrating target molecule production and optimizing their titer, rate, and yield. One key focus area in this task is to enhance the Learn functionality so that it will be able to effectively analyze key data from Design-Build-Test and make nonintuitive predictions that can be used to improve titer, rate, and/or yield of these crop molecules. The technical accomplishments to date in this task include the development of robust, baseline strains that produce either terpenes or fatty alcohols, most of these molecules at g/L titers. The bisabolene strain was examined in the first DBTL cycle with multiomics Test, and several nonintuitive predictions from Learn are currently being tested in the second DBTL cycle for their ability to improve in strain performance. New DBTL cycles in this vein include "Learn-friendly" Test experiments for both terpenes and fatty alcohols, designed specifically for machine learning, with the goal to optimize either pathway dynamics or growth conditions toward increased titers, respectively. In several mini-DBTL cycles, the project has identified key Design-Build strategies for rapid optimization of terpene production and for fatty alcohols, and identified several key host genes to modulate for enhanced production. Overall, these efforts have shown that the ABF concept works, and, most importantly, have identified areas where improvements can be made to increase process efficiency and decrease cycle time, both metrics that will enable the ABF to reach its primary goal of stimulating the bioeconomy by reducing time and cost for deployment of bioproducts into the market.

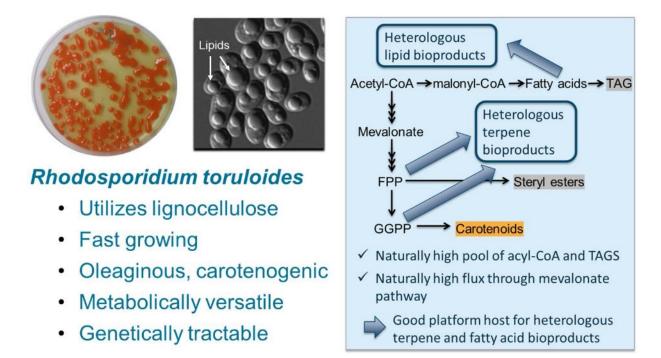


Photo courtesy of Agile Biofoundry Consortium

### OVERALL IMPRESSIONS

• As a testbed for the ABF, this team reports significant process in using DBTL to aid in the development of the expression of terpenes and fatty alcohols in *R. toruloides*. Through large-scale testing (100–200 strains constructed), they have shown improvements in production of both of these target compounds. Particularly noteworthy are the impacts of computational methods on their progress; simple regression models validate predictions regarding the impact of expression level on yield and by developing new, quantitative metabolic models and kinetic models for this organism and combining them with omics

data, they have shown that they can identify nonobvious genetic targets for optimization, some of which have been validated experimentally.

- This goal of the subproject is to produce terpenes and fatty alcohols in *Rhodosporidium toruloides*. This is a great target organism, as little is known about its metabolism. The team is making good progress. The dynamic proteomic data sets will be very useful for the Learn step. The initial Learn prediction regarding transcription factor overexpression seems promising.
- Great progress so far. Same as other subsections in ABF projects, it would be great if the PI can expand on time reduction (10 times) and their proposed approach claiming to achieve that reduction. Overall, subprojects are missing the connection to their project to the overall goal/target in a clear way.
- *Rhodosporidium toruloides* is a fungal host being developed for terpenes and long-chain fatty alcohols. The organism readily consumes not only C5 and C6 sugars, but also aromatics; thus it can be used in lignin conversion. This project showcases several capabilities of the ABF:
  - o Iterative rounds of strain construction and screening
  - Metabolic modeling and machine learning
  - Multiomics analysis
  - Fermentation development.

One particular novel application of machine learning was the "kinetic learn" method, using protein time series data in conjuction with a metabolic model to predict metabolite levels. The first DBTL cycle was completed for both products, and used to inform designs for the next cycle. Mini cycles were also used to screen strains and conditions prior to a full experiment where omics data were collected. It is still uncertain how useful the machine-learning approach was compared to rational intuition and the metabolic model alone. This will be clearer once the recommended modifications are tested and evaluated.

• *R. toruloides* is a good host choice for ABF objectives (e.g., for DBTL demonstration) and complements other host choices across the ABF. Target choices are also sensible and reflect pathways that lead to target-rich classes of compounds (terpenes and fatty acids) with wide commercialization potential.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thanks for your comments. The ABF has certainly accelerated development of this organism.
- Thanks for your comments. We agree that this is a great target organism for the ABF.
- Our ultimate goal within the ABF is to reduce the time to bioprocess scale-up by 50% through improvements in DBTL cycle efficiency. Reduction of DBTL cycle time is one of several metrics that will contribute to increased DBTL cycle efficiency. One of our goals for the initial DBTL cycles implemented for each target/host pair was to identify areas where efficiency gains can be made. This exercise has allowed us to identify many areas for improvement. Specifically regarding time, improvements can be made in Design through the assembly and validation of a library of engineering parts, which can then be more rapidly refactored into new Designs with a greater likelihood of being functional. Within Build, improvements can be made with streamlined transformation and screening protocols as well as development of high-throughput plate-based protocols to enable examination of a greater number of samples in a shorter timeframe. For Test, now that analysis of baseline samples has been conducted and protocols validated for this host, sample analysis can be expediated. In addition, reliance on mini-DBTL Test analysis (high-performance liquid chromatography, gas

chromatography/mass spectrometry, etc.) can be expedited by high-throughput Testing of strains constructed in the aforementioned plate-based Build efforts. For Learn, we now have a metabolic model to put our multiomic data into context, which can be analyzed both manually and computationally. We are in the process of assessing several machine-learning platforms for data analysis, which should also expediate Learn and lead to better predictions for improvements to be made in subsequent DBTL cycles, reducing the time it takes to optimize titer, rate, and yield.

- Regarding connection to the broader ABF milestones, while not specifically called out in our presentations, all the ABF hosts have multiple specific milestones within the ABF. To assess the overall progress of the ABF, these milestones were specified to be met through the combination of all three ABF host organisms and their targets. So, rather than host-specific milestones, we aggregated host milestones. The milestones defined both the number of target molecules selected to be engineered into these host organism and specific titer, rate, and yield targets.
- While we are very excited about some of the machine-learning Learn methods, we are still in the early phases of validating and optimizing these approaches in *R. toruloides*. The ABF offers a great testbed for these approaches, and as time goes on, will provide the large data sets some of these methods require. We are in the process of dedicating a significant portion of our Test and Learn resources to generate those data, in consultation with the Learn team experts. We are also assessing less data-intensive Learn approaches in parallel to ensure we have multiple routes to success. Where possible, we will leverage the same data sets for different Learn approaches but will also generate tailored data as needed. We are in the process of vetting different Learn approaches, and will focus resources toward those that are determined to be the most promising after this initial vetting phase. We are excited to experimentally validate these approaches in upcoming DBTL cycles.
- Thanks for your comments. We agree that this is a good host to help us meet our ABF objectives.

# ABF – ASPERGILLUS PSEUDOTERREUS

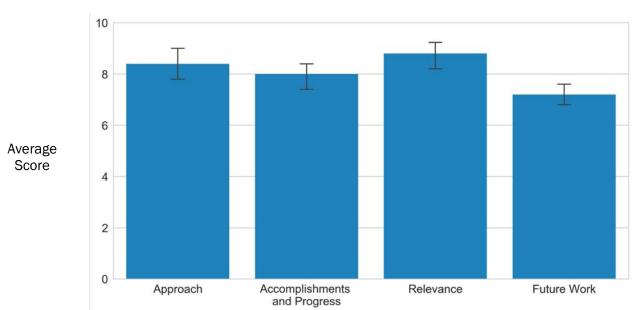
### Agile BioFoundry Consortium

### **PROJECT DESCRIPTION**

The goal of the target-host pairings in the ABF is to employ the DBTL cycle to engineer promising microbial hosts to produce target molecules of interest to the bioeconomy. This will aid in the establishment of the distributed foundry, highlight key bottlenecks in the DBTL process, and enable accomplishment of critical milestones toward the foundry concept. *Aspergillus pseudoterreus* has been selected as one of three hosts in the ABF because it is a readily engineered, highly acid tolerant, and filamentous fungus that is used in industry for the production of native organic acids in their free acid form. It can grow on a wide variety of sugars, as well as oligosaccharides and polysaccharides with inorganic sources of other nutrients.

| WBS:                      | 2.5.3.104d          |
|---------------------------|---------------------|
| CID:                      | NL0030036d          |
| Principal Investigator:   | Dr. Jon Magnuson    |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$5,720,000         |
| DOE Funding FY16:         | \$20,000            |
| DOE Funding FY17:         | \$1,900,000         |
| DOE Funding FY18:         | \$2,000,000         |
| DOE Funding FY19:         | \$1,800,000         |
| Project Status:           | Ongoing             |
|                           |                     |

For Target 1 of the ABF, 3-hydroxypropionic acid (3HP) was selected. This molecule can be converted into a major commodity chemical, acrylic acid, by technology existing within the ABF partner laboratories to serve as a direct replacement molecule. For Target 2 of the ABF with *A. pseudoterreus*, aconitic acid from the six-carbon tricarboxylic acid family, which includes citric and isocitric acids, was selected as the primary target compound. This family of six-carbon tricarboxylic acids are used as acidulants and chelators in the food, cement, and other industries.

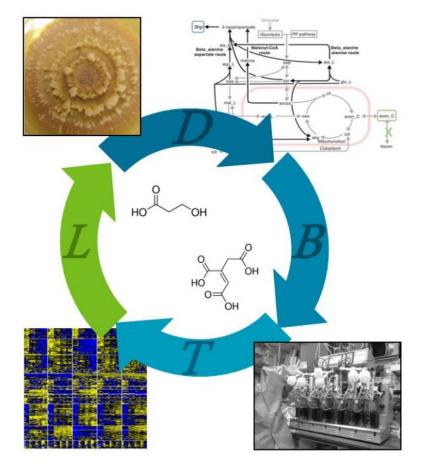


### Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

The approach in this task in the ABF closely mirrors that of the other target-host pairings, bringing a multilaboratory team together to implement various aspects of the DBTL cycle and to promote tool development, with the aims of first demonstrating target molecule production and then optimizing their titer, rate, and yield. A key focus in this task is to enhance the Learn functionality so that it will be able to effectively analyze key data from Design-Build-Test and make nonintuitive predictions that can be used to improve titer, rate, and/or yield of these crop molecules. The technical accomplishments to date in this task include the development of acid-tolerant (pH 1-3) baseline strains that are able to produce 3-hydroxypropionic acid via the beta-alanine pathway. Strains containing one or two copies of the pathway at different locations in the chromosomes were examined in the first DBTL cycle with the multiomics Test and both traditional and nonintuitive Learn approaches. These have identified gene targets for another DBTL cycle in FY 2019 aimed at improving titer, rate, and/or yield of the target 3HP. Multiomics testing has also identified a list of candidates potentially involved in 3HP degradation that will be targets for deletion to increase net titer, rate, and yield. Similarly, transporter genes that may be involved in increasing aconitic acid transport between cell compartments and exports from the cell have been identified and will be the subject of another DBTL cycle for this target. Overall, these efforts have shown that the ABF concept works, and most importantly, have identified areas where improvements can be made to increase process efficiency and decrease cycle time, both metrics that will enable the ABF to reach its primary goal of stimulating the bioeconomy by reducing time and cost for deployment of bioproducts into the market.



# Aspergillus pseudoterreus

Photo courtesy of Agile Biofoundry Consortium

### OVERALL IMPRESSIONS

- The goal of this subproject is to produce 3HP and aconitic acid in *Aspergillus pseudoterreus*. The inclusion of a filamentous fungus provides a useful test for the ABF. The team is making solid progress. It is difficult to evaluate the Learn component of this project at this stage, though it is clearly an important step. More details should be provided given the focus on Learn. While clear milestones are presented, the project would benefit from competitive benchmarks, particularly with regards to 3HP.
- Overall, significant portions of work were done (more than 80%), however future work still pictured significant research, which does not seem to be achievable within less than a year left in the project. IP was mentioned in the first slide, so if there is any IP associated with this project, the principal investigator would need to touch on potential IP.
- As a testbed for the ABF, this team reports in-process results in applying DBTL to aid in the development of the expression of organic acids in an industrially relevant fungus, *A. pseudoterreus*. Initial mini-DBTL cycles have established baseline strain performance of 1.3 g/L and 10 g/L for respective targets, and they have started to analyze omics data in order to guide genetic modifications for subsequent design cycles. The group has also started to develop new genetic constructs in order to streamline strain construction.
- *A. pseudoterreus* is a fungal host related to strains historically used for enzyme expression and production of citric acid. Due to its acid tolerance, it is a suitable host for producing organic acids in the free acid form. Here, it is being considered for aconitic acid and 3HP. The pathways to these molecules are well established, so the team is focused on solving the key challenges of improving timelines for genetic manipulation and reducing byproduct formation. For the latter, they have leveraged a variety of omics techniques in conjunction with metabolic modeling and machine learning. This has led to identification of targets for knockout or overexpression, many of them not intuitive. However, the value of these techniques cannot really be evaluated until these manipulations are made and results provided. The team has also greatly reduced the amount of time needed for testing strains, and has taken steps to improve translation and reproducibility from shake flask to fermentation.
- The selection of a filamentous fungus, especially *Aspergillus*, is an excellent inclusion in the host-target development programs due to industrial relevance and as an opportunity to optimize a DBTL cycle. This organism has inherent handling and growth challenges that impose time and throughput limitations, which perhaps can be overcome with improved Learn (including deep-Learn) capabilities that seem to be the focus. In this respect, it may be a good example of how DBTL can be flexible to garner improvements by emphasizing certain elements of the cycle because of limitations in others. Progress has been good and the outcome of potentially exciting unintuitive learnings is pending. It might be of benefit to develop relationships with external entities who are developing (other, but related) strains and tools for similar hosts to move towards high-throughput use.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We believe filamentous fungi are very important, as evidenced by their wide use within industry. "Traditional" Learn techniques using metabolic models as a framework for analyzing omics data and to support flux balance analysis for identifying bottlenecks and targets has been a major emphasis and has resulted in both intuitive and nonintuitive targets. Advanced Learn techniques, such as Artificial Neural Networks (ANN), have been employed in the last year to identify nonintuitive targets, and this effort will expand in the future with increasing numbers of large Test data sets. A number of targets already suggested by Learn remain to be Designed, Built, and Tested. We will be able to address the highestpriority targets in FY 2019. Milestones pertaining to all of the targets have been satisfied, but we realize we are still well short of handing off the 3HP strain for commercialization.

- The demarcation between work to be accomplished in the remainder of FY 2019 and moving beyond into FY 2020 could have been clearer. A provisional patent was filed, and a full patent will be filed before the end of April. Since this was a public presentation, few details were discussed.
- We agree with this assessment and we have a significant number of high-priority targets in regard to improving titer, rate, and yield for both target molecules. The highest-priority targets will be constructed and tested before the end of FY 2019 (see response above). We are excited to have the opportunity to report on those results in the literature and at peer review two years hence.
- We appreciate the guidance with regard to exploring external collaborations for development of highthroughput tools for these challenging but highly useful hosts. We also have work in a project outside of BETO exploring high-throughput methods for transformation that will be leveraged within the ABF.

# ABF – DESIGN-BUILD-TEST-LEARN INFRASTRUCTURE

### Agile BioFoundry Consortium

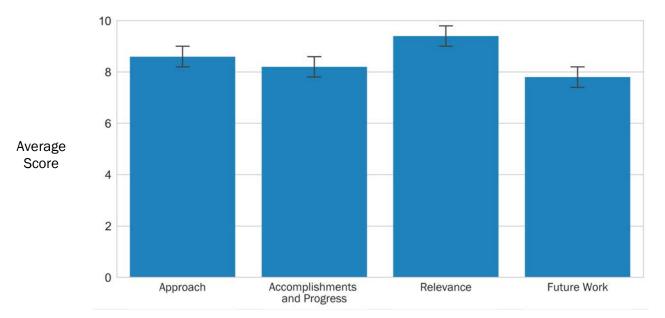
### PROJECT DESCRIPTION

One of the key tasks of the DOE ABF is to design, implement, operate and maintain DBTL infrastructure that enables the efforts of the ABF, as well as industry and other BETO projects and consortia. This talk will provide an overview of the ABF's DBTL infrastructure (in a more detailed and deliberate fashion than in previous or subsequent ABF presentations), and provide some DBTL infrastructure R&D highlights from the first 2.5 years of the ABF's operations.

| WBS:                      | 2.5.3.104e          |
|---------------------------|---------------------|
| CID:                      | NL0030036e          |
| Principal Investigator:   | Dr. Nathan Hillson  |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$15,200,000        |
| DOE Funding FY16:         | \$1,000,000         |
| DOE Funding FY17:         | \$5,000,000         |
| DOE Funding FY18:         | \$4,500,000         |
| DOE Funding FY19:         | \$4,700,000         |
| Project Status:           | Ongoing             |
|                           |                     |

### Weighted Project Score: 8.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 $\square$  One standard deviation of reviewers' scores

# **Highlights – DBTL infrastructure**

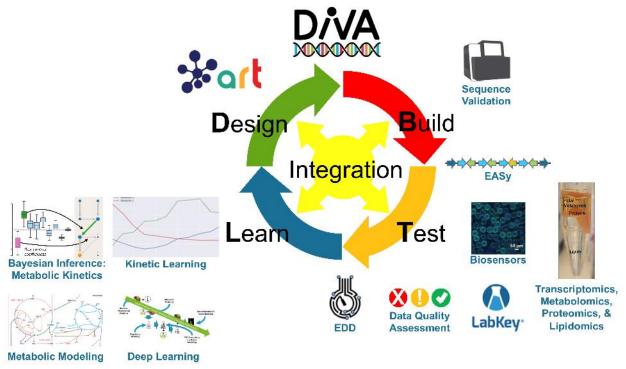


Photo courtesy of Agile Biofoundry Consortium

### OVERALL IMPRESSIONS

- This subproject is focused on developing the DBTL infrastructure within the ABF. The main contribution is bringing together multiple tools into a common platform. The focus on reproducible unit operations across different institutions is a valuable goal and key strength of the foundry.
- Great management. It is great to see an overview of the projects and how each has contributed to the DBTL cycle in detail.
- The team presented highlights of over a dozen novel capabilities under development under the ABF umbrella. These efforts span the entire DBTL cycle and include at least eight different software projects, in recognition of the importance of establishing high-quality maintained software as an enabling capability for the community. Layered on top of these technology development efforts are strategic plans to ensure their relevance, including multifaceted industry engagement (especially including CRADAs), TEA-driven project prioritization, and a commitment to wide dissemination of the software.
- The DBTL infrastructure is the core of the ABF and supports all other tasks. Having this infrastucture in place and streamlined is critical for reducing both DBTL cycle time as well as overall project timelines. This is dependent on having a good software platform to maintain data and enable Learn activities, and the team has built or aquired a number of tools. These include DNA construct design and assembly, various types of metabolic modeling, deep-learning algorithms, and laboratory information management systems for data storage and sharing. New Build tools are next-generation sequencing to verify construct accuracy and a novel method for gene evolution based on duplication and recombination. Sample processing for omics analysis has also been streamlined. The DBTL cycle time has been improved, but is

still too long. Now that all the computational and experimental tools are in place, effort should be spent on developing a streamlined workflow. Also, the current ABF projects may be too early to really gain full benefit from DBTL. As a test case, it would be useful to apply this to a mid-stage project with an organism with well established genetic tools.

• Development of the DBTL infrastructure to realize efficiency gains in project execution and delivery is at the heart of the ABF engine design room. The software, tools, processes, and other assets combine to optimize the project development cycle and can greatly enhance productivity and success at the ABF and, if made available, to external stakeholders such as industry and academia. It will be important to identify the appropriate business model to achieve this.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that our DBTL cycle time (as of the 2019 BETO Peer Review) is too long. We are now quantitatively defining what constitutes a DBTL cycle (vs. mini-DBTL) beyond the qualitative definitions provided at peer review. We will be working towards increasing the coverage and granularity of our cycle-time metrics capture, and use the resulting data to prioritize our DBTL workflow streamlining efforts. We agree that some ABF projects may be too early stage to benefit from DBTL (which might otherwise be better served by mini-DBTL); finding the transition point (in terms of project maturity needed in order to benefit from DBTL) is a good idea.
- The ABF's philosophy is to use methods, instruments, software, etc., that are accessible (and develop those that will be accessible) to industry and academia, either through commercial vendors or through licensing from the ABF itself (via the national labs). This enables our industrial and academic collaborators to practice these same methods, instrumentation, and software behind their own corporate or institutional firewalls without persistent reliance on the ABF. There are established licensing models and mechanisms (e.g., exclusive in a field of use or nonexclusive, freely open source) that enable this, with the general broad objective to maximize impact and market transformation (which determines the licensing mechanism). For the ABF in particular, the nonexclusive (including freely open source) mechanisms are strongly preferred (so that multiple companies and academic groups can benefit from them) with the exception of exclusive licenses to technology platform companies that will make the technologies broadly accessible. Part of the sustainable business model for the ABF, then, is to incentivize its collaborators to opt for nonexclusive licensing options in CRADAs, and we plan to explore these options in the next phase of the ABF.

# ABF – INTEGRATED ANALYSIS

### Agile Biofoundry Consortium

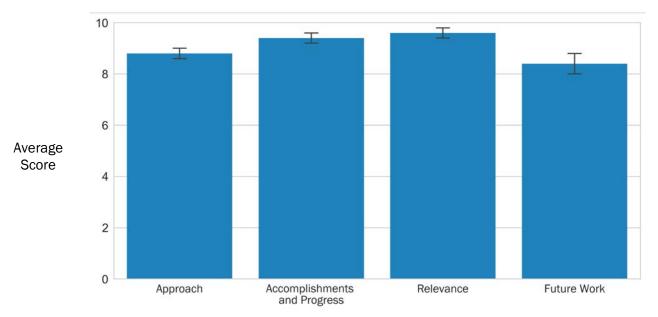
### PROJECT DESCRIPTION

The Integrated Analysis task is incorporated within the DBTL approach with a goal of providing an analysis-based foundation to the science and research of the ABF. The collaborative team develop TEA and LCA for the pairs of chemical targets and host microbes being pursued. To date, the team has performed analyses on over 10 different target chemical host-microbe combinations. This talk will summarize the ongoing analysis work and will detail how TEA and LCA have been integrated to support ABF goals with a focus towards developing bio-based products that are sustainable and economically viable. Future work plans for the Integrated Analysis project also will be outlined.

| WBS:                      | 2.5.3.104f          |
|---------------------------|---------------------|
| CID:                      | NL0030036f          |
| Principal Investigator:   | Dr. Mary Biddy      |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$500,000           |
| DOE Funding FY16:         | \$100,000           |
| DOE Funding FY17:         | \$200,000           |
| DOE Funding FY18:         | \$100,000           |
| DOE Funding FY19:         | \$100,000           |
| Project Status:           | Ongoing             |
|                           |                     |

### Weighted Project Score: 9.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

# Integrated Analysis: Molecule Cycle

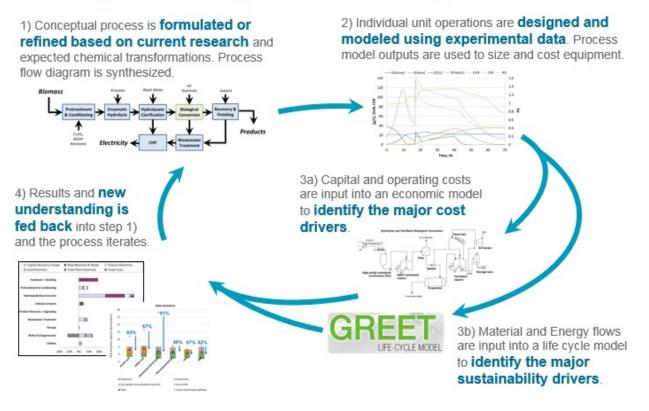


Photo courtesy of Agile Biofoundry Consortium

### **OVERALL IMPRESSIONS**

- The goal of this subproject within the ABF is to provide TEA and LCA in order to evaluate the economics and sustainability of proposed molecules. In addition, they will develop conceptual process designs. Such analysis will be useful for determining the feasibility of different host-target pairs. This is an essential service and should be a central activity. The budget is small and likely insufficient to support these critical activities.
- The project and projects similar to these are well needed to provide clear understanding of manufacturability, cost, and LCA of the biological product. The principal investigators did a great job creating clear analysis for a variety of products and it would be great to see more of these analysis/projects in the future.
- The Integrated Analysis team has provided critical guidance to the ABF project through careful technoeconomic and sustainability analyses. This work helps ensure that ABF efforts attain relevance to the bioproducts industry and by prioritizing targets for testbed, help bolster relevance even for projects still at the proof-of-principle stage. These continuing efforts are vital for ABF success.
- The goal of this function is to assess economic and sustainability drivers for the ABF work, analyzing individual host-target pairs. This provides a consistent, unbiased framework for evaluating and prioritizing processes, and is thus critical to choosing successful projects. In addition, it can help drive decisions during a development project to determine which metrics have the strongest impact on cost. The team completed TEA and LCA on 10 host-target pairs and observed clear trends on the factors

influencing both economics and sustainability. In the future, these models will be refined with data gathered from the projects.

• Meaningful TCAs and LCAs are the currency of fact-based decisions for downselection and prioritization within and across projects. The value that this program is bringing is critical to the success of the ABF, provided that inputs are sound and that the results and recommendations are acted upon by those making program decisions. This program is not only important, but should probably be expanded.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their helpful and supportive feedback. We will work to incorporate these suggestions in future analysis efforts.

# **ABF – HOST ONBOARDING**

### Agile BioFoundry Consortium

### **PROJECT DESCRIPTION**

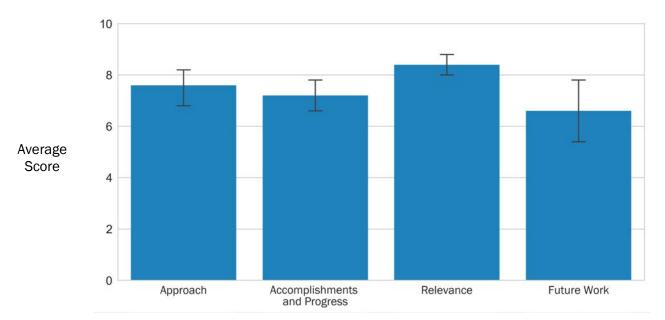
Non-model microorganisms often have advantageous physiological traits that could be leveraged for advanced bioprocessing, such as the ability to thrive at low pH or to utilize uncommon substrates such as syngas or oligomeric sugars. However, a lack of genetic tools and fundamental knowledge about these organisms hinders strain development. The role of the Host Onboarding team is threefold: (1) evaluate proposed hosts for new host-target pairs within the ABF, (2) develop genetic tools that allow new hosts to be used for DBTL cycles within the ABF and by outside stakeholders, and (3) improve genetic tools for BETO "State Of Technology" (SOT) organisms to increase DBTL cycle efficiency across the BETO

| 2.5.3.104g         |
|--------------------|
| -                  |
| IL0030036g         |
| Dr. Adam Guss      |
| 0/1/2016-9/30/2019 |
| 3,500,000          |
| 5100,000           |
| 51,200,000         |
| 5700,000           |
| 51,500,000         |
| Ingoing            |
|                    |

portfolio. In this talk, the Host Onboarding team will discuss the development of a "Tier System" to evaluate the readiness of an organism for DBTL cycles, as well as current progress on developing new hosts such as *Bacillus coagulans* and *Clostridium carboxidivorans*. Future work on these organisms and SOT organisms such as *Zymomonas mobilis* and *Clostridium tyrobutyricum* will also be discussed.



Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

### OVERALL IMPRESSIONS

- The goal of this subproject is to develop new non-model organisms for chemical and fuel production. A key step involves developing a ranking system for evaluating the potential of new non-model organisms. Overall, this project addresses an important problem. Many tasks are proposed. The project would benefit by clearly ranking the importance of these tasks and explaining how effort will be allocated toward achieving them. Otherwise, it is difficult to evaluate progress.
- This project aims to fill important gaps not addressed elsewhere in the BETO portfolio regarding host onboarding by developing analytical tools for pragmatic, data-driven downselection of non-model organisms with new and useful phenotypes and developing genetic manipulation tools to provide access to these phenotypes. The team has successfully developed a principled prioritization system and applied it to identify three non-model organism targets, for which it has now started the process of developing genetic tools.
- This group prioritizes new host organisms for bioprocessing, and develops genetic tools and basic knowledge to make them tractable. Novel host organisms can extend the range of feedstocks and products due to the ability to utilize novel carbon sources and tolerate inhibitors or extreme conditions. In order for these host organisms to find applications, genetic tools must be developed so they can be manipulated. It is good that these tools are being developed early, so they are ready when needed. The team created a ranking system for organisms to help prioritize, and also a tier system to determine which organisms are ready to enter the DBTL process. Furthermore, a web portal will give protocols and lab contacts for methods of each organism. They developed a methodology to overcome host restriction modification systems, and have made progress on two difficult organisms.
- The new host onboarding program is creating significant value and ideally will expand the pool of industrially relevant hosts (and host-target pairs). A sensible tiered set of criteria to downselect to approprite selections has been developed and a good, diverse set of initial host targets have been put into play. Consideration toward upgrading biosafety/regulatory criteria to the selection process, as well as a biosafety board, should be considered.
- Good to see the principal investigator mentioned where this project fits in the overall ABF goals. New hosts and new tools seem ambitious. Can the principal investigator select one (either a new host or new method) and focus on and move to the next after success in the first one?

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the useful comments. We feel that the both (1) the web portal detailing the ABF capabilities, protocols, and data sets; and (2) the development of new host organisms for use in the ABF and the community at large are of equal importance, and so we are devoting substantial efforts on both fronts to make sure each task is accomplished. To facilitate this, Oak Ridge National Laboratory has taken the lead on developing the genetic tools, which is a core area of expertise for the lab. Similarly, Los Alamos National Laboratory has taken the lead on finalizing and making public the tier system. For onboarding new hosts in FY 2020, we are targeting the development of genetics for a targeted number of targeted microbes (*Bacillus coagulans*, which catabolizes hydrolysate very well, and *Clostridium carboxidivorans*, which catabolizes sugars and syngas) to expand the types of hosts available within the ABF. We are also targeting improvement of genetic tools in organisms that are important for other BETO projects like *Zymomonas mobilis* and *Clostridium tyrobutyricum*. In future years, we will identify new hosts that would bring unique capabilities to the ABF for targeted development.
- Thanks for these comments. We do have a biosafety plan in place, wherein any new organism that is used needs to be evaluated by our home institutions, which have rigorous regulations. We also utilize Lawrence Berekely National Laboratory-developed software called BLiSS to identify biosecurity/biosafety concerns of synthetic DNA in advance. Our current goal is to only use Biosafety

Level 1 organisms, and so the biosafety risk is inherently low. However, the reviewer's point is an important one, and we will work on formalizing a process within the ABF itself, particularly taking into consideration how biosafety might affect use of such organisms by industry.

• Thank you for the comment. Given the importance of developing new organsims and the scope of the ABF, we feel that it is important to develop multiple hosts and methods in parallel. We think there is synergy in parallel development, where new learnings in one system can help accelerate development in all systems.

# ABF – PROCESS INTEGRATION AND SCALE-UP

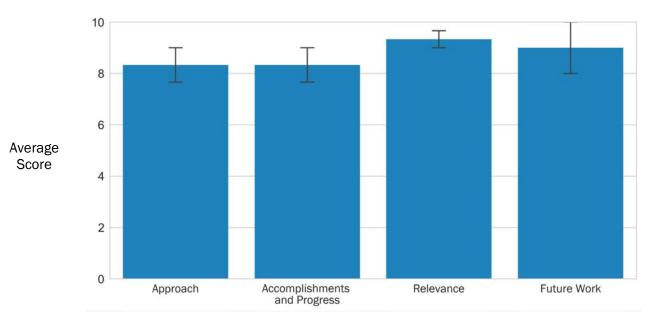
### Agile BioFoundry Consortium

### **PROJECT DESCRIPTION**

The aim of the ABF Integration and Scaling task within the overall project is severalfold: (1) to produce a consistent sugar hydrolysate for the ABF to use across the target-host pair demonstration and scaling efforts, (2) to conduct hydrolysate-based cultivations for the target-host pair teams to provide feedback to the DBTL efforts and to meet critical project milestones related to strain performance, (3) to expand Test capabilities via the onboarding and maintenance of new bioreactor capacity, (4) to conduct pan-scale DBTL efforts with the target-host pairs, and (5) to provide process data to the Integrated Analysis team for TEAs and LCAs to inform DBTL priorities. Overall, this task leverages BETO investment in scale-up and scale-

| WBS:                      | 2.5.3.104h            |
|---------------------------|-----------------------|
| CID:                      | NL0030036h            |
| Principal Investigator:   | Dr. Deepti Tanjore    |
| Period of<br>Performance: | 10/1/2016 - 9/30/2019 |
| Total DOE Funding:        | \$1,900,000           |
| DOE Funding FY16:         | \$0                   |
| DOE Funding FY17:         | \$400,000             |
| DOE Funding FY18:         | \$400,000             |
| DOE Funding FY19:         | \$1,100,000           |
| Project Status:           | Ongoing               |
|                           |                       |

down activities at the Advanced Biofuels and Bioproducts Process Development Unit (ABPDU) and the Integrated Biorefinery Research Facility (IBRF), as well as other partner institutions with existing bioprocess development capabilities (e.g., bioprocess development with filamentous fungi at Pacific Northwest National Laboratory). Additionally, the Integration and Scaling task acts as a liaison to other BETO-funded consortia, such as the Bioprocessing Separations Consortium, the Chemical Catalysis for Bioenergy Consortium, and the Consortium for Computational Physics and Chemistry.



### Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

Technical accomplishments to date include two pilot-scale runs of the deacetylation, mechanically refining, and enzymatic hydrolysis process at the IBRF to produce a self-consistent, highly characterized hydrolysate stream for the ABF, the majority of which has been distributed to the partner institutions for use in DBTL and scale-up experiments. Ongoing work in hydrolysate production includes leveraging new separations techniques being implemented at the pilot scale to be able to produce highly concentrated, clarified sugar streams for the ABF partners. For all three target-host pairs, the Integration and Scaling task has conducted bioprocess development in direct support of DBTL efforts to improve strain performance and to benchmark the difference between shake flasks and bioreactor cultivations. Additionally, a critical round-robin experiment was conducted between the ABPDU and IBRF using the Pseudomonas putida-muconic acid target-host pair as an initial example. These results highlighted good agreement between the facilities, indicating that the ABF is able to produce internally consistent results at different institutions, even with some differences in equipment configuration. Additional round-robin experiments are planned in FY 2019 for the Rhodosporidium toruloidesterpene target-host pair and the Aspergillus pseudoterreus-3-hydroxypropionic acid target-host pair. In FY 2019, a pan-scale test was also initiated to inform DBTL efforts using the *P. putida*-muconic acid target-host pair as an initial example. Lastly, onboarding new bioreactor capacity has significantly increased the Test capability of the ABF by multiple folds.

# **Outline of Technical Accomplishments**

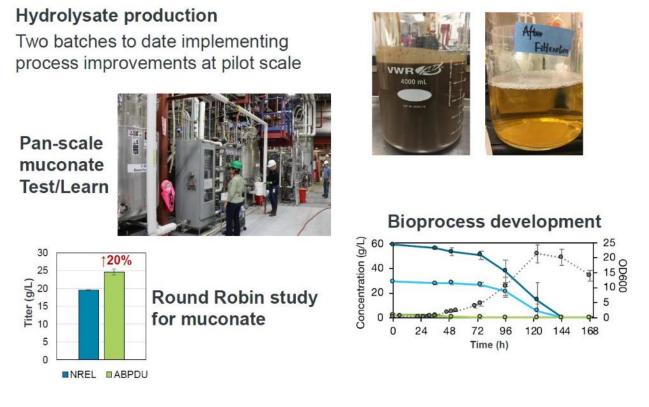


Photo courtesy of Agile Biofoundry Consortium

### **OVERALL IMPRESSIONS**

• This subproject focuses on process scale-up and providing standardized deacetylation and mechanical refining hydrolysates for members and external partners. Overall, the team is making good progress. A

major suggestion would be to develop a more systematic procedure for facilitating scale-up. In particular, the team should focus on identifying the key factors involved in scale-up and optimization in order to accelerate this process and improve the broader impact of this work.

- This group focuses on providing hydrolysate feedstocks, testing ABF strains at various scales, and providing fermentation data to the Learn team. Scaling up a process is an important step in de-risking, and collecting fermentation data at bench scale is important for guiding project decisions. The team is making a strong effort to generate high-quality data and fully characterize the system; for example, omics analysis at multiple scales, closing the carbon balance, and cross-site validation. They are working on a better understanding of the impact of different scales on cell physiology, and are implementing new small-scale culturing techniques. Improvements could be made by defining clear goals and integrating this team better into the overall DBTL workflow.
- Process and integration is an underserved area and often an afterthought in new projects and products. In particular, a lack of scale-up and scale-down consistency is often hard to come by. This project is developing a core competency by standardizing substrates (especially relevant to biomass-derived complex substrates) and pan-scale test methods. So-called "round-robin" testing across sites is helping to develop what is more broadly known to industry as technology transfer expertise, which is how success (or failure) is often determined (e.g., for milestone testing, go-no-go decisions). In a multisite environment, this is an absolute must-have competency for measurable and fact-based success. As more projects come online, more host-target pairs and substrates will need to be put through this process, so it is likely this area will emerge as a priority for additional funding and effort.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewer for the positive and constructive feedback. We agree with the reviewer that there should a systematic procedure for facilitating scale-up. At this time, as we are working with non-canonical hosts, we are still in the process of developing unique cultivation protocols for the scale-up of each target-host pair and at economically viable titers, rates, and yields. Our end-of-project goal is to "Demonstrate target-host pair production of at least 3 molecules at 10 g/L, 100 mg/L/hr, at 40% of theoretical yield from deacetylation and mechanical-refining and enzymatic hydrolysis (DMR-EH) at 10 L." During the process of achieving this goal, we will be learning many nuances of scale-up, some of which can be broadly applied to both canonical and non-canonical hosts. We are documenting these results and look forward to publishing them. In FY 2020 and beyond, given continued support, we should be able to develop a procedure that can be adopted widely for many target-host pairs. We are hopeful that the omics approach to identifying variances in microbial culture behavior and thereby performance with scale will be insightful and provide the necessary guidance to design target-host pairs for robustness during scale-up.
- We appreciate the positive feedback from the reviewer. The reviewer identifies a particular aspect of this task to be essential, namely integration with the DBTL cycle. We are in complete agreement with this feedback, and as described during the presentation, we are actively working on this with the pan-scale Test and Learn activities in *P. putida* and *R. toruloides*. At this time, we consider the scale-up task to be a part of the Test arc of the DBTL cycle. Our most recent scale-up campaigns, generating muconic acid (at 600 L) and fatty alcohols (at 300 L), provided us with the samples and necessary omics and fermentation data to engage with the Learn team. This coordination with the Learn team will allow us to integrate better with the Design and Build arcs in the future. We expect to be more fully integrated in the full DBTL cycle by the end of FY 2021, by which point some of the design principles would be based on our learnings from the scale-up studies.
- We thank the reviewer for this comment. We agree with the feedback and will further our round-robin studies by including target-host pairs such as 3-hydroxypropionic acid-*Aspergillus niger* in FY 2020. We will also publish our learnings for industrial and academic entities to benefit from our findings. Further,

the FY 2020 milestone of ABF is being constructed such that reproducibility at separate locations is a prime subject of our studies: "Reproducibility of three distributed Test unit operations, including bioreactor scale-up quantified through comparison of results post data quality assurance for on-site vs. off-site sample analysis." Future scale-up and round-robin studies will allow us to develop a standard template with necessary know-how that can benefit future endeavors in industrial biotechnology.

# ABF – INDUSTRY ENGAGEMENT AND OUTREACH

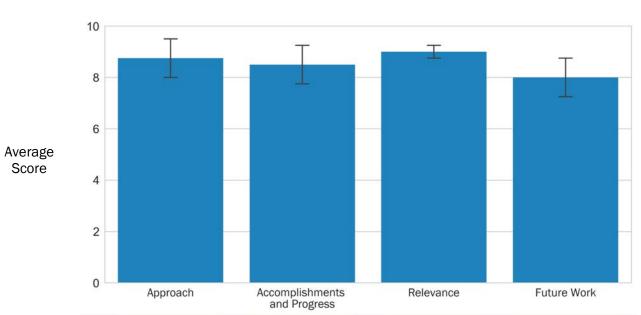
### Agile BioFoundry Consortium

### PROJECT DESCRIPTION

The objective of the ABF is to develop infrastructure to support industrial biotechnology, while understanding the needs of the industry is critical to achieving this goal. In support of this, the ABF Industry Engagement and Outreach (IEO) team organizes and facilitates interactions with industry, providing feedback from the industry stakeholder community to the ABF and BETO, which supports decision making and project planning. The activities of the team also aim to increase the visibility of the ABF and attract collaborators from academic and industrial communities. The goals of this task are accomplished through the workings of three highly interwoven, strategic focus areas (SFAs): Assessment,

| WBS:                      | 2.5.3.104i          |
|---------------------------|---------------------|
| CID:                      | NL0030036i          |
| Principal Investigator:   | Dr. Phil Laible     |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$900,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$200,000           |
| DOE Funding FY18:         | \$300,000           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

Outreach, and Interactions. For the Assessment SFA, an Energy I-Corps approach is used to understand the needs of the biomanufacturing industry by interviewing and surveying its members. In the Outreach SFA, members work to manage the ABF public profile and disseminate ABF information and resources to industrial, academic, governmental, and public stakeholders. For the Interactions SFA, the main goal is the coordination of community-building activities. This includes Industry Days and workshops to ensure research effectiveness and industry responsiveness. This SFA also facilitates interactions with the IAB. The IEO team collectively plans panels and sessions at key industry conferences. Overall, the IEO task contributes to the alignment of



### Weighted Project Score: 8.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

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.



Photo courtesy of Agile Biofoundry Consortium

### OVERALL IMPRESSIONS

• The goal of this subproject is to identify and remove obstacles for technology transfer. In addition, they proposed to expand the number of industrial partners. This task is necessary to broaden the impact and relevance of the ABF. Overall, the team is making solid progress. The project would benefit by including explicit milestones in order to evaluate progress and to define success.

- It is heartening to see industry engagement as a "first-class citizen" component of the ABF strategy. The team describes a comprehensive approach to promoting ABF and gaining guidance from industry to ensure future relevance. This approach is built on pillars of passive engagement, active engagement, and third-party assessment and based on quantitative measures of engagement. It appears to be impactful.
- The industry engagement group ensures the ABF is working on projects that are of interest to industry, and that the technologies can be transferred. They are looking to attract academic and industry collaborators and licensees. Knowledge is gathered through interviews, surveys, and listening days. The team is well coordinated at gathering this information, and providing the industry feedback to the experimental groups. More activities are planned for the future, such as hosting panel discussions at conferences.
- Maintaining and refining a customer focus and relevance is a critical objective to be achieved, in part, by gaining highly valuable industry feedback and via IAB interactions. The current effort is doing so with its outreach, interactions, and assessment approach. Real traction will depend on to what extent the results influence stakeholders to evolve/refine the ABF approach and mission.

### **RECIPIENT RESPONSE TO REVIEWER COMMENTS**

• Regarding milestones, we could have explicitly shown that we have a detailed project plan that includes quarterly IEO task milestones. Each IEO subtask has two or three specific, measurable, attainable, realistic, and time-related (SMART) milestones throughout the year. Joint monthly IEO/management discussions help to keep the subtask on track and accountable. Since these internal milestones might have been confused with formal ABF milestones, we erred on the side of not showing them. They can be made available to the review team upon request.

# **ABF – DIRECTED FUNDING OPPORTUNITY MANAGEMENT**

### Agile BioFoundry Consortium

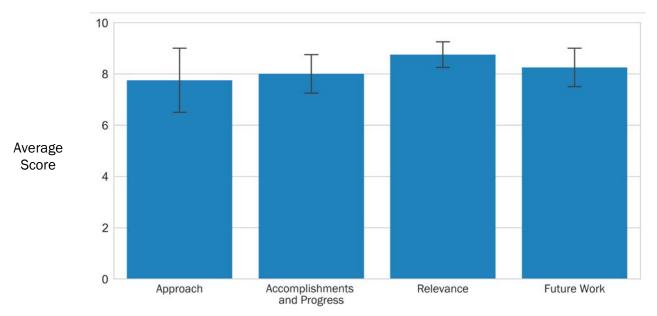
### **PROJECT DESCRIPTION**

This presentation will present a summary of all CRADAs between the ABF and industry as a result of the ABF Directed Funding Opportunity (DFO) and the recent BioEnergy Engineering for Products Synthesis (BEEPS) Funding Opportunity Announcement (FOA). This will include a review of how the ABF leadership team managed the proposal review process for the ABF DFO.

| WBS:                      | 2.5.3.104j          |
|---------------------------|---------------------|
| CID:                      | NL0030036j          |
| Principal Investigator:   | Dr. Blake Simmons   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$5,000,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$5,000,000         |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Ongoing             |
|                           |                     |

### Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

### OVERALL IMPRESSIONS

- This subproject focuses on external engagement through partnerships and external funding agreements. The major success was the creation of a template for the CRADA process that works with all of the ABF partners. This resulted in a streamlined process and increased transparency. Overall, these activities are critical to the success of the ABF. In addition, opening up the ABF to external partners though different funding mechanisms is a critical step in broadening the impact of the foundry. Developing robust management and review/evaluation protocols is clearly important.
- ABF/BETO has established FOAs/DFOs in order to establish formal engagements that will be critical for dissemination of ABF approaches ensuring they maintain relevance, and for providing feedback to ABF regarding its technical strategy and operations. The funding mechanism is effective in that it incentivizes industry while mainly providing funds within the national laboratory system. This, along with cost share, ensures that industrial partners are vested in the research and in its success. Throughout the process, the ABF team has noted ways to improve the engagement. In particular, the administrative burden for establishing these CRADAs has been substantial, which has led the team to innovate on the process for future engagements.
- Development of funding opportunities to drive the industry-oriented mission of the ABF is critical to its success. The description of DFO and FOA successes shows progress in fulfilling this mission, as well as establishing a scoreboard. Difficulty in bringing some CRADAs to closure highlights the challenges of working with customers with different business needs. A nonnegotiable CRADA template was developed and may streamline this process in the future. What level of traction this provides remains to be established, as well as whether it changes the customer landscape going forward. This should be tracked to determine impact/benefit, and fed back into business development to refine messaging, funding, and collaborative opportunity development.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for these comments and agree with all of the issues raised.
- We hope that the lessons learned from this DFO process will assist in future efforts. In particular, the development of a template CRADA should significantly improve overall efficiency of getting projects underway in a timely fashion.
- We agree that tracking projects and monitoring the rate of placing contracts and initiating projects will be a key metric, and we will be sure to collect and share those data.

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# **BIOCHEMICAL CONVERSION**



# TECHNOLOGY AREA

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## INTRODUCTION

The Biochemical Conversion Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 30 projects were reviewed in the Biochemical Conversion session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$82,692,210, which represents approximately 9.6% of the BETO portfolio reviewed during the 2019 Project Peer Review. During the Project Peer Review, the principal investigator (PI) for each project was given 25–30 minutes to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the Biochemical Conversion Technology Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. Ian Rowe as the Biochemical Conversion Technology Area Review Lead, with contractor support from Mr. Clayton Rohman (Allegheny Science & Technology). In this capacity, Dr. Rowe was responsible for all aspects of review planning and implementation.

### **BIOCHEMICAL CONVERSION R&D OVERVIEW**

The Biochemical Conversion Technology Area focuses on research and development (R&D) of biological processes that convert biomass to biofuels and bioproducts. Biochemical processes within the BETO portfolio can either stand alone as an entirely biological operation from feedstock to final product, or they can act as single steps within larger pathways that employ other nonbiological conversion technologies. Projects presented in the Biochemical Conversion session cover a wide variety of scientific disciplines, generally targeting one or more of four purposes: (1) to deconstruct lignocellulose into biochemical intermediates, such as cellulosic sugars (both five-carbon [C5] and six-carbon [C6]) and lignin; (2) to biologically upgrade such intermediates into fuels and bioproducts; (3) to biologically upgrade thermochemical intermediates (gaseous or aqueous); and (4) engineering bioprocesses to valorize waste streams.

Since Fiscal Year (FY) 2016, BETO's state-of-technology (SOT) model for tracking technological progress has assumed that all C5 and C6 sugars would be converted to fuels, while lignin would be valorized to bioproducts. This is the framework in which most of the core "pathway-specific" research done within the biochemical conversion R&D portfolio fits. The assumptions associated with the SOT are critical for certain national laboratory annual operating plan (AOP) projects that seek to verify BETO SOT pathways. Other projects within the biochemical conversion portfolio aim to enable the bioeconomy more broadly; most of the competitive funding opportunity announcement (FOA) projects fall within this "enabling" category.

Cost-effective and energy-efficient biochemical deconstruction is the first half of most of the efforts represented in this chapter. The low-temperature deconstruction of biomass by dilute acid or mild deacetylation treatment followed by enzymatic hydrolysis is the common process for generating intermediates within the biochemical conversion R&D portfolio. Other intermediates, such as those produced from the processing of algal biomass or from the biological deconstruction of plastics, represent additional enabling approaches to generating intermediates that can then be upgraded. The second half of the conversion processes discussed here involve a biological upgrading approach. Projects which upgrade cellulosic sugars are the focus of the portfolio; however, processes that use other intermediates such as syngas, lignin, and plastic-derived monomers are also being investigated.

A key to developing cost-competitive cellulosic biofuels is reducing the processing and capital costs and improving the efficiency of separating and converting cellulosic biomass into fermentable sugars. Current R&D focuses on high-yield feedstocks, more efficient enzymes, and more robust microorganisms to advance biochemical conversion processes. The resulting advanced biochemical conversion technologies will increase fuel yields in future biorefineries and enable a bioeconomy that leverages an abundant, renewable carbon feedstock.

## **BIOCHEMICAL CONVERSION REVIEW PANEL**

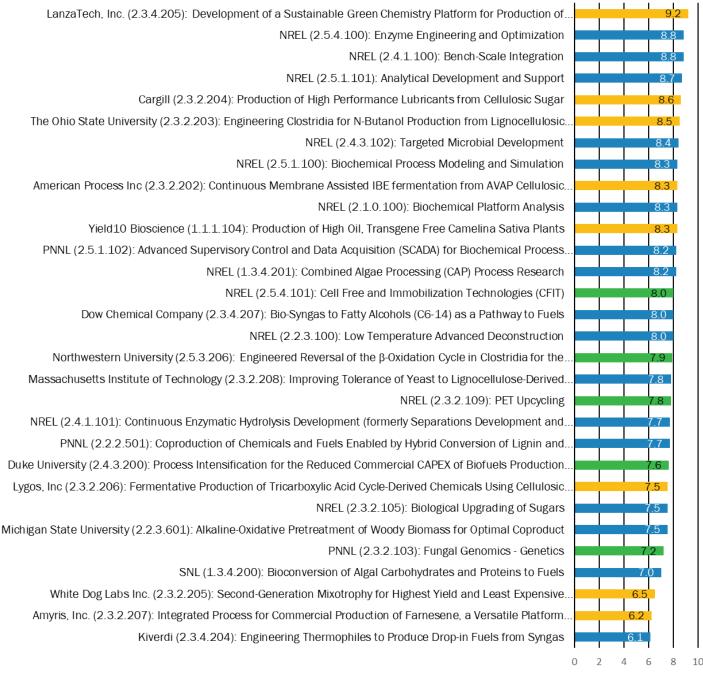
The following external experts served as reviewers for the Biochemical Conversion Technology Area during the 2019 Project Peer Review:

| Name            | Affiliation                                |
|-----------------|--|
| Charles Abbas*  | iBiocat                                    |
| Farzaneh Rezaei | Pivot Bio                                  |
| Chris Rao       | University of Illinois at Urbana-Champaign |
| Ben Gordon      | Broad Foundry                              |
| Steve Van Dien  | Persephone Biome, Inc.                     |
| Lood Doviouor   |  |

\*Lead Reviewer

# **TECHNOLOGY AREA SCORE RESULTS**





Sunsetting Ongoing New

## BIOCHEMICAL CONVERSION REVIEW PANEL SUMMARY REPORT

#### Prepared by the Biochemical Conversion Review Panel

The Biochemical Conversion Review Panel was tasked to provide feedback using criteria selected by BETO to assess the biochemical conversion projects based on project outlines, abstracts, and updates provided in oral and written presentations by project PIs and teams. Based on the summary provided from the different reviewers, most reviewers shared similar assessments of the projects reviewed, with five projects that the lead reviewer feels were underrated or overrated based on deliverables. Some of these discrepancies can be explained on the basis of technical success versus commercial viability or the projects being outside of a reviewer's areas of expertise. That is expected given the makeup of the review committee and the criteria used to analyze the projects.

The projects reviewed represented work done at DOE national labs, private well-established companies, small startup companies, and/or university-led research. The projects had different start and completion dates with a range of budgets, levels of difficulty, and challenges. With few exceptions, most of the PIs and project teams responded well by providing responses to the criteria in BETO guidelines, with some providing extensive details that assisted the reviewers in responding to criteria selected. The projects that did not follow the required format for reporting progress achieved an overall lower average score in spite of the fact that they had technical depth and showed good progress on achieving the targets outlined. The review process went smoothly, and presenters did a great job highlighting the progress of their work and technical merits and deliverables while allowing sufficient time for reviewers' questions and answers. The reviewers were impressed with the quality of the presentations that further provided clarity on the soundness of technical plans and deliverables.

#### IMPACT

The current funded projects in the Biochemical Conversion Technology Area represent several parallel approaches that deploy a range of bio-based omics technologies that have been developed over the past two decades to help address the economic challenges for the processing of biomass lignocellulosic feedstocks. The investment made by BETO is necessary in light of the knowledge gaps that increase the uncertainty of economic viability for the use of these feedstocks. These gaps are not being addressed by industry as they require mid- to long-term funding, and as a result compete with short-term industrial projects that increasingly focus on making existing biorefineries more efficient for conventional feedstocks.

The BETO-funded projects attempt to address challenges to industrial development presented by biochemical conversion in achieving cost-effective bioprocessing of biomass to biofuels, chemicals, and polymers at a biorefinery. This requires the development of cost-effective, rapid methods for compositional analysis of the starting incoming materials and the processed separated streams, as well as hydrolysis components which include sugars, phenolic compounds, and cations. It also requires cost-effective commercial enzymes that can be used to effectively hydrolyze pretreated or untreated biomass to release and separate the carbohydrates from the lignin and other organic and nonorganic constituents. Additionally, a biorefinery requires robust microbes that can withstand industrial processing conditions, can operate at pH and temperatures under anaerobic or microaerophilic conditions that are far from optimal conditions, and that can survive common process upsets. The selection of robust microbes that can be developed for biofuel and bio-based chemicals must take into account the resistance to inhibitors that are generated during pretreatment steps such as degraded sugars (furfural, hydroxymethyl furfural, levulinic acid, formic acid); lignin degradation products (phenolic compounds); and acetic acid and other cations (sodium, calcium, iron, magnesium, etc.) that are toxic, required for growth, or can result in imbalanced growth. For optimized conversion, improved online process tools need to be available, as well as biochemical process modeling and simulation capabilities. The current projects within the Biochemical Conversion portfolio address these issues directly and indirectly.

The analytical development and support platform at the National Renewable Energy Laboratory (NREL) is at the forefront of developing analytical methods for compositional analysis of biomass feedstocks. While these methods are well developed for research purposes, they are still costly and require a dedicated research lab staff with technical expertise—something that is not readily available to industry. The emerging lignocellulosic biomass industry also faces challenges in the cost and availability of effective cellulase enzymes. The enzyme engineering and optimization platform at NREL seeks to optimize a cellulase-enzyme blend that is more effective at hydrolysis of sodium hydroxide-treated corn stover deconstructed through low-temperature deacetylation and mechanical refining (DMR). This effort is necessary and worthwhile. BETO should continue to support and expand cellulase enzyme development to provide more cost-effective enzymes.

The development of new microbes for production of cellulosic ethanol, *n*-butanol, other alcohols, and lipids from sugars, as well as the use of syngas as a feedstock, is an active area of industrial research. Some of these projects are carried out in partnership with DOE national labs and university-based research. Among the projects funded within the biochemical conversion theme that look promising are:

- The engineering of acetogenic *Clostridia* to improve syngas utilization for the production of acetone and other downstream fuel and commodity products directly from biomass syngas using a novel energy-conserving route (LanzaTech, Oak Ridge National Laboratory [ORNL])
- The Ohio State University project for engineering *Clostridia* for *n*-butanol production from lignocellulosic biomass and recaptured CO<sub>2</sub>
- The production of high-performance lubricants from lignocellulosic sugars (Cargill)
- Biosyngas to fatty alcohols (C6–C14) as a pathway to fuels (Dow Chemical Company/LanzaTech/Northwestern University)
- The Continuous Membrane-Assisted isopropanol, butanol, and ethanol (IBE) fermentation from American Value Added Pulping (AVAP<sup>TM</sup>) cellulosic sugars (American Process Inc.). The production of high oil, transgene-free camelina hybrids (Yield10 Bioscience).

All of these five projects should be further evaluated for technology transfer and commercial scale-up opportunities.

### INNOVATION

Most of the innovative projects reviewed received a score lower than 8.0. This reflects the higher degree of risk and technical challenges inherent in innovation that need to be addressed in funding these projects. These projects were primarily led by universities or small to midsize startup companies. Some examples of these are:

- Amyris project focused on the production of farnesene from lignocellulosic sugars (Amyris/Renmatix/Total)
- Engineering of thermophilic bacteria for production of drop-in fuels from syngas (Kiverdi/Lawrence Berkeley National Laboratory [LBNL]/NREL)
- The use of a Dynamic Metabolic Control (DMC) approach for production of biofuels and chemicals from lignocellulose with lower capital expenditures (CAPEX) (Duke)
- Engineering the reversal of β-oxidation cycle for the production of fuels and chemicals from syngas (Northwestern University/LanzaTech)
- Use of mixotrophs for highest yield and lowest cost for biochemical production (White Dog Labs)

- Fermentative production of tricarboxylic acid cycle (TCA)-derived chemicals from cellulosic sugars (Lygos)
- Improving tolerance of yeast to lignocellulose-derived sugars (Massachusetts Institute of Technology).

By funding these projects, BETO has shown a higher tolerance to risk to ensure new disruptive technologies are developed. A common weakness in some of these higher-risk projects is the use in some cases of novel microbes, poorly characterized or highly toxic feedstocks, and/or novel processes and staging. The target product selected and cost associated for recovery of finished products and detoxification of feedstocks were some of the challenges encountered, as well as low productivity, low yields, and low titers of products. These projects could have benefited greatly by providing a proof of concept or short feasibility study and a detailed techno-economic analysis (TEA) prior to multiyear funding.

Some examples of innovative projects that incorporated risk-management approaches and therefore were more successful technically are:

- The production of high-performance lubricants from lignocellulosic sugars (Cargill)
- Biosyngas to fatty alcohols (C6–C14) as a pathway to fuels (Dow Chemical Company/LanzaTech/Northwestern University)
- Production of high oil, transgene-free camelina hybrids (Yield10 Bioscience)
- Continuous Membrane-Assisted IBE fermentation from AVAP cellulosic sugars (American Process Inc.)
- Development of a sustainable green chemistry platform for production of acetone (LanzaTech).

A closer look at the more successful projects indicate that these projects were well executed. Two of these projects involved strong partners and industrial know-how. The American Process Inc. project is a good example of a highly integrated project that uses lignocellulosic sugars for the production of IBE and what looks like a promising, cost-effective recovery of end products. These projects adapted their plans to meet research needs using a stage-gate approach with deliverables and milestones, thereby incorporating appropriate risk management into the innovation process to facilitate and accelerate innovation as opposed to hindering or curtailing it.

### SYNERGIES

There are several projects that were well developed with sound technical approaches and synergies that focused on a range of topics, including the development of processes for the production of biofuels and chemicals from lignocellulosic-derived sugars and syngas produced from lignocellulose, that use cellular or algal biomass as feedstocks. These synergies can be used to advance the use of these feedstocks by grouping the projects together based on the carbon source used as a fermentation feedstock. They can also be grouped based on the choice of microbial system and processing aids used. For example, some of these projects aim to develop new strains of the conventional yeast *Saccharomyces cerevisiae* for the production of ethanol from lignocellulosic hydrolysate sugars, other nonconventional oleaginous yeasts (*Lipomyces, Cryptococcus*, etc.) for oils, the use of bacteria (both aerobic and anaerobic; mesophilic and thermophilic), or selected strains of microalgae. These projects can also be grouped based on the target product(s). The products include—in addition to ethanol, algal oils, fatty acid alcohols, acetone, *n*-butanol, isopropanol, farnesene, mono and C15 terpenes—organic acids such as lactic and butyric, other TCA organic acids, the amino acid aspartic acid, 2,3-butanediol (BDO), the biopolymer polyhydroxyalkanoate (PHA), and monoethylene glycol (MEG).

Although the original goals of these funded projects involved multiple approaches and parallel platforms to use lignocellulosic feedstocks with different microbes for different target products, it may be possible to aid these projects to more effectively achieve their goals. This can be accomplished through a collaborative approach to

assess bottlenecks in each project. BETO can provide support by assisting with TEA, the development and implementation of analytical tools, improving process monitoring, and process design and engineering. These capabilities already exist within DOE labs, in particular at NREL and Pacific Northwest National Laboratory (PNNL), but are not currently deployed to support external projects supported by BETO. Creating a mechanism for this open collaborative exchange would be worth pursuing, and the projects can be helped by providing access to DOE in-house capabilities. Other tools that the external projects may need that are not available at DOE labs can be pursued with external partners as necessary.

An example of how this approach is used are the platform projects focused on the development of processes that use all of the constituents of lignocellulose to improve processing of these feedstocks by greater valorization of lignin and other byproducts such as fermentation-derived microbial biomass. There are four complementary projects that use a fungal genomics platform: the production of a C15 terpene hydrocarbon for use as a fuel and the organic acid maleic acid at PNNL; the Hybrid Conversion of Lignin and Bioconversion Intermediates at Idaho National Laboratory (INL), NREL, and PNNL to produce oleaginous yeast and other cellular biomass; the combined algal processing (CAP) to produce precursors to polyurethane, butyric acid, or hydrocarbons at NREL; and the bioconversion of algal carbohydrates and proteins to PHA and lactic acid at Sandia National Laboratories (SNL). These projects, while unrelated, have great synergies and can benefit from an open collaborative approach across the four DOE labs. The above projects, when taken in the collective, bring together an excellent dedicated team of scientists within the DOE national laboratory system. BETO can use a similar approach to group other external projects to assist these projects in achieving their targets through an open innovation model by facilitating the dialogue and exchange between these different projects.

### FOCUS

There are several gaps that need to be addressed with greater support from BETO. The areas that come to mind are:

- Developing new cellulases and supporting more enzyme discovery work, as the current cellulase cost needs to be reduced and effectiveness needs to be improved to cover a broad range of lignocellulosic feedstocks. Enzymes form extremophilic organisms that are well suited to industrial applications but have not been used much within industry. Greater use of directed evolution and rational protein design and engineering tools are needed to improve enzyme stability and performance.
- **Developing more robust, cost-effective analytical tools to measure composition of lignocellulose.** The current wet chemistry approaches require a considerable investment of funds and manpower while the new spectroscopic analytical approaches are expensive and require routine instrument calibration by an experienced operator. Expediting this work with companies that are providing the equipment and funding of nanoscale measuring instruments can drive innovation and cost down.
- Exploiting more of the fungal genomes that have been sequenced by the DOE's Joint Genome Institute (JGI) to use and mine additional microbes and genes for metabolic engineering using the fungal genome portal or MycoCosm.<sup>1</sup> Since the publication in 2011 in *Mycology Journal* of the article on fueling the future with fungal genomics, there has been little progress on industrial applications using the fungal sequences analyzed.<sup>2</sup> The fungal genomics projects within PNNL need to be expanded to include other DOE labs and university-based and private company research. There are many nonconventional yeasts where genomics tools are now available. The Lygos project attempted to

<sup>&</sup>lt;sup>1</sup> U.S. Department of Energy Joint Genome Institute. "MycoCosm: The Fungal Genomics Resource." http://jgi.doe.gov/fungi.

<sup>&</sup>lt;sup>2</sup> Grigoriev, Ivor V., Daniel Cullen, Stephen B. Goodwin, David Hibbett, Thomas W. Jeffries, Christian P. Kubicek, Cheryl Kuske,, et al. 2011. "Fueling the Future with Fungal Genomics." *Mycology Journal* 2:3, 192–209. https://doi.org/10.1080/21501203.2011.584577.

engineer the yeast *Pichia kudriavzevii* for the production of aspartic acid but these efforts were abandoned prematurely in favor of *Corynebacterium glutamicum*.

• Adopting the use of TEA and in-depth modeling for all projects. It was not clear from the presentations that all of the projects have received rigorous in-depth analysis. Some of the PIs mentioned that a TEA was carried out but there does not seem to be a consistent approach. An independent TEA should be used to confirm some of the assumptions made by researchers on what represents technical targets for a successful project.

As a point of emphasis, BETO has endeavored to find a careful balance between new high-risk projects at universities and startup companies that are not easily funded by industry and other government granting agencies, while supporting lower-risk projects with the involvement of industrial partners from well-established companies. The preceding summary clearly represents the need to support new, potentially disruptive technologies.

### TECHNOLOGY DEVELOPMENT PIPELINE

Most of the projects reviewed were at the early- to mid-stage development. Some of the BETO-funded earlystage development projects represent higher risk when compared to industrial in-house projects that are funded at existing biorefineries. They also lacked an in-depth techno-economic modeling analysis or TEA that is required for industrial projects. The more advanced mid-stage projects had already gone through a proof-ofprinciple or feasibility study, and therefore had a lower inherent risk. While most of these projects will be technical successes, without a much more in-depth analysis it is difficult to determine commercial viability in the biofuels and bio-based chemical markets. Based on past experience, companies seek funding for higherrisk projects when there is a lack of clarity on new technology and uncertainty about the markets.

### RECOMMENDATIONS

1. Increase investment in the development of rapid analytical tools to lower costs and create more effective cellulases and more robust industrial organisms.

The absence of cost-effective analytical methods that can be readily deployed and used for routine analysis continues to hinder industrial development of lignocellulosic biofuels. This is illustrated in the current situation with processes outlined by the U.S. Environmental Protection Agency (EPA) for renewable identification number (RIN) credit applications from first-generation ethanol plants that aim to use the corn fiber component in corn kernels.

Beyond the analytical challenges that the emerging lignocellulosic biomass industry faces are the cost and availability of effective cellulase enzymes. The enzyme engineering and optimization platform seeks to optimize a cellulase-enzyme blend that is more effective at hydrolysis of low-temperature deconstructed corn stover. While addressing the current limitations to DMR hydrolysis has great relevance to this feedstock, it is not clear if there is also a direct benefit that will reduce the cost of cellulases for other lignocellulosic feedstocks. Expanding the testing of the new cellulase-enzyme blend to other feedstocks including corn kernel fiber would be a positive development in supporting the existing U.S. corn-based biofuels industry. Beyond the current commercial suppliers of cellulase, there has been limited recent development of cellulases outside of the efforts by some research universities, small enzyme manufacturers, startup companies, and NREL. This effort is worthwhile and needs continued BETO support to spur and expand cellulase enzyme development to provide more cost-effective enzymes.

There is also the need to ensure that the strains of microbes being engineered can meet chemical and physical stresses that are common in large-scale fermentation such as the presence of toxic inhibitors and toxic end products, nutrient deficiency, poor mixing condition, poor heat transfer, and vessel back pressure. Successful fermentations also require good temperature, sufficient aeration, and pH control, which are not readily attainable in high-solid lignocellulosic fermentations. There are well-developed industrial microbes in wide use

and tapping into genes to engineer new pathways should be used when necessary, thereby reducing the risk associated with using novel organisms with poor productivity. Gene-editing technologies that have recently gained acceptance will help pave the way for more efficient, well-targeted genes that improve metabolic flux. The BIOREFINE-2G European Union-funded project that was recently completed is a good example of the use of gene-editing technology to develop more commercially attractive processes for efficient conversion of pentose-rich side streams from biorefineries into dicarboxylic acids for use as precursors for bio-based polymers (https://cordis.europa.eu/project/rcn/110369/reporting/en).

#### 2. Implement a rigorous, independent TEA process for all projects.

End-product titers need to be quantified, process yields from all sugars/carbon sources need to be determined, and productivity needs to be calculated. All yields and productivity measurements should be clearly specified and not reported on the basis of unspecified inputs or baseline numbers that are not provided.

# **3.** Expand the advisory team from the existing industries and work towards greater industrial involvement.

All project teams need to have chemical engineers, preferably with industrial scale-up experience. This is necessary in view of the fact that technical successes in engineering microbes do not always lead to commercial success. Greater emphasis should be placed on the cost-effective recovery of end products. Bridging the gap between bench scale and industrial scale is needed for deployment of research projects at industrial biorefineries.

## **BIOCHEMICAL CONVERSION PROGRAMMATIC RESPONSE**

### INTRODUCTION/OVERVIEW

The Biochemical Conversion Program expresses its immense gratitude to the reviewers for their thoughtful recommendations and the significant time and effort they each put into the panel and the subsequent feedback sessions. The reviewers stated that the investments made by BETO into Biochemical Conversion R&D are important mechanisms for addressing the higher-risk gaps in capabilities and knowledge that carry a significant amount of uncertainty. The funding of such technologies that have a mid- or long-term time horizon often compete for the immediate needs of industry and are thus underexamined. The panel also identified the analytical development tasks within the portfolio as a specific strength which can enable the field of in-line compositional analysis of biochemical processes to advance.

The synergies that exist within the portfolio were also specifically pointed out by the panel. The active connection between the projects that work biomass pretreatment and deconstruction techniques and those that focus on microbial development was seen as a strong collaborative effort. Similarly, praise was given to the portfolio connection between efforts on deacetylation and mechanical refining pretreatment with the enzyme engineering project, which focuses on designing an enzyme blend that specifically works with that pretreatment strategy.

The panel pointed toward more effective cellulase enzymes as a potential area of the portfolio that may require additional resources. The reviewers stated that BETO could address the industrial gap in capabilities and the development of robust microbes that can tolerate chemical and physical stresses present in many biochemical processes.

The following section specifically address the three major recommendations from the review panel.

# Recommendation 1: Increase investment in the development of rapid analytical tools and lower-cost/more effective cellulases.

The program agrees with the panel's assessment that in-line, rapid analytic tools are vitally important to advancing the bioeconomy. Such technologies are essential to allowing real-time measurements and process control within intricate biochemical conversion processes. BETO continues to fund our existing projects devoted to analytical development and support and we are specifically motivated to enable industrially relevant in-line analysis tools. This is reflected in recently established efforts on this subject at PNNL. BETO also continues to fund efforts in cellulase development and points toward the long history of successful enzyme development from BETO-funded work as substantial progress already made toward this recommendation.

### Recommendation 2: Implement a rigorous, independent TEA process for all projects.

BETO acknowledges the vital importance of TEA in ensuring that the efforts undertaken by this Office are sound and justified. Every competitive project within the biochemical conversion portfolio has rigorous TEA requirements and must pass an initial verification (including a robust TEA discussion) prior to receiving the bulk of the awarded funds. Similarly, our AOP efforts at the national labs often have required TEA components associated with individual projects. Lastly, there are several AOPs within the portfolio that are specifically dedicated to performing such analyses for large portions of the portfolio and comparing them to each other. Given all of these current extensive efforts, BETO believes that our existing efforts in TEA are sufficient; however, BETO will make efforts to better communicate our existing TEA efforts to future reviewers.

### **Recommendation 3: Improved industrial involvement.**

As often as possible, BETO targets stakeholder input in the form of workshops, listening days, requests for information (RFIs), and one-on-one informal discussions with external partners in the bioeconomy. Given the smaller scale of much of the work within this R&D portfolio, requiring dedicated chemical engineers on each project within given funds would not be feasible or suitable. Although there is no dedicated "advisory team" for the biochemical conversion portfolio, members of the conversion team regularly attend relevant industrial and academic events to stay abreast of the current SOT within the industry. We feel that this is an area in which BETO excels.

# PRODUCTION OF HIGH-OIL, TRANSGENE-FREE CAMELINA SATIVA PLANTS

### Yield10 Bioscience

### **PROJECT DESCRIPTION**

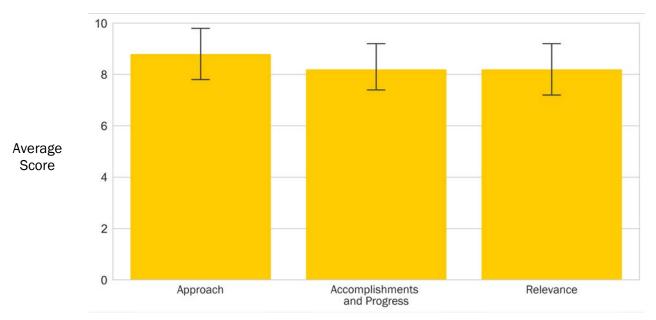
The objective of this project was to develop a *Camelina sativa* feedstock with significantly increased seed yield and oil content to maximize oil yields per acre. *Camelina* is an oilseed crop with high potential as a bioenergy feedstock due to its high oil content, low inputs for cultivation, frost tolerance, and short growth cycle (80–110 days). To accelerate market entry, a next-generation technology was used to develop genetically-modified-organism-free plants to provide an expedited path through regulatory approval. This is anticipated to significantly decrease the time and thus the costs of commercialization of these lines.

| WBS:                       | 1.1.1.104               |
|----------------------------|-------------------------|
| CID:                       | EE0007003               |
| Principal<br>Investigator: | Dr. Kristi Snell        |
| Period of<br>Performance:  | 10/1/2015-<br>9/30/2018 |
| Total DOE Funding:         | \$1,996,598             |
| Project Status:            | Sunsetting              |

For this program, current *Camelina* lines were considered to yield, on average, 1,500 lb of seed per acre and possess a seed oil content of 40%. The program had two oil production benchmarks: (1) increase production of seed to 2,500 lb per acre with seed containing 45% oil, and (2) increase production of seed to 3,500 lb per acre with seed containing 60% oil. Hitting the first benchmark would significantly expand the potential of *Camelina* as a crop and would provide the profitability necessary to incent farmers to grow *Camelina*, resulting in the production of renewable feedstock for the bio-based energy and chemical industries. The second benchmark (3,500 lb of seed per acre with 60% oil content) would have a huge impact on the availability of renewable *Camelina* oil for the biodiesel and aviation fuel markets.

### Weighted Project Score: 8.3

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



L One standard deviation of reviewers' scores

The accomplishments of this program demonstrated that genome editing of multiple targets in *Camelina* is technically feasible, despite the complexity of the *Camelina* genome. It also demonstrated that it is possible to increase seed yield while maintaining seed oil content using genome editing. Genome-edited lines achieving up to a 40% increase in seed yield were demonstrated in greenhouse growth studies. In separate experiments, the program also achieved increases of up to 38% in the seed oil content of individual seeds. This increased seed oil content was, however, often accompanied by a decrease in seed yield. These observations demonstrate that carbon flow in *Camelina* can be significantly shifted to seed oil production but that additional research is necessary to concurrently increase or maintain seed yield. Yield10 Bioscience plans to continue to build on these results after the BETO program. During the course of this program, Yield10 Bioscience also demonstrated that lines with single edits, as well as lines with multiple edits, generated using genome-editing technology can be designated as nonregulated by the U.S. Department of Agriculture (USDA) Animal and Plant Health Inspection Service (APHIS) through their "Am I Regulated?" process. Two separate "Am I Regulated?" letters were submitted to USDA-APHIS and edited *Camelina* lines described in the letters were deemed nonregulated by the agency, demonstrating a reduced regulatory path.

The technology developed in this program contributes to the overall understanding of seed oil biosynthesis in oilseed crops and how seed yield and seed oil content can be improved using genome-editing techniques. The technology is thus also relevant to increasing seed and oil yield in related oilseed crops, such as canola.

### **OVERALL IMPRESSIONS**

- The goal of this project is to develop a *Camelina* strain with both increased yield and oil content using a genome-editing technique that would have facilitated regulatory approval compared to other modified crops. The team made increases in both yield and oil content but determined that with the current approach there is a tradeoff between these two metrics, so the final goals were not achieved. Plans are in place for field testing of the best strains. The team also obtained confirmation from the USDA that plants modified using *Agrobacterium* transformation of the clustered regularly interspaced short palindromic repeats (CRISPR)-associated protein 9 (Cas9) were not regulated, as long as no foreign genes were introduced. This could have huge implications for other modified crop development. It would be good to see more projects on crop development, not only to improve yield but also to make them more amenable to downstream conversion.
- The goal of this project was to engineer *Camelina sativa* with increased seed yield and lipid content using a transgene-free approach. While the project did not meet all of its objectives, the results were very promising and merit future work. The major accomplishment was to increase seed yield by 39% while sustaining the oil content. Increasing oil content was more challenging, as this resulted in a reduction in yield. The next step will be to evaluate these lines in the field to demonstrate commercial viability.
- The Yield10 Bioscience team has applied new gene-editing technologies to define a new state-of-the-art process for *Camelina* engineering to produce non-food seed oils. Seed oil yields are not yet at desired levels, but if the team can achieve them, it could provide a new and important feedstock.
- This project attempts to promote *Camelina* as an alternative crop and to demonstrate the use of geneediting technology, as well as the identification of target genes. Work is incomplete as it stands, and further research and development is needed. Without that, the investment made in this work may not materialize or generate interest from the current seed development companies.
- Refreshing to see a focus on the crop, which is a different aspect but as important. It is great that the PI included regulatory piece in the project as well.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# BIOCONVERSION OF ALGAL CARBOHYDRATES AND PROTEINS TO FUELS

### Sandia National Laboratories

### **PROJECT DESCRIPTION**

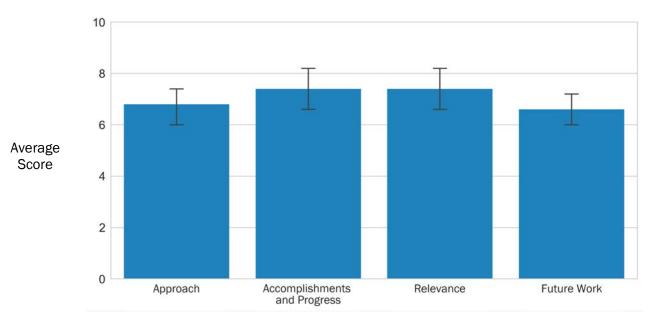
A key challenge for scale-up of algal biomass production for renewable commodities is efficient utilization of all of the major biochemical fractions of the biomass, including carbohydrates, proteins, and lipids. Development of a combined algal processing biorefinery would facilitate coproduction of petroleum-displacing chemicals with the intermediate- to high-value products that are currently produced from algae. To overcome issues involved with highly variable feedstock composition, our group is developing means for single-pot bioconversion of amino acid and sugar oligomers from algal hydrolysates to generate a variety of petroleum-displacing end products. Through these efforts we have recently demonstrated

| WBS:                      | 1.3.4.200           |
|---------------------------|---------------------|
| CID:                      | NL0026336           |
| Principal Investigator:   | Dr. Ryan Davis      |
| Period of<br>Performance: | 10/1/2015-9/30/2019 |
| Total DOE Funding:        | \$1,100,000         |
| DOE Funding FY16:         | \$350,000           |
| DOE Funding FY17:         | \$350,000           |
| DOE Funding FY18:         | \$200,000           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

pretreatment and bioconversion of a variety of whole-algae hydrolysates, including raceway-cultivated *Nannochloropsis sp.* and filamentous periphyton obtained from algal turf flow ways. To enable high-efficiency utilization of multiple fermentation substrates, we have developed an engineered *E. coli* biocatalyst consortium with each cohort optimized for utilization of either sugar or amino acid oligomers. A quantitative polymerase chain reaction (qPCR)-based method was developed for tracking the relative abundance of the biocatalyst cohorts during fermentation trials and was subsequently used to optimize the inoculum composition for

### Weighted Project Score: 7.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

maximum bioconversion yields. Using this strategy, we have demonstrated production of fusel alcohols, terpenes, and hydroxyalkanoates from diverse algal biomass, and found that retention of algal lipids as an extractive overlay in the bioprocessing provides process-intensification benefits by alleviating product inhibition and allowing co-extraction of the algal-derived products. Downstream testing of these products for fuel applications indicate that in several cases the algal-derived bioconversion products have attractive properties in both spark- and compression-ignition engines. Furthermore, TEAs suggest that the demonstrated yields of multiple bioconversion product options should offset the algal biomass production cost estimates from n<sup>th</sup>-plant models.

### OVERALL IMPRESSIONS

- The goal of this project is to extract additional value from algal biomass, which is currently expensive to produce. The basic idea is to use algal biomass as a substrate for a microbial fermentation process. Initial work was focused on the production of fusel alcohols. Current work is focused on the production of ethyl lactate using an engineered microbial consortium. Overall, the project is very innovative. The team is making reasonable progress. It is not clear how the metabolic engineering work fits into this project—the details are somewhat vague. The project would benefit from TEA and more focus on product recovery.
- This team has demonstrated important improvements in the production of alkanoates and fusel alcohols from microalgal biomass. So far, they have achieved near-theoretical yields in pretreatment, demonstrated the first *in vivo* production of ethyl lactate, and are well on the road toward demonstrating a two-times yield improvement over their previous target.
- On the overall, this project is technically sound and aims to add value from the refining of algal biomass from non-oil streams. Identifying the right product mix and markets for these products will be challenging.
- This project, the way it is presented, seems like a complicated one with stretch goals/targets. Better project management, clear go-no-go decision making, and a better explanation of current progress is needed to make it clear what the project status is, and how the team is planning to meet milestones.
- The goal of this project is to utilize algal biomass as a feedstock for producing chemicals. After extraction of lipid products from algal cultures, an abundance of protein and carbohydrates remains that can be used as a substrate. The team has focused on making hydroxyalkanoate esters from algal protein and carbohydrate. This is a complicated process, requiring organisms to take up a complex mixture of substrates and make two different compounds and then condense them by esterification. The team has made very commendable progress given the modest budget and is in a position to make a very high impact if the progress continues. The team has a good vision for future work, but specific tasks associated with improving product titer are not described. In the future, they should focus on some of the metabolic challenges in getting all the pathways to work in coordination. Growing multiple strains in coculture at scale is high risk and has no commercial validation.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# COMBINED ALGAL PROCESSING (CAP) PROCESS RESEARCH

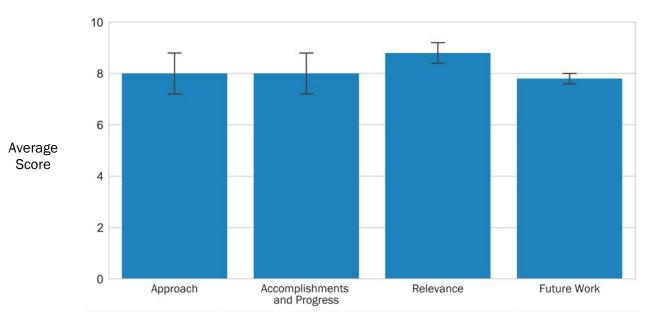
### National Renewable Energy Laboratory

### **PROJECT DESCRIPTION**

The CAP scheme has been developed to reduce the Minimum Fuel Selling Price (MFSP) through the development of technology for the production of a portfolio of fuels and coproducts. This work has combined a number of unit operations arising from the Biochemical Conversion Program along with novel conversion steps specific to algal biomass in order to develop an integrated process to establish a conceptual multiproduct algal biorefinery. Acid pretreatment enables wet lipid extraction with high yields and efficiently hydrolyzes algal carbohydrates with no need for enzymes, allowing for efficient fermentation of the sugars to fuels and chemicals. Additional products have also been identified by

| WBS:                      | 1.3.4.201           |
|---------------------------|---------------------|
| CID:                      | NL0026469           |
| Principal Investigator:   | Dr. Phil Pienkos    |
| Period of<br>Performance: | 10/1/2014-9/30/2021 |
| Total DOE Funding:        | \$2,100,000         |
| DOE Funding FY16:         | \$600,000           |
| DOE Funding FY17:         | \$500,000           |
| DOE Funding FY18:         | \$500,000           |
| DOE Funding FY19:         | \$500,000           |
| Project Status:           | Ongoing             |
|                           |                     |

conversion of the residual biomass following fermentation and extraction, rounding out the complete valorization of the algal biomass. Recent improvements in process sustainability have been achieved through adaptation of the CAP process for use with algal biomass grown in saline media, and approaches for further cost reduction are being developed to take advantage of low-cost wet wastes to serve as blendstocks for algal biomass.



### Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

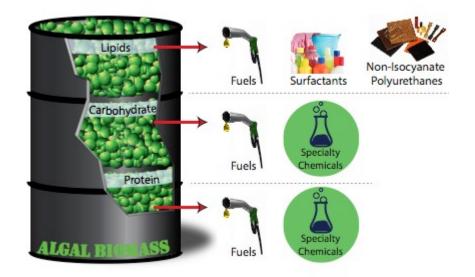


Photo courtesy of National Renewable Energy Laboratory

### **OVERALL IMPRESSIONS**

- The goal of this project is to improve the economics of an algal-based process by generating a portfolio of products. Unlike cellulosic biomass, the composition of algal biomass is tunable, thereby enabling a range of potential products. One promising example is the development of a process enabling the conversion of lipids to polyurethane polymers, using a mixture of chemical and biological approaches. The focus for the next year will be to develop protein conversion processes to make diesel. In addition, the team proposes to develop halotolerant algae in order to reduce the need for fresh water. Overall, this is a very compelling project and the team is making excellent process. The partnerships with Patagonia and Algix are also very promising.
- This project is making impressive progress toward demonstrating an approach to significantly reduce MFSPs from algal feedstocks by integrating conversion technologies for fuel and coproducts. A major driver of the success of this project will be in matching CAP-accessible products from different algal components with industry.
- The project performers have addressed several of the challenges for the cost-effective production and use of algal biomass. They have also relied on experience gained from the processing of lignocellulose. In the long term, CAP may provide additional revenue for product and coproducts. Before that can be accomplished, a commodity supply chain with a low cost of production is needed.
- Clarification on the quad chart overview (project start date) would help understand the percentage of work completed so far (it is stated that the project started in 2013). The project needs to rely on various other projects within BETO; however, it is not clear how the project interacts with other teams, and therefore, clearer paths/approaches to work more closely with other projects for quick adaptation of their learning would be needed in this project and all other projects working in the consortia. From manufacturability, it would be great to investigate costs associated with production of various products

(fermentation and separation/purification) and if there are combinations that would make the most sense and feasibility in regard to cost of operation.

• CAP is using various approaches to extract as much value as possible from algae, because TEA has shown that algal biofuels without coproducts will never be economically viable. Having a detailed understanding of the algal biomass composition is important for this goal. This biomass can also be combined with other waste streams as a feedstock. There is a clear path to a \$2.50 per gasoline gallon equivalent (GGE) biofuel cost if the goals of this project can be achieved. The team has demonstrated three different products made from algal material using biological or chemical conversion: butyric acid, polyurethanes, and hydrocarbons. The team has a good approach and has made great progress. They have a solid understanding of the economics and algal processing technology, but it is not clear that they appreciate all of the challenges associated with downstream fermentation.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thanks to all the reviewers for their positive feedback and constructive criticism.
- We apologize for the confusion created by the quad chart. Due to time limitations, we were unable to cover this in great detail. The project started back in 2013 but is now in the first year of a three-year annual operating plan cycle indicating a 17% completion of that cycle. Interaction with other teams is summarized in slide 28 in the supplemental section. Interactions with biochemical project leads take place formally at biweekly program meetings and with algal project leads at monthly algal program meetings. There was not enough time to provide more details on how this project interfaces between biomass production, composition, and TEA across the Advanced Algal Systems platform. Some background is missing due to the separation of this presentation from the other algal projects, including the algal TEA work. We included four supplemental slides from the algal TEA presentation (slides 29–32). Ryan Davis of NREL is responsible for TEA modeling of both biochemical processes and algal processes, and so the modeling of fermentation and product recovery costs uses the same process assumptions though with different feedstock and product metrics based on the data generated in this project.
- The comment regarding insufficient appreciation of the challenges associated with fermentation is certainly true, and in my experience every scale-up project presents a new learning curve. As noted above, the algae program uses the same TEA modeling modules for our fermentation work as are used for the biochemical program, though modified for the differences in feedstock input. It may be worth noting that our approach is to establish the applicability of various fermentation options in our integrated CAP scheme to determine the potential value based on relative contributions to MFSP, and to maximize fitness within the BETO strategic framework. As in any early-stage R&D program, the ultimate goal is to establish a conceptual process, within an appropriate TEA framework, that would warrant addressing the various challenges that occur during scale-up.

# **BIOCHEMICAL PLATFORM ANALYSIS**

### National Renewable Energy Laboratory

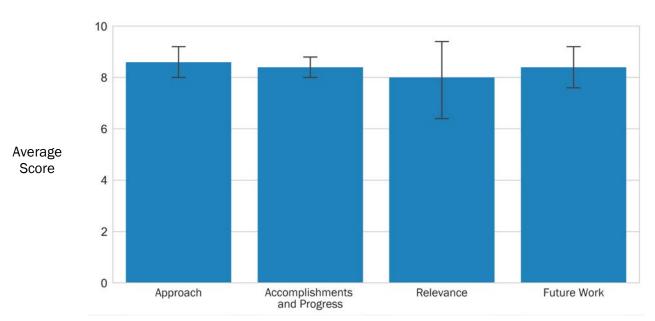
### **PROJECT DESCRIPTION**

The objective of this project is to perform TEA to support and guide biochemical platform R&D efforts, through use of process and economic models which translate key process parameters into overall economics for purposes of setting future R&D targets and tracking performance progress against those targets. Outcomes of integrated TEA modeling are utilized by BETO to guide program plans, as well as by other NREL/partner projects to quantify the impact of research on key technology barriers and to prioritize future efforts.

| 2.1.0.100<br>NL0008202 |
|------------------------|
|                        |
| Dr. Duar Davia         |
| Dr. Ryan Davis         |
| 10/1/2016-9/30/2019    |
| \$2,702,000            |
| \$750,000              |
| \$750,000              |
| \$852,000              |
| \$350,000              |
| Ongoing                |
|                        |

This work is highly relevant to BETO program goals, in that "bottom-up" conceptual modeling conducted under

this project serves as a basis for understanding the technical feasibility to meet "top-down" program cost targets set by BETO. By providing a framework to translate technical performance to cost reductions within a biorefinery, our TEA models may be leveraged to direct R&D towards the most economically impactful priorities. This helps to maximize the efficiency of research funding, ultimately in support of demonstrating 2030 fuel cost targets below \$2.50/GGE.



### Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${f I}$  One standard deviation of reviewers' scores

This project has made significant achievements since the 2017 BETO Peer Review, including: (1) a go-no-go decision to downselect for the most economically promising pathways for sugar fermentation to hydrocarbon fuels, (2) establishment of a new Biochemical Design Report to highlight paths to achieving \$2.50/GGE fuel cost targets in the future (based on two separate integrated process approaches reflecting the prior downselect guidance), and (3) providing state-of-technology (SOT) updates to benchmark progress towards those targets based on current experimental performance data. This work demonstrated the technical potential to achieve BETO's fuel cost goals and associated key gaps/barriers that must be overcome relative to current benchmarks, most notably including the need to maximize biomass utilization through opportunities to valorize lignin for value-added coproducts.

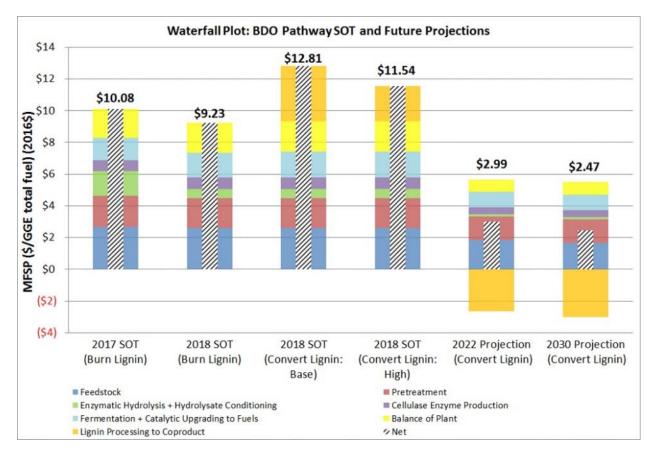


Photo courtesy of National Renewable Energy Laboratory

### **OVERALL IMPRESSIONS**

• The objective of this project is to conduct process modeling, TEA, and sustainability assessment to support all biochemical platform R&D activities. This is an essential function towards reaching the BETO Multi-Year Plan (MYP) goals, as it enables choice of target molecules and processes with the highest probability of successfully meeting cost targets and defines performance metrics needed to accomplish them. The team is well integrated with other projects, regularly communicating with experimentalists to understand technical challenges. This project underscores BETO's increasing commitment toward ensuring commercialization potential of the funded work. One of this project's key accomplishments was to determine that anaerobic processes should be emphasized over the aerobic lipid pathways, and as a result developed case studies for two anaerobic processes: 2,3-BDO and butyric acid. Both can be converted to fuel molecules. It was also clear that lignin-upgrading technology must be improved to be cost advantaged relative to burning it. In addition, the team can serve as a valuable

resource among all projects to ensure economic viability and sustainability. Future projects are well defined and are focused on activities with the best impact on cost. It is recommended to increase funding to this effort so they can work on more projects, including those done externally.

- This project provides process designs and economic analysis for many existing BETO projects. This analysis is then used to identify worthwhile projects, in particular helping identify go-no-go decision points. A key success of this analysis is the identification of two promising processes (2,3-BDO and organic acids) and to deemphasize aerobic processes focused on fatty alcohol production. Overall, the team is making excellent process and addresses a key need within the BETO portfolio. The project would benefit from more input from industry and an increased focus on the costs of product recovery, which will influence upstream design decisions.
- This project addresses a critical ongoing need across the biochemical conversion platform to incorporate process/cost modeling into the decision making that guides research prioritization and project tracking. The project has already demonstrated success by guiding downselection of pathways and shift of focus toward anaerobics. Moreover, its Design Report Update work product is a valuable resource for BETO, and an exemplar study of how to pursue comprehensive, quantitative strategic guidance. Finally, the project's goals to extend its purview to other BETO projects, develop new models, and disseminate models to the community will greatly add to the impact of the work.
- Biochemical platform analysis is key to establishing commercial viability of a process, as it provides TEA that is necessary to evaluate uses of biomass-derived feedstocks for the bioproduction of chemicals and drop-in fuels, as well as the use of thermochemically treated products and residues as biocrude or upgraded advanced fuels. This activity provides BETO with the tools to establish progress in funded projects as well as greater diversification of the portfolio of products made from biomass.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their positive feedback in recognizing the impact of this project for BETO and the utility in guiding R&D priorities for NREL and the community. We welcome the suggestions to increase collaborations with and feedback from industry to help refine the TEA models, particularly for more new/novel process operations, including key separation and product recovery steps. Two such mechanisms for this include subjecting our draft design reports to a thorough peer-review vetting process (including stakeholders from industry) and subcontracting with engineering firms or other expert consultants to improve process understanding for such operations. For example, at present we are working with one such consultant from industry to improve current design and cost estimates for carboxylic acid recovery via membrane pertraction, to be incorporated into future TEA model iterations.

# COPRODUCTION OF CHEMICALS AND FUELS ENABLED BY HYBRID CONVERSION OF LIGNIN AND BIOCONVERSION INTERMEDIATES

### **Pacific Northwest National Laboratory**

### **PROJECT DESCRIPTION**

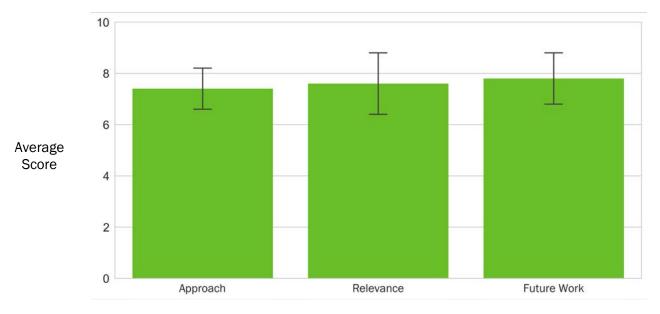
Contemporary biorefinery designs for bioconversion of lignocellulosic feedstocks to fuels and chemicals treat residual lignin and microbial cell mass as waste streams, and route them to combustion and wastewater treatment operations for production of heat and power. The opportunity and challenge are to optimize the value obtained from all streams within the biorefinery to increase total profitability, while retaining a high yield of liquid fuel from biomass. To meet this challenge, we have developed a new "hybrid conversion" biorefinery concept in which hydrolysate sugars are used to produce high-value commodity chemicals via bioconversion. Residual lignin and microbial cell mass are then routed to continuous

| WBS:                      | 2.2.2.501           |
|---------------------------|---------------------|
| CID:                      | NL0034399           |
| Principal Investigator:   | Dr. Jim Collett     |
| Period of<br>Performance: | 10/1/2018-10/1/2020 |
| Total DOE Funding:        | \$300,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | New                 |
|                           |                     |

hydrothermal liquefaction (HTL) for the production of biocrude oil, which may be upgraded via hydrotreating to a distillate blendstock for diesel and jet fuel. BETO has already played a major role in bioconversion R&D on commodity chemical production from biomass, and in the reinvention of HTL for continuous conversion of wet-waste streams such as mixed algae and sewage sludge. Combining these approaches provides a genuinely innovative and more efficient conversion process. As such, the goal of this new, two-year seed project is to demonstrate the potential for profitable bioconversion of corn stover hydrolysate sugars to a model commodity chemical (e.g., carboxylic acids), and co-conversion of the residual cell mass with corn stover lignin via HTL

### Weighted Project Score: 7.7

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

to biocrude oil for the production of distillate fuels with an MFSP of \$3/GGE. This seed project builds upon preliminary experimental work and TEA of the hybrid conversion biorefinery concept, which projected a distillate fuel yield of 63 GGE/ton of dry corn stover without coproduction of a commodity chemical. Achieving the objectives of this project will decrease risk in the BETO portfolio by providing a new, less complex route for lignin valorization in cellulosic biorefineries with lower installed costs compared to other current biorefinery designs, while maintaining a high yield of high-quality distillate blendstock for use in diesel and jet fuels.

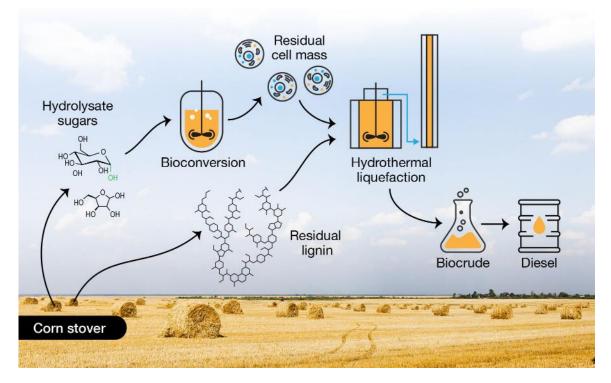


Photo courtesy of Pacific Northwest National Laboratory

### OVERALL IMPRESSIONS

- Overall interesting concept; more work is needed to work through logistics in large-scale plants and how the outcome of this study will/can be manufacturable. PIs are encouraged to consider applying proper project management with relevant milestones and go-no-goes.
- New project aims to apply HTL of yeast and lignin biomass to enable coproduct production, which should approximately double yields. Cost estimates based on modeling and prior HTL work supports the aims of this project.
- The goal of this project is to develop a proof-of-principle biorefinery process, where fuels will be made from lignin, biomass, and other leftovers. This is a new seed project. The process will involve the oleaginous yeast *Lipomyces starkeyi* and HTL of lignin. The work looks promising, and clearly addresses key needs within the BETO portfolio.
- Organic acids are currently produced by fungal fermentations (yeast and mold) from cost-effective refined streams of sugars (molasses from cane/beets or corn dextrose syrups). The refining of sugars for production of food-grade chemicals would add cost to nonconventional feedstocks, as in this case. A similar challenge is faced for recovery of organic acids for non-food applications unless a cost process is possible. This is usually possible only using a low-pH/high-acid-tolerant strain. The aerobic production

of organic acids represents a significant cost. Titer, rates, and yields, as well as CAPEX considerations, need to be addressed further.

• This project seeks to use HTL to convert combined lignin and waste-cell mass to diesel-fuel molecules. The biorefinery concept presented is to use the higher-quality sugars to make a higher-value product, while using these lower-quality mixed streams to make the fuel. Task 1 is to characterize the residual broth from a model organism/product fermentation so it can be used as a substrate for HTL. Task 2 is to run the HTL process using the model biomass to understand the critical process parameters. Task 3 is to perform TEA to determine sensitivity of product/fuel ratio. The milestones for the next year are well defined, but the technical risks and challenges are not presented.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

## LOW-TEMPERATURE ADVANCED DECONSTRUCTION

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

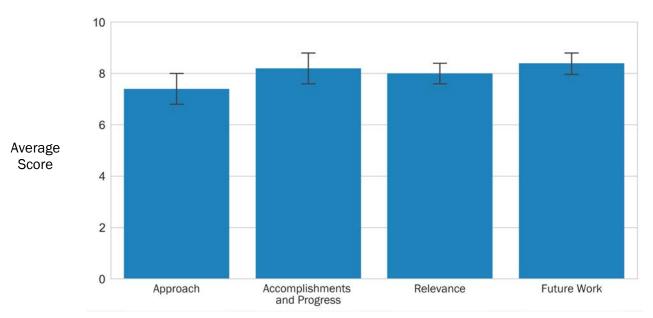
The overarching Low-Temperature Advanced Deconstruction project goal is to develop industry-relevant low-temperature biomass deconstruction and fractionation processes that produce low-toxicity, high-concentration sugar syrups, and reactive lignin streams at low CAPEX and operational expenditures (OPEX) using relevant feedstocks for biological and catalytic upgrading to meet BETO's 2022—and beyond—targets and goals. We have demonstrated high-solids (33 wt % insoluble solids), enzymatic hydrolysis (EH) reactions with the NRELdeveloped DMR pretreated corn stover substrates. This process has achieved titers of over 270 g/L of fermentable monomeric sugars at greater than 80% yields (at an

| WBS:                      | 2.2.3.100           |
|---------------------------|---------------------|
| CID:                      | NL0006288           |
| Principal Investigator:   | Dr. Mel Tucker      |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$5,915,368         |
| DOE Funding FY16:         | \$1,400,000         |
| DOE Funding FY17:         | \$1,400,000         |
| DOE Funding FY18:         | \$1,615,368         |
| DOE Funding FY19:         | \$1,500,000         |
| Project Status:           | Ongoing             |
|                           |                     |

enzyme loading of 20 mg protein per g of cellulose). These sugars are highly fermentable using recombinant *Zymomonas* to produce ethanol or 2,3-BDO at high titers and yields. In recent developments, we have achieved over 80% monomeric sugar yields at an enzyme loading of 12 mg of protein per g of cellulose using least cost formulation (LCF) blended (corn stover, switchgrass, sorghum) feedstocks provided by INL. A differential deacetylation process option was applied to the LCF biomass feedstocks, increasing overall process sugar yields as high as 9% compared to the single-severity deacetylation process control. A continuous counter-current deacetylation (CCCD) process option further increased EH sugar production rates and yields, as well as reduced xylan losses and lignin condensation reactions, using a shaftless screw reactor to replace the current

#### Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

batch deacetylation process. The improved mass and heat transfer and decreased residence times in the CCCD process option resulted in lowering xylan solubilization and losses by 66%, while sugar yields in EH increased over 15%. Furthermore, a low-consistency disk-refining process option has been introduced to replace Szego milling in a multistage DMR process to solve the potential equipment scale and vibration issues. Low-consistency disk refining, which has been practiced at the commercial scale, shows similar sugar yield improvements as compared to Szego milling, with sugar yields increased by as much as 13% compared to EH of single-stage DMR pretreated corn stover substrates. Collaborations with the University of Colorado at Boulder and Princeton University have developed novel microbial electrochemical technology (MET) systems shown to recover 90% of the salts (especially sodium ions [Na+]) and 60% of the lignin using electrons generated by degradation of the dilute organic waste in the deacetylation black liquor (after removing the solubilized lignin), saving chemicals and reducing the environmental and life cycle assessment (LCA) footprints. Collaboration with Washington State University has shown successful upgrading of the technical lignin isolated from the black liquor waste stream to high-energy, high-density jet fuel blendstocks using super Lewis acid metal triflates combined with ruthenium on carbon or ruthenium on aluminum oxide metal catalysts, increasing the carbon efficiency and decreasing the quantity of waste streams at a biorefinery.

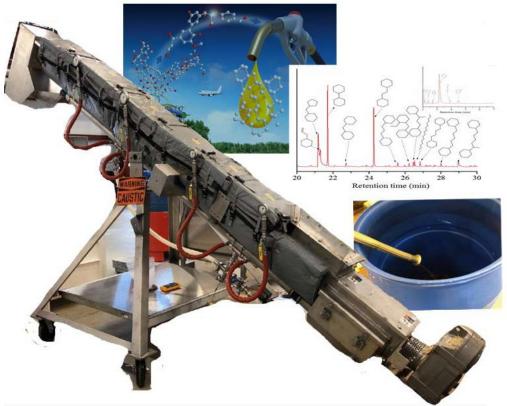


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• This project seeks to develop a biomass deconstruction process that produces high-quality, cost-effective sugars as well as a tractable lignin stream that is more amenable to processing than that resulting from conventional high-temperature methods. The project is divided into two tasks, one for biomass

deconstruction and the other for black liquor (deconstruction waste stream) recovery and upgrading. Work has proceeded on track, and they have a solid plan for future work.

- The goal of this project is to develop a cost-effective, low-temperature deconstruction process for sugar and lignin recovery. A key advance is the transition to continuous operation, as this will provide better yields and require less sodium hydroxide (NaOH). Overall, the team is making excellent progress. The project would benefit by comparing their process with existing ones. In particular, competitive benchmarks are lacking. In addition, more emphasis should be placed on NaOH recovery, as this will be critical for commercial viability.
- This project seeks to develop a low-temperature deconstruction process by combining a novel DMR with a novel method to utilize black liquor (waste). So far, the researchers have developed several interesting innovations to address technical barriers they have encountered, enabling them to make considerable progress toward both of these aims. Still, in order to attain direct industrial relevance, more progress is needed over the remainder of the performance period to attain the project's desired sugar yields and waste utilization targets.
- The project outlined progress in the development of a low-alkali process for deacetylation and two-step mechanical refining from corn stover that is less toxic to fermenting organisms to produce a DMR slurry that can be readily digested by enzymes and used as a fermentation feedstock. Good progress has been made in this process, but additional work is necessary for commercial viability.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers. Our project will continue developing novel, industry-relevant, low-temperature biomass deconstruction processes to improve sugar yields while reducing enzyme, chemical, energy, and water usages. In an earlier BETO FY 2017 Peer Review, we directly compared the enzymatic hydrolysis performance of the DMR process in head-to-head competition with deacetylation followed by dilute acid pretreatment on a variety of feedstocks (corn stover, switchgrass, and sorghum) and feedstock blends, but time constraints prevented presenting those data here. The DMR process achieved equivalent, or better, enzymatic hydrolysis and process sugar yields when compared to deacetylation followed by dilute acid pretreatment on various corn stover lots and blends. We also agree with the reviewers that NaOH recovery is one of the keys to the commercial success and application of the DMR process to biorefineries where we are continuing our research efforts in METs to recover water, sodium, lignin, and other chemicals for recycling back into and use by the biorefinery. To improve the DMR process, we are moving away from batch processes to developing continuous process options that are scalable. We chose to investigate low-temperature deconstruction processes to mitigate many issues that result from hightemperature pretreatments (e.g., hydrolysate toxicity, lignin condensation, operational reliability of feeding biomass into high pressure reactors, etc.). In order to achieve BETO's 2022 and beyond yields and targets, we will continue our research into scalable approaches as outlined in the presentation with guidance from TEAs and LCAs.

## ALKALINE-OXIDATIVE PRETREATMENT OF WOODY BIOMASS FOR OPTIMAL COPRODUCT

#### **Michigan State University**

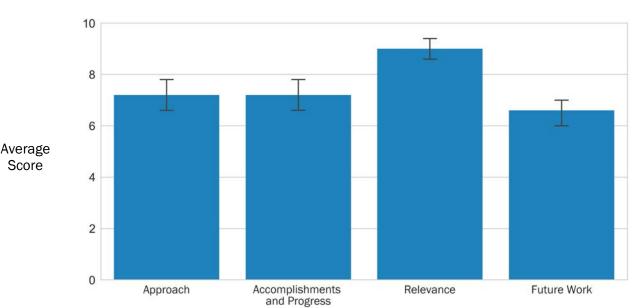
#### **PROJECT DESCRIPTION**

Woody biomass represents a vast source of carbohydrates and aromatics and it is envisioned as a key feedstock for the sustainable production of biofuels and bioproducts. We recently demonstrated that combining an alkaline pretreatment with an alkaline-oxidative post-treatment is a promising strategy for the delignification of hybrid poplar to generate (1) sugars in high yields that can be converted to hydrocarbon biofuels, as well as (2) a largely

| WBS:                      | 2.2.3.601            |
|---------------------------|----------------------|
| CID:                      | EE0008148            |
| Principal Investigator:   | Dr. Eric Hegg        |
| Period of<br>Performance: | 10/1/2017-12/31/2020 |
| Total DOE Funding:        | \$1,800,000          |
| Project Status:           | Ongoing              |
|                           |                      |

unmodified lignin stream suitable for valorization to bioproducts, including aromatic monomers and polyurethane coatings. In addition, we identified a novel approach to lignin depolymerization that resulted in high yields of aromatic monomers from lignins, and we demonstrated that hybrid poplar lignins generated by our mild catalytic alkaline-oxidative pretreatment resulted in the highest monomer yields obtained from the many process-derived lignins screened.

Motivated by this promising route for integrated deconstruction and lignin valorization, the goals of this project are to (1) optimize the two-stage alkaline-oxidative deconstruction approach to generate both a sugar stream and a lignin stream from hardwoods, (2) understand how pretreatment conditions impact lignin properties and how these properties can be linked to lignin suitability for coproduct applications, (3) employ TEA and LCA to inform the experimental work and to ascertain the tradeoffs between processing costs and



#### Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

environmental costs associated with generating high-value coproduct streams at high yields, and (4) identify strategies to decrease the MFSP. Successful completion of this project will demonstrate the possibility of using this process to achieve the target of \$3/GGE by generating both a low-cost sugar stream and a relatively clean lignin stream that is ideally suited to depolymerization and coproduct production.

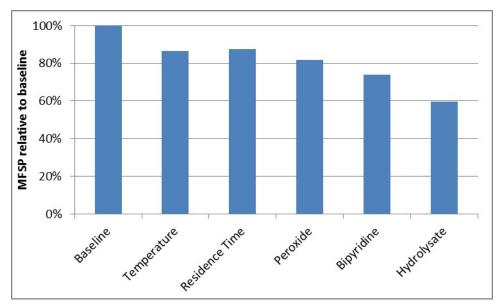


Photo courtesy of Michigan State University

#### OVERALL IMPRESSIONS

- The goal of this project is to produce pure sugars and lignin from woody biomass using a two-stage alkaline-oxidative deconstruction process. The project focuses on optimizing the process. The main advance and innovation are that the process can recover clean lignin, which can subsequently be depolymerized. The project appears to be on schedule. It is not clear if the process will be commercially viable. Competitive benchmarks and more transparent cost estimates would be useful. In addition, it is not clear how milestones relate to commercial viability.
- The team is developing a two-stage deconstruction process (called alkaline hydroperoxide [AHP]) to generate clean sugars along with lignins suitable for valorization from woody biomass. Thus far, they have established an initial system and optimized conditions for each of the two steps of the AHP process. It is too early to evaluate the eventual success of the project, but they have achieved all of their intermediate milestones to date. TEA/LCA is in progress and process integration is part of their future plans.
- The stepwise depolymerization of woody poplar with conversion of sugars post-enzyme treatments to hydrocarbon fuels and the alkaline oxidation of lignin to yield at least a target of 25% monomer is promising. The targeting of a range of products from lignin should aid in developing a cost-effective lignin biorefinery.
- This seems to be a great project. Having clear milestones, timelines, and a well-described project plan enables the project to be more accountable and the accomplishments more relevant to the overall goal. PIs are encouraged to work on those items more.
- The goal of this project is to optimize a biomass deconstruction process to generate both a clean sugar stream for fuel production and lignin suitable for coproducts. The technology is intended to produce a

higher-quality lignin stream that is very compatible with the oxidation/depolymerization process, which provides monomers to be used for upgrading. The two-stage process was optimized by evaluating the influence of process conditions on both yield and quality of the products. The two stages have to be optimized in parallel, because they are interdependent. Good progress has been made on both overall yield and monomer generation, estimated to reduce total cost by 25%. The project seems to be going in the right direction, but challenges and goals for the future are not clearly defined.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewers' time and thoughtful comments. Our milestones and go-no-go decision points are linked to decreasing the MFSP. Progress on reducing the MFSP as well as other TEA data is reported to DOE quarterly.
- Our goals for the future include (1) scaling up the process, (2) integrating the different components, and (3) continuing to lower MFSP.

## **FUNGAL GENOMICS – GENETICS**

#### **Pacific Northwest National Laboratory**

#### **PROJECT DESCRIPTION**

The challenge facing biological conversion routes from carbohydrates to hydrocarbon biofuels is that they are inherently carbon inefficient, because oxygen must be removed as carbon dioxide (CO<sub>2</sub>) or water, or both. Our goal is to engineer the yeast *Lipomyces starkeyi* to maximize carbon efficiency by conversion of biomass sugars to the easily separated hydrophobic phase biofuel zingiberene and aqueous phase bioproduct malic acid, in parallel.

In a previous project we developed genetic engineering tools for *L. starkeyi* that enable us to accomplish the task of coproduction of fuels and chemicals for greater carbon

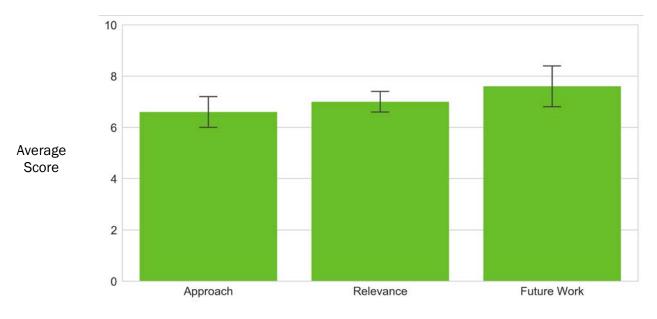
| WBS:                      | 2.3.2.103           |
|---------------------------|---------------------|
| CID:                      | NL0011937           |
| Principal Investigator:   | Dr. Jon Magnuson    |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$4,333,275         |
| DOE Funding FY16:         | \$1,650,000         |
| DOE Funding FY17:         | \$1,500,000         |
| DOE Funding FY18:         | \$743,275           |
| DOE Funding FY19:         | \$440,000           |
| Project Status:           | New                 |
|                           |                     |

efficiency. In true biological fermentation processes, a sugar is converted into one highly oxidized and another highly reduced molecule (e.g., glucose to ethanol and  $CO_2$ ). We are applying that biological principle, coupled with carbon-fixing enzymatic steps, to generate a more carbon-efficient process for production of the highly reduced hydrocarbon biofuel zingiberene and the oxidized product malic acid.

In the first quarter of the project we succeeded in introducing the zingiberene synthase gene into *L. starkeyi* and obtained an initial titer of 18 mg/L in the best strain. Further media and culture condition optimization has increased the titer to 100 mg/L of zingiberene in a hydrophobic phase overlay. A strain with both the zingiberene synthase and farnesyl pyrophosphate synthase genes has been generated, and initial results indicate

#### Weighted Project Score: 7.2

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

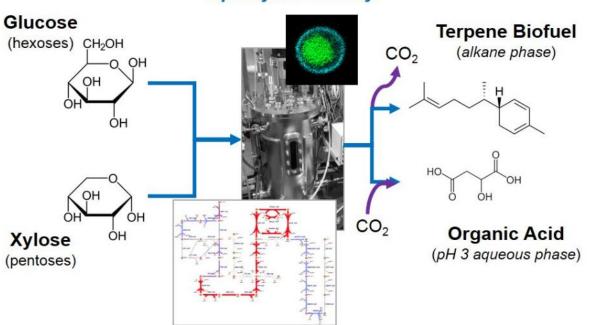


 $oxed{I}$  One standard deviation of reviewers' scores

an increase in titer relative to the control strain with only the zingiberene synthase gene. By the end of FY 2019 our milestone is to produce 300 mg/L of zingiberene. In addition, in FY 2019 we will overexpress the pathway to convert three-carbon central metabolites and  $CO_2$  (released during zingiberene synthesis) into our four-carbon target bioproduct L-malic acid. Subsequent years will focus on increasing titers of both compounds and merging the two pathways into a single strain for coproduction.

Another challenge addressed in this project is driving down the gas-handling requirements of the bioprocess through two approaches. First is to continue bioprocess development with our engineered *Lipomyces* strains to determine the minimal aeration requirement throughout the process. Second is identifying and characterizing additional yeast species that may perform better than *Lipomyces* in regard to microaerobic growth. We started with a diverse set of 28 different yeasts for which we had sequenced genomes in collaboration with the DOE Joint Genome Institute from across the fungi kingdom. We have selected the 10 most promising candidates from initial screens for a final selection of the two most promising species by March 31, 2019. The selected strains must have microaerobic growth characteristics superior to *Lipomyces*, as well as a wide substrate range, and antibiotic sensitivities to enable genetic tool development.

TEA will be utilized throughout the project to guide our research toward the most impactful challenges and identify likely paths forward, during, and beyond the 36-month tenure of the project. One measure of project success at 36 months will be the production of 5 g/L of both the biofuel and the bioproduct in a single strain, preferably under much reduced aeration relative to the starting case of two vessel volumes per minute. This will be a significant milestone indicating the modified strain is worthy of further development, driving toward transfer of the technology and commercial development by industry.



#### Lipomyces starkeyi

Photo courtesy of Pacific Northwest National Laboratory

#### OVERALL IMPRESSIONS

• This project leverages extensive research at PNNL in fungal genomics to develop a process for production of an oxidized bioproduct and reduced biofuel in the same fungal organism. By fixing CO<sub>2</sub> in

the reductive tricarboxylic acid (TCA) cycle branch, it maximizes carbon efficiency. They have chosen a terpene fuel molecule that can also be a valuable flavor compound in the short term. The acid tolerance of *Lipomyces* is leveraged to make the product, malic acid, in the free-acid form. The team has a clear path to a proof-of-concept demonstration, and milestones are clearly defined. A combination of metabolic and process modeling is used to inform the design, indicating a preference to get a microaerobic or anaerobic organism. This is an early-stage effort, with a goal to produce 5 g/L of each compound. If this proof of concept is successful, a larger project will be required to de-risk commercial viability. This will be particularly difficult if a new anaerobic yeast is used, requiring development of new tools. Although an anaerobic strain will have lower operating costs, it is not clear this would be worth the setback associated with a new organism.

- The goal of this project is to improve the carbon efficiency of fermentation processes by reducing losses due to CO<sub>2</sub> production. The team specifically proposes to produce terpenes and organic acids using *Lipomyces*. Overall, this is a high-risk proposal that is still far away from commercialization. In particular, it may not be possible to introduce a nonoxidative pathway into *Lipomyces*, because the genetic tools are still very limited. In addition, the team will likely run into issues associated with compartmentalization within the cell. Aside from *Lipomyces*, the team also proposes to look at alternate yeasts capable of growing during microaerobic conditions. This aspect of the project is not well developed or well motivated. Moreover, it is not clear whether such yeasts provide good platforms for making the proposed compounds. In general, this is a high-risk, potentially high-reward project still in the early phases of development.
- This new project has made good initial progress toward its goals to build the necessary capabilities to demonstrate a system that maximizes carbon utilization efficiency by producing oxygen-utilizing phase-separated coproducts. Already, they have established initial production strains.
- This is a highly challenging project that aims at the coproduction of a solvent-soluble terpene with a maleic acid that partitions to the aqueous phase. Targets for commercial viability need to be established once proof of concept can be demonstrated in a single strain that is adapted to use corn stover DMR.
- Great project and plan. Milestones need more clarification, organizing future work is needed with providing more detail on upcoming tasks and only high-level vision for far-future tasks. The project was great during the technical slides. It would be great to see more balance between the project management and technical slides.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that this is a higher-risk and high-reward project that is just beginning. The genetic tools are modest in comparison to a model organism, thus requiring more effort, but fortunately they allow us to manipulate the organism effectively. Compartmentalization is always something we consider in working with fungi and it is built into our metabolic model and design considerations. The strategy for increasing production of malate will be primarily directed at increasing the cytosolic pool. Mitochondrial transporters to address metabolic species imbalances are present in the organism. NADPH/NADH imbalance may be an issue and a transhydrogenase would be one possibility for addressing that issue. We agree that the task on assessing and developing alternative microaerobic yeasts accompanied by genetic tool development is high risk. In recognition of this risk, it was made the subject of the 18-month decision point. The LCA suggesting reduced carbon emission impacts by decreasing the need for gas handling suggests these alternative platforms are worthy of exploration.
- The terpene biofuel and malic acid coproduct will be the subject of a TEA, as we collect sufficient data in the latter two-thirds of the project. We recognize that the target titers, though ambitious for a project of this size, are not commercial titers. We anticipate they would need to be at least 10 times greater for

commercial viability, but the TEA will help assess that assumption and focus out-year efforts on the highest-impact parameters.

• With the first half year of the project behind us, we will add second-year milestones for increased clarity of the project direction. We fell into the familiar trap of scientists excited to talk about our early technical achievements but will seek greater balance at the next BETO Peer Review. We note that the project is of an intermediate size, involving a team at PNNL that has worked together for many years, so the project management is relatively straightforward.

## **BIOLOGICAL UPGRADING OF SUGARS**

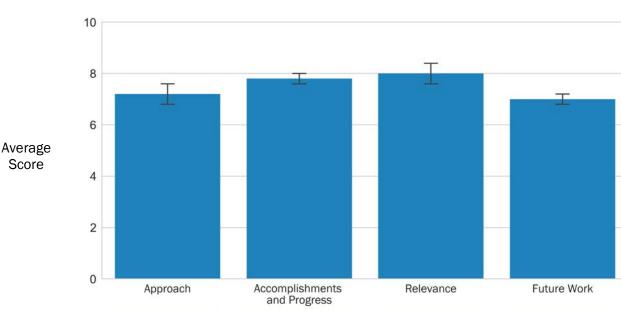
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

The goal of the Biological Upgrading of Sugars project is to develop robust microbial strains to convert lignocellulosic sugars to fuel precursors at titer, rate, and yield targets set by TEA and which are fully integrated into a complete process to produce biofuels at the BETO 2022 goal of \$2/GGE and future MYP targets. Our technical focus is on the anaerobic production of carboxylic acids using non-model bacteria and yeast that exhibit beneficial phenotypes for industrial bioprocesses. Carboxylic acids are readily catalytically upgraded to fuel molecules through known, well-studied chemo-catalytic transformations being developed in collaborating projects. Specifically, we focus on holistic process development and integration via collaborations with the BETO-funded Bioprocessing Separations Consortium

| WBS:                       | 2.3.2.105           |
|----------------------------|---------------------|
| CID:                       | NL0028598           |
| Principal<br>Investigator: | Dr. Jeff Linger     |
| Period of<br>Performance:  | 10/1/2015-9/30/2020 |
| Total DOE Funding:         | \$6,781,256         |
| DOE Funding FY16:          | \$1,800,000         |
| DOE Funding FY17:          | \$1,800,000         |
| DOE Funding FY18:          | \$2,031,256         |
| DOE Funding FY19:          | \$1,150,000         |
| Project Status:            | Ongoing             |
|                            |                     |

(for separations of intermediates) and the Chemical Catalysis for Bioenergy Consortium (for catalytic upgrading of intermediates to hydrocarbon jet fuel and diesel), along with industrial and academic partners. Regarding carboxylic acids, we are primarily focused on the biological production of butyric acid. *Clostridium butyricum* and *Clostridium tyrobutyricum* are bacteria that naturally produce butyric acid from the principal sugars found in corn stover hydrolysate. In addition to native butyric-acid-producing bacteria, we are also exploring the use of acid-tolerant yeasts that demonstrate great potential for economically viable routes towards carboxylic acid production.



#### Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- In order to develop industrially relevant yeasts, the research team screened 32 strains against acidic, hydrolyzed feedstocks to find new acid-tolerant strains, and subsequent omics analysis identified a gene that might be responsible for acid tolerance. In parallel, the team has developed *Clostridium* strains capable of achieving high titers of organic acid via pertractive fermentation using mock hydrolysates. Demonstration of complete conversion (from hydrolysate to organic acids) has not yet been fully demonstrated for yeast but should be coming soon.
- The goal of this project is to produce butyric acid from cellulosic sugars, which can be catalytically converted to diesel and jet fuel. Two processes are being considered, one involving bacteria and the other involving yeast. Overall, the team is making excellent process with the bacterial route. Excellent titers and productivities are being achieved. Developing a process involving continuous distillation will be an important step for establishing feasibility and connecting with TEA. The route involving yeast is far less developed and does not integrate well with the bacterial work. It is also not clear whether these strains can produce butyric acid at high rates and titers. This work is still in the discovery phase. As such, this part of the project is not very compelling.
- Developing a robust production organism, whether bacterial or yeast, for production of 150 g/L butyrate is challenging. There are drawbacks for both systems, as well as challenges inherent in both. Focusing on one system would allow for more rapid progress. For all organic acid production, the cost associated with recovery of the acid should be considered in choosing the production strain. Based on that, the choice of organism can be different from an anaerobic *Clostridium*.
- This program develops microbial strains to convert cellulosic sugars to fuel molecule precursors. Due to input from the TEA performed by the integrated analysis team, the focus was shifted in the last two years from fatty acids to short-chain carboxylic acids, in particular butyric acid. They are currently evaluating two options, a yeast and bacterial strain. The bacterial (*Clostridium*) fermentation requires protractive fermentation to remove acid, while yeast can operate at low pH. However, the yeast strain tends to produce ethanol, does not readily take up C5 sugars, and is very sensitive to the organic acid products. Significant progress was made with strain and fermentation development of the bacterial process, and the pertractive fermentation gave reasonable titer, rate, and yield. Progress with the yeast strain has been slower, but they were able to achieve xylose utilization. Tolerance to the product remains a key challenge in yeast. If this is not solved soon, all resources should be shifted to the bacterial process.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The reviewers have provided valuable guidance, which is well aligned with our own self-assessment of the project. When we pivoted from fatty-acid-based routes towards carboxylic routes, we opted to pursue two complementary approaches: (1) using top-candidate Clostridium strains, which natively produce butyric acid but have limited ability to grow at low pH; and (2) a higher-risk but potentially gamechanging approach using acid-tolerant yeast, which can grow at low pH but do not natively produce carboxylic acids. TEA analysis suggests that the cost savings from employing bioprocesses with low-pH carboxylic acid production could be dramatic, thus we performed early work to determine the feasibility of this approach. While our top yeast strains are indeed tolerant to low pH (2.0), and to high concentrations of butyric acid (0.4 M) at neutral pH, the combination of high acid concentrations at low pH has thus far proven too harsh of conditions to present a viable path forward. Accordingly, once we publish this research, we will intensify efforts exclusively on the Clostridial platform, which has yielded promising results thus far. Notably, our lab-directed evolution campaign and multiomics data sets should enable development of these yeasts for production of a wide array of organic acids, and we have had discussions with commercial and academic entities related to future collaborations. Thus, while we will be focusing efforts on Clostridial production of butyric-acid-derived fuels moving forward, we still view this research pursuit as a worthwhile endeavor that will help move the field as a whole in a positive direction. Finally, regarding the comment that our targets of 150 g/L butyrate will be challenging, we agree that we still have some hurdles to overcome, but we have already demonstrated this titer via pertraction in a glucose medium with *Clostridium*. We are currently transitioning our process to hydrolysate and are ultimately aiming for even higher titers.

### **PET UPCYCLING – NREL**

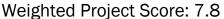
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

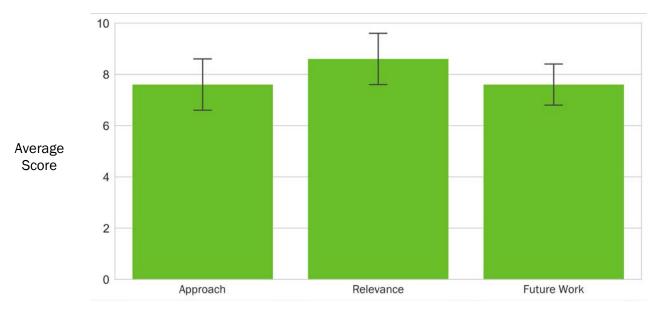
More than 300 million metric tonnes of plastics are produced each year. The volume of waste generated from plastics use is an enormous global problem, as plastics wreak massive environmental damage on terrestrial and aquatic ecosystems. Moreover, recycled products are most commonly lower in value than the original plastics due to a reduction in key material properties upon recycling, creating a disincentive for increased recycling rates relative to the use of virgin plastic materials. Accordingly, drastic changes in plastics recycling technologies will be essential to enable a more circular materials flow in plastics.

| WBS:                    | 2.3.2.109           |
|-------------------------|---------------------|
| CID:                    | NL0034397           |
| Principal Investigator: | Dr. Gregg Beckham   |
| Period of Performance:  | 10/1/2018-10/1/2020 |
| Total DOE Funding:      | \$350,000           |
| DOE Funding FY16:       | \$0                 |
| DOE Funding FY17:       | \$0                 |
| DOE Funding FY18:       | \$0                 |
| DOE Funding FY19:       | \$350,000           |
| Project Status:         | New                 |
|                         |                     |

To that end, the aim of this project is to deliver cost-effective solutions to deconstruct and upcycle the massive plastic waste stream, polyethylene terephthalate (PET). PET is comprised of ethylene glycol (EG) and terephthalic acid (TPA) and is used for single-use beverage bottles, carpet, and other textiles. PET recycling rates are low around the world, and PET bottle recycling results in a loss in advantageous material properties, such that recycling is "downcycling." This work will leverage BETO investments in overcoming biomass recalcitrance, interfacial biocatalysis, metabolic engineering of aromatic-catabolic bacteria, and bioprocess development to ultimately enable the Circular Materials Economy for this plastic.



Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

Specifically, we are targeting upcycling of PET carpet fibers as a nonrecyclable plastic. The challenges in PET biological or chemical deconstruction closely mirror that of cellulose depolymerization. Namely, the PET polymer is crystalline and is connected by C-O (ester) bonds that are difficult for (bio)catalysts to access. Like cellulose, there are natural enzymes (esterases) active for PET degradation to TPA and EG. Two potential strategies to upcycling are the enzymes that degrade PET, namely PETase and mono-2-hydroxyethyl terephthalate (MHET)ase, and chemo-catalytic solutions using easily recyclable catalysts (such as catalyzed glycolysis). We are pursuing two parallel, closely related aims to convert PET into higher-value chemical building blocks using a wholly biological strategy (Task 1) and a hybrid chemo-catalytic-biological strategy (Task 2). For both aims, we will leverage an engineered strain of *Pseudomonas putida* KT2440 that is able to readily consume EG, developed with BETO support in the Biological Conversion of Thermochemical Aqueous Streams project. We are actively engineering this strain to secrete two PET bis-hydroxyethyl terephthalate (BHET)-degrading enzymes, PETase and MHETase, and engineered variants of these enzymes. We are also engineering the baseline strain to consume the aromatic monomer TPA, first for growth and ultimately for conversion and upcycling to an exemplary performance-advantaged monomer, namely ßketoadipic acid, which is being researched heavily in the Performance-Advantaged Bioproducts miniconsortium. P. putida is an excellent chassis strain for both strategies because it already harbors genes for robust aromatic catabolism and for EG consumption, it is genetically tractable, both NREL and ORNL have extensive metabolic engineering experience with the strain, and it has previously been industrially scaled up for several applications by multiple companies. In addition, we are also pursuing enzyme discovery, evolution, and engineering. It is likely that more efficient enzymes exist in nature already, and they are waiting to be discovered and characterized. Working with colleagues at Montana State University and ORNL, we are prospecting existing metagenome libraries from various thermal and pH extrema across known microbiological samples. To date, we have already developed a set of putative PETases from these databases that are taken from thermal environments above the glass transition of PET, which represents an excellent starting point for enzyme screening. The purpose of this component of the project will be to discover more effective enzymes for PET degradation and BHET degradation, as well for the hybrid process.

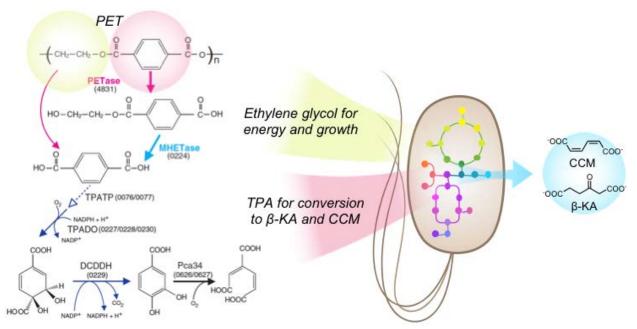


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- Overall relevance of the project to BETO and how the project plan can tackle the issue is not clear. There are a lot of technical challenges in the proposed work and the timing of the project might not be sufficient to address these challenges. But good start.
- This exciting new project seeks to leverage discoveries of PET-metabolizing microbes to develop processes for industrial-scale PET upcycling. Thus far, the team has demonstrated production and secretion of key enzymes in a *P. putida* host and has built genetic constructs for transport. If successful, this project will have a broad impact by converting plastic waste into a new feedstock for industrial production.
- The goal of this exploratory project is to develop processes for the upcycling of PET plastic. This project represents a new and promising direction for BETO. Overall, this is a fantastic project that is exploring both biological and chemical approaches. Many exciting ideas are proposed. The team is also outstanding. More importantly, it addresses a key environmental problem of concern to the general public.
- Overall, this a good project; while not a perfect fit for bioenergy sector, it is focused on using a biological approach to treat a recalcitrant material and in the process produce a chemical by bioconversion. Most short- to mid-term opportunities for chemical production can follow a similar approach and help establish bioconversion-based manufacturing as a viable industry while seeking greater deployment of plant-derived materials, as is the case for lignocellulosics.
- This project is aimed at breaking down PET and then using the resulting carbon monomers to make
  small molecules by fermentation and/or catalysis. Both chemical and biological processes will evaluate
  PET breakdown. The conversion to the exemplary product, β-ketoadipate, will be done using *P. putida*,
  leveraging tools developed for engineering this organism. This is a very challenging program because it
  requires heterologous pathways to consume novel substrates, as well as producing a product. It should be
  considered high risk, high reward. However, this team is very experienced, and if anyone can be
  successful with it, they can. This will likely take many years to develop, but if successful could be
  revolutionary in the conversion of waste to value-added products.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Plastics are a major component of municipal solid waste, which is relevant to the BETO portfolio. Moreover, many process and scientific concepts that are core elements of the BETO portfolio can be leveraged towards this key environmental problem, which is essentially the conversion of waste, polymeric, recalcitrant, low-value, diffusely available solids into small-molecule intermediates that can then be upcycled to higher-value materials. In terms of the timing, we agree that our milestones are aggressive, but we have assembled an excellent team of researchers from NREL and ORNL to tackle this problem and have been able to deliver and exceed our milestones thus far.

## CONTINUOUS MEMBRANE-ASSISTED IBE FERMENTATION FROM AVAP CELLULOSIC SUGARS

#### American Process Inc.

#### **PROJECT DESCRIPTION**

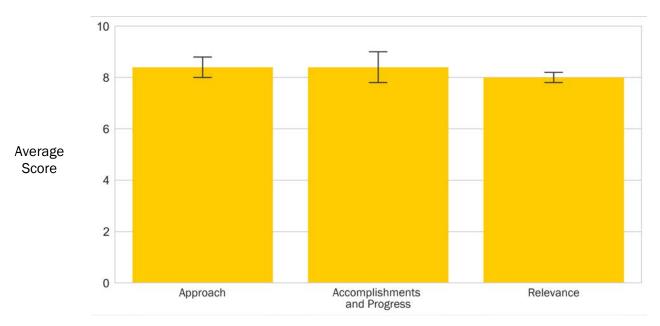
The process demonstrated in this project consisted of continuous membrane-assisted isopropanol, butanol and ethanol (IBE) fermentation of American Value Added Pulping (AVAP) cellulosic sugars and recovery of the IBE fuel mixture. The overall goal of the project was to demonstrate the process in an integrated pilot plant so as to collect data that demonstrates the ability to scale up production of IBE as a transportation fuel in an economical manner. It was further demonstrated that the targeted final MFSP of \$3/GGE (corresponding to \$2.27/gallon, or \$745/ton of IBE) can be achieved in a plant using 1,200 bone dry (BD) tons per day of corn stover feed stock.

| WBS:                       | 2.3.2.202          |
|----------------------------|--------------------|
| CID:                       | EE0006879          |
| Principal<br>Investigator: | Dr. Vesa Pylkkanen |
| Period of<br>Performance:  | 7/1/2015-3/31/2018 |
| Total DOE Funding:         | \$3,088,632        |
| Project Status:            | Sunsetting         |

The proprietary AVAP pretreatment technology, based on fractionating biomass in a sulfur dioxide-ethanolwater fractionation was used to produce cellulosic and hemicellulosic sugars. A conditioning step was developed for the hemicellulosic sugars, which allowed the utilization of the xylose fraction to increase to 50%. The membrane-assisted recycle fermentation process developed increased the fermentation volumetric solvent productivity to 8.85 g/L/hr with an average titer of 14.75 g/L, and a yield of 0.36 g/g of utilized sugar. The production of isopropanol by genetic modification of *Clostridium acetobutylicum* was demonstrated for short periods.

#### Weighted Project Score: 8.3

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $\square$  One standard deviation of reviewers' scores

A novel liquid-liquid extraction technology was applied for the recovery of the alcohols from the fermentation broth. A butanol recovery of 90% was achieved at a low organic-to-aqueous ratio—as low as 0.4:1 during integrated operation. Reactive distillation to produce butyl butyrate extractant was also demonstrated.

Pinch analysis was conducted on the fundamental process to increase the energy efficiency though heat integration. Following the Pinch analysis, an LCA showed that equivalent CO<sub>2</sub> emission was about 85% lower than gasoline blend stock and 70% lower than the first-generation butanol from corn. The coproduct acetone-replacing petroleum equivalent generated a carbon credit that was larger than the emissions during IBE manufacture (e.g., a carbon-negative fuel).

The commercial plant scale-up was simulated using an American Process Inc. proprietary biorefinery simulator, apiMAX<sup>™</sup>, and was further optimized using value engineering and heat integration. The TEA established that in the base case, an MFSP for the IBE mixture of \$4.88/gallon is necessary in order to obtain positive net present value (NPV) for the project. A number of realistic improvement assumptions were then superimposed in the base case scenario to develop an optimized case scenario. In the latter, a plant making about 57 kilotons per annum (kta) of IBE fuel and 22 kta of acetone coproduct from 420 BD kta of corn stover priced at \$60/ton would have a positive NPV at an MFSP of \$3/gallon of IBE. The NPV can be further significantly increased if the capital cost were further decreased through integration to an existing facility with infrastructure and boiler house.

#### **OVERALL IMPRESSIONS**

- The goal of this project is to develop a process to produce butanol from various domestic cellulosic feedstock sources with economics that do not require any subsidy. Continuous membrane-assisted fermentation and liquid-liquid extraction were novel methods used to increase productivity and remove butanol *in situ* so concentration remains low. The team engineered *Clostridium* to produce isopropanol instead of acetone for a higher-value coproduct. Acetone conversion to isopropanol was not as high as projected, so this requires more work on the strain. Productivity and yield goals were achieved, and most of the challenges associated with parallel fermentation of two sugar streams and butanol separation were solved at the lab scale. Overall, this was a very successful project. The process should be de-risked at a larger scale when possible.
- The goal of this project was to create a continuous IBE process using membrane separations. The team achieved most of their milestones. In these regards, the project was successful. The team is now looking to license their technology. Many innovative ideas were explored in this project; key among them was the use of reactive distillation to make the extractant for product separation. Much was also learned from project failures, such as the need for better biomass sensors, better foam control, and less process intensification, particularly at this stage of process development.
- The novelty of this project is that it combines in-depth process optimization with continuous membraneassisted fermentation to attain up to 20-times increases in productivity of the generation of alcohols from cellulosic sugars. The process is enhanced by further introducing a low-temperature, recycling-friendly liquid-liquid extraction system, which could cut thermal energy use in half. The team has produced several compelling technical achievements, including getting the model system operational, demonstrating continuous fermentation, and nearly optimal extractant recovery, but the acetone-toisopropanol conversion is still lagging and requires additional enhancement, which might include strain engineering.
- On the overall, the project progressed reasonably well in spite of the challenges of integrating fermentation, cell recycle, and solvent recovery. Improvement in solvent recovery in g/L/hr looks good for a continuous system and the 500 hours of continuous operations is a step in the right direction.

• The project was clear on technical and financial targets and designed project plans to test the targets. The projects worked both on upstream process improvement (fermentation) as well as downstream recovery and fractionation.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# ENGINEERING CLOSTRIDIA FOR N-BUTANOL PRODUCTION FROM LIGNOCELLULOSIC BIOMASS AND CO<sub>2</sub>

#### The Ohio State University

#### **PROJECT DESCRIPTION**

| The goal of this project was to develop engineered                            |
|---|
| Clostridia strains and fermentation process that can                          |
| directly utilize cellulose and fix CO <sub>2</sub> for <i>n</i> -butanol      |
| production from lignocellulosic biomass. To achieve this                      |
| goal, the project included the following specific objectives:                 |
| (1) engineering <i>Clostridia</i> for <i>n</i> -butanol production from       |
| cellulose and CO <sub>2</sub> hydrogen (H <sub>2</sub> ) (years 1 and 2); (2) |
| fermentation kinetics studies and process optimization; (3)                   |
| amia analysis of mutants in formantation, and (4) process day                 |

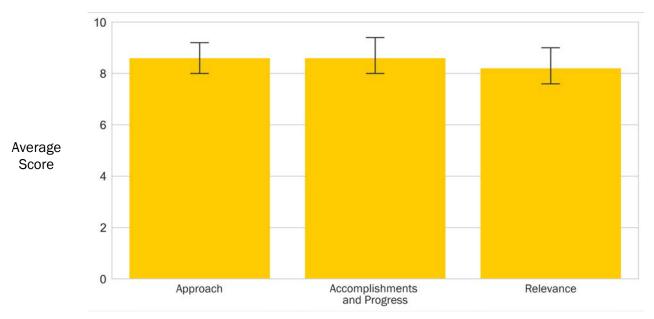
| WBS:                      | 2.3.2.203           |
|---------------------------|---------------------|
| CID:                      | EE0007005           |
| Principal Investigator:   | Dr. Shang-Tian Yang |
| Period of<br>Performance: | 10/1/2015-9/30/2018 |
| Total DOE Funding:        | \$1,232,148         |
| Project Status:           | Sunsetting          |
|                           |                     |

omic analysis of mutants in fermentation; and (4) process design and cost analysis.

More than 20 engineered strains of *Clostridium cellulovorans* and *Clostridium carboxidivorans* were generated and evaluated for butanol production from cellulose and  $CO_2$  H<sub>2</sub>. Among all engineered strains, *C. cellulovorans* co-expressing the gene for aldehyde–alcohol dehydrogenase (adhE2) with thl and hbd genes showed the greatest potential for butanol production from cellulose, with the highest butanol titer (5.5 g/L), yield (0.27 g/g), butanol-ethanol ratio (6.63 g/g), alcohol-acid ratio (1.32 g/g), and C4-C2 ratio (2.84 g/g) in batch fermentation with glucose and the addition of methyl viologen (MV). The strain overexpressing adhE2 and fnr genes produced 5.28 g/L butanol and 1.93 g/L ethanol from cellulose, with a high butanol yield of 0.33 g/g, alcohol-acid ratio of 5.30 g/g, and C4-C2 ratio of 2.35 g/g in batch fermentation with MV. These mutant strains meet our target of 5 g/L butanol with a yield of 0.3 g/g cellulose in batch fermentation. However, butanol production was inhibited by butanol and impaired by sporulation under butanol stress. It is thus

#### Weighted Project Score: 8.5

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

necessary to further engineer the strain to improve its butanol tolerance. Metabolic flux analyses for selected mutants and fermentation conditions also suggested the necessity to further improve NADH availability and to knock down acid production. Comparative proteomics and metabolomics analyses, along with the fermentation kinetics data, provided the basis for developing a novel dynamic model, which can be used to guide further metabolic engineering strategies. Through further process and medium optimization, butanol production from lignocellulosic biomass and CO<sub>2</sub> H<sub>2</sub> would be economically viable, as indicated by the cost model developed for the consolidated bioprocess. A well-to-pump LCA shows that the integrated biobutanol production process can potentially reduce CO<sub>2</sub> and greenhouse gas (GHG) emissions by ~75% compared to a traditional chemical process.

Strain development via metabolic engineering and fermentation process optimization, assisted by omic analysis of the mutation and process effects, helped us to achieve our goal of producing *n*-butanol and ethanol (biofuel) from lignocellulosic biomass at a cost of \$3/GGE or less. The co-fermentation technology using both cellulose and  $CO_2$  H<sub>2</sub> for biofuel production can greatly increase product yield from the biomass feedstock while also reduce GHG emissions, and is novel and advantageous compared to existing ethanol and acetone-butanol-ethanol fermentation technologies.

#### **OVERALL IMPRESSIONS**

- This project is a collaboration with Green Biologics to improve butanol titer, rate, and yield using both strain engineering and process development. They converted an acetogenic *Clostridium* into an ethanol/butanol producer and used a novel approach to have a second strain to fix CO<sub>2</sub> using the Wood-Ljungdahl pathway. Using two organisms rather than putting both pathways in a single organism is a good approach, since the Wood-Ljungdahl pathway is very difficult to engineer into other organisms. Cocultures with organisms using different substrates should be stable, and results were demonstrated at lab scale. Industry involvement indicates there is confidence in scale-up ability of the process. Milestones were clearly defined, and most were accomplished.
- The goal of this project was to increase butanol production from cellulose using engineered strains of *Clostridia*. In addition, they also proposed to capture the CO<sub>2</sub> produced in the fermenters using homoacetogens. The team was able to increase butanol production and achieve most of their milestones. In addition, they were able to capture some of the CO<sub>2</sub> produced. However, they will need to supplement with hydrogen or potentially syngas. Overall, the project was successful. The TEA appears overly optimistic and would have benefited from external evaluation.
- This project sets a high bar for thorough strain development and process development for biobutanol production from lignocellulosic biomass. By merging gene mining, metabolic engineering, and omics/flux analysis, they demonstrate a coculture system capable of producing high levels of butanol. Their success appears to be aided by the employment of a coculture technique to instantaneously reclaim CO<sub>2</sub> produced during fermentation, although the evidence of this is indirect.
- On the overall strain development, work is good but not sufficient for commercial deployment, as there are several challenges. A critical review of this work and TEA would help in assessment and cost sensitivity analysis with side-by-side comparison to the current Green Biologics acetone-butanol-ethanol process.
- If the project continues, it would be great to see plans on further production cost reductions (profit margin is still low) and learn more about scalability and manufacturing success of the proposed process/strain.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# PRODUCTION OF HIGH-PERFORMANCE LUBRICANTS FROM CELLULOSIC SUGAR

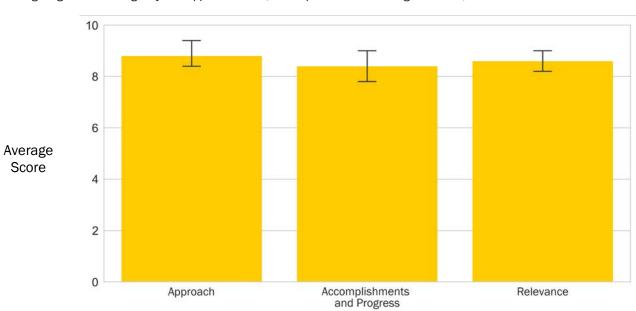
#### Cargill

#### **PROJECT DESCRIPTION**

Certain classes of fatty acids are valuable raw materials that can be used to produce bio-based lubricants; however, their broader use has been limited by high cost and limited availability. This project was focused on producing a fatty acid methyl ester (FAME) of a specific chain length from cellulosic sugars. Development of a biological pathway and engineered organisms for production of low-cost FAMEs from cellulosic sugar is a novel and potentially

| WBS:                      | 2.3.2.204           |
|---------------------------|---------------------|
| CID:                      | EE0007007           |
| Principal Investigator:   | Dr. Tom McMullin    |
| Period of<br>Performance: | 1/1/2016-11/14/2017 |
| Total DOE Funding:        | \$2,000,000         |
| Project Status:           | Sunsetting          |
|                           |                     |

disruptive technology that is supportive of BETO's mission to displace all fractions of a barrel of crude oil. The project was organized around four tasks that focus on (1) production pathway engineering, (2) host strain engineering, (3) assembly of a production pathway in the host strain, and (4) fermentation process development. Pathway engineering focused on discovery and improvement of two key pathway enzymes, namely 3-ketoacyl coenzyme A (CoA) synthase and wax ester synthase. Both enzymes were improved using a variety of enzyme engineering and mutagenesis approaches and assembled into a host strain with relevant additional pathway genes and genome modifications. Assembled strains were evaluated in two-liter benchtop fermenters using a commercially produced cellulosic hydrolysate to supply carbon source for FAME production. These evaluations demonstrated that performance targets and final milestones were met or exceeded for sugar uptake rate, product titer, product specificity, and production rate.



#### Weighted Project Score: 8.6

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%

 ${f I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- The goal of this project was to produce lubricants from cellulosic sugars. The project was successfully completed. The technical approach was very impressive. The team exceeded their final milestones by 2.5-fold, which is outstanding. Future work is unfortunately on hold due to changes in the caprylic acid market and business priorities.
- Cargill has developed pathways in *E. coli* capable of processing hydrolysates to C8 caprylic fatty acids, which can be used in a variety of industries. Impressively, they paired screening of hundreds of natural enzymes with rational protein design to more than double the activity of the needed enzymes *in vivo*. It is also noteworthy that they pursued process development through to the fermentation process, successfully exceeding their production targets. The work is relevant to BETO in that it successfully transforms renewable biomass into a bioproduct with commercial viability.
- Overall, the research expands uses of a hydrolysate for production of lubricants of commercial value. It is hard to judge from the titers, rates, and yields, as well as the process parameters necessary for commercial scale-up production.
- Great progress even with lower-than-expected 3-ketoacyl-CoA synthase activity. It would be great to include TEA.
- The team is developing a process for producing caprylic methyl ester from cellulosic hydrolysate. The product and others of different chain lengths have a potential application as high performance lubricants that are biodegradable. The use of an acyl carrier protein-independent fatty acid pathway removes product synthesis from native fatty acid regulation and esterification with methanol reduces toxicity of the C8 fatty acid. The project is well structured with specialized functional teams, and goals are well defined. Much of the effort was focused on improving the pathway enzymes to achieve needed specific activity and chain specificity so cycle stops at C8. This was accomplished by a combination of natural enzyme screening, rational modifications, and random mutagenesis. With the improved enzymes combined with fermentation optimization, production targets were reached. Progress was made on cellulosic sugar utilization, but there was not full co-consumption of glucose and xylose.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# SECOND-GENERATION MIXOTROPHY FOR HIGHEST YIELD AND LEAST EXPENSIVE BIOCHEMICAL PRODUCTION

#### White Dog Labs Inc.

#### **PROJECT DESCRIPTION**

The primary economic driver for second-generation biochemical biofuel processes is feedstock cost and cost associated with the conversion to fermentable carbohydrates, and therefore it is crucial to maximize conversion of the feedstock into a product of interest. However, biomass (particularly sugar) is less reduced than the majority of biochemical products of interest, particularly non-oxygenated fuels and alcohols.

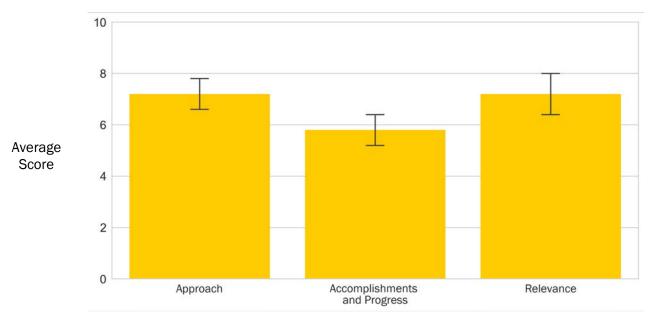
| WBS:                      | 2.3.2.205           |
|---------------------------|---------------------|
| CID:                      | EE0007564           |
| Principal Investigator:   | Dr. Shawn Jones     |
| Period of<br>Performance: | 9/1/2016-12/31/2018 |
| Total DOE Funding:        | \$1,539,826         |
| Project Status:           | Sunsetting          |
|                           |                     |

Accordingly, fermentation processes must oxidize a portion of the biomass, thus releasing  $CO_2$  and decreasing the potential mass yield of the product of interest. White Dog Labs Inc. is developing a technology to help mitigate this loss to  $CO_2$  termed Anaerobic Non-Photosynthetic (ANP) Mixotrophy, or just Mixotrophic Fermentation. This technology consists of using specific microorganisms that can concurrently consume both a sugar feedstock and the  $CO_2$  evolved, thus limiting the amount of  $CO_2$  released from the process.

As a first demonstration of this technology, White Dog Labs is targeting acetone production, an important commodity chemical and a feedstock for poly(methyl methacrylate) (PMMA) production. Using traditional fermentation technology, the theoretical maximum conversion of sugar into acetone is only 32 wt %, thus wasting a significant fraction of the carbon feedstock. However, applying a Mixotrophic Fermentation process will increase the mass yield to 45 wt %, a similar yield to commercial ethanol facilities, which dramatically changes the economic outlook for a bio-acetone facility. Importantly, this is a technology that can be applied to

#### Weighted Project Score: 6.5

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 ${f I}$  One standard deviation of reviewers' scores

a wide variety of biochemical biofuel molecules, making many of these molecules economically viable when produced through a biological route.

#### **OVERALL IMPRESSIONS**

- The goal of this project is to produce acetone from cellulosic sugars with increased mass yields. Increased yields would be achieved by capturing CO<sub>2</sub> produced during fermentation using acetogenic microorganisms. This is an interesting idea that, if successful, would greatly improve yields. Acetone was chosen as a proof-of-principle molecule, which is a good target given the organisms being explored. While the team was able to produce acetone using an engineered microorganism, they failed to meet their final milestones due to a number of technical problems. The project was technically ambitious, and the performers were unable to achieve their goals. Nonetheless, they developed a promising platform of organisms for future work.
- The team attempted to beat theoretical yield maximums by recovering CO<sub>2</sub> during fermentation. Data from plasmid-transformed strains indicate that the approach has promise, but unfortunately difficulties associated with integration into the genome prevented the team from realizing a strain to demonstrate industrial relevance.
- This project is technically and commercially challenging. Acetone is a commodity chemical and is produced commercially. The fermentation route requiring engineering of a *Clostridium* strain that cometabolizes C5/C6 sugars in hydrolysates to produce commercially viable quantities is a major undertaking. Green Biologics is already producing acetone by acetone-butanol-ethanol fermentation. The advantage of Mixotrophic Fermentation resides in combining aspects of both conventional fermentation and gas fermentation into a single microbe. The microbes can fix CO<sub>2</sub> produced during catabolism of sugar to produce more product, thereby increasing carbon yields. This assumption is valid for a robust strain with high titer, rates, and yields that can be commercially competitive with other routes. It is not clear the limit of tolerance of the selected strain to acetone.
- It seems the project is continuing under a different program. If that is the case, PIs are encouraged to address the remaining issues in this project and complete evaluations/tests of the integrated system.
- The Mixotrophic Fermentation platform technology utilizes the CO<sub>2</sub> produced during glucose catabolism to increase product yield. The team constructed an acetogen that could consume all C5 and C6 sugars and evolved to cellulosic hydrolysates. However, this mutant was not readily transformable. Growth of the organism is slow, so a cell retention system was used to maximize productivity. After solving problems with membrane fouling, the team got stable continuous operation of the bioreactor, but production was low. They did not reach fermentation titer and yield goals, but progress was demonstrated. Overall, most of the individual challenges were addressed but could not be combined in a single strain. The concept is a great idea, though acetone may not be the most profitable target product. Given the challenges so far, it is going to be difficult to reach commercial metrics.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# FERMENTATIVE PRODUCTION OF TRICARBOXYLIC ACID CYCLE-DERIVED CHEMICALS USING CELLULOSIC SUGARS

#### Lygos, Inc.

#### **PROJECT DESCRIPTION**

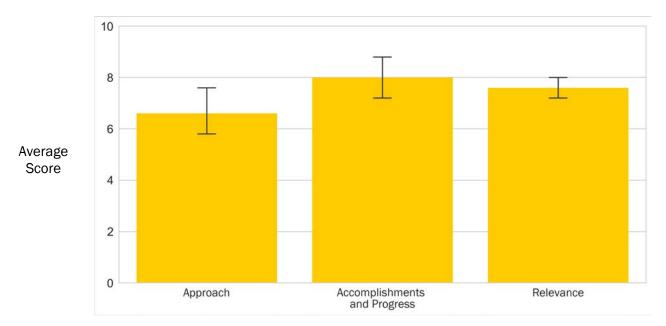
| Lygos, Inc. has demonstrated the fermentative production     |  |  |
|--|--|--|
| of a tricarboxylic acid cycle-derived organic acid product   |  |  |
| from cellulosic glucose. Furthermore, we also                |  |  |
| demonstrated the ability to separate and purify this product |  |  |
| from the fermentation broth. More recently, we made          |  |  |
| significant strides in the area of strain engineering and    |  |  |
| process optimization, as evident by the steady               |  |  |
| improvements in the overall production metrics from our      |  |  |

| WBS:                      | 2.3.2.206            |
|---------------------------|----------------------|
| CID:                      | EE0007565            |
| Principal Investigator:   | Dr. Jeffrey Dietrich |
| Period of<br>Performance: | 10/1/2016-1/1/2019   |
| Total DOE Funding:        | \$1,709,464          |
| Project Status:           | Sunsetting           |
|                           |                      |

engineered production host. Currently, successful scale-up is at the forefront of our engineering efforts to ensure that we are on a track to achieve the techno-economics that support cost-effective production from cellulosic sugar at commercial scales.

#### Weighted Project Score: 7.5

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 ${f I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- The goal of the project is to produce aspartic acid from cellulosic glucose. The motivation for producing aspartic acid is that it can potentially be produced at high yields from glucose, in part by capturing the CO<sub>2</sub> produced during glycolysis. Initial work was done in *Pichia* yeast; the initial results were not promising. The team then switched to *C. glutamicum*, which is an industrial amino-acid-producing strain. The team was able to achieve target yields and titers using engineered *C. glutamicum*. Process was demonstrated at the two-liter scale. Overall, the team is on track to meet all of its project milestones. The project would benefit from TEA and comparison to existing amino acid processes given that a lot of work has already been done in this area.
- Lygos, Inc. has demonstrated a novel design for production of aspartate from TCA (via aspartate dehydrogenase) and achieved all performance targets. Lack of TEA makes it hard to judge the broader
- Great outcomes, clear plan, and clear progress. It would be great if the PIs can do a TEA to estimate cost of production, and if that would be a feasible process.
- This project is intended to develop a full process from cellulosic sugars to aspartic acid. The pathway is redox balanced and high yielding (2:1 molar from glucose), so it is a good choice for a low-cost, carbon-efficient process. Originally a *Pichia* strain was chosen, but this did not transport the product well, so they switched to *C. glutamicum*, which is well suited for amino acid production. All milestones were met, indicating that the pathway is de-risked. However, only the C6 stream of the cellulosic feedstock was utilized. It is also not clear how their work compares to the current state of the art in the amino acid industry.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# INTEGRATED PROCESS FOR COMMERCIAL PRODUCTION OF FARNESENE, A VERSATILE PLATFORM CHEMICAL, FROM DOMESTIC LIGNOCELLULOSIC FEEDSTOCK

#### Amyris, Inc.

#### **PROJECT DESCRIPTION**

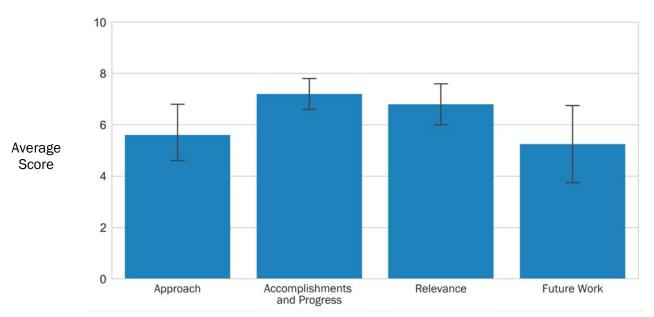
The goal of this project has been to develop an engineered yeast strain and a scalable, lignocellulosic-based manufacturing process for the production of farnesene for fuel and bioproducts from woody feedstocks. This work has been carried out by Amyris, Renmatix, and Total, three commercial entities with complementary capabilities. Renmatix has employed its Plantrose<sup>®</sup> process using supercritical hydrolysis to fractionate hemicellulosic and

| WBS:                      | 2.3.2.207            |
|---------------------------|----------------------|
| CID:                      | EE0007729            |
| Principal Investigator:   | Dr. Joel Cherry      |
| Period of<br>Performance: | 10/1/2016-12/31/2019 |
| Total DOE Funding:        | \$7,000,000          |
| Project Status:           | Ongoing              |
|                           |                      |

cellulosic sugars from pine. Amyris has developed yeast biocatalysts and fermentation processes for conversion of Renmatix's cellulosic sugars into farnesene that is of equal quality to that produced from cane syrup feedstocks. This involved engineering a farnesene manufacturing strain to consume the xylose and to be resistant to growth inhibitors present in biomass-derived sugars. Total has conducted a thorough engineering study and TEA to provide production cost estimates and has developed a rigorous LCA to assess environmental impact. The final project goal was to develop a manufacturing-ready process to produce farnesene from cellulosic sugar in the United States for a manufacturing cost of \$2/L. Such a production cost would allow immediate access to existing farnesene markets.

#### Weighted Project Score: 6.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

Progress on the project has been very positive, but final cost targets now appear impractical. Amyris biocatalyst improvements have met milestone targets for xylose consumption, cellulosic hydrolysate tolerance, and consumption of organic acid growth inhibitors present in hydrolysates. Amyris has also adapted their fermentation processes for non-syrup feedstocks, and developed technologies for the analytical measurement and biological assessment of hydrolysate components. Renmatix has developed a viable and scalable strategy for fractionation of their sugar streams in case further purification is still required after biocatalyst improvement. Total has modeled a fully integrated U.S. manufacturing plant to assess reductions in carbon emissions and overall production costs. This last activity reveals unanticipated CAPEX costs that make final cost targets infeasible for now.

#### OVERALL IMPRESSIONS

- The goal of the project was to produce farnesene from lignocellulosic sugars. This work builds on Amyris's technology for producing farnesene from cane syrup. Farnesene is a promising target as it has many applications, from fuels to cosmetics. The strength of the project was that the milestones include realistic cost targets. The major challenge was that engineered strains did not grow well due to inhibitors in hydrolysates. The team was able to generate a strain that could partially tolerate inhibitors in hydrolysates. The project failed to achieve its objectives and was terminated early, mostly due to high capital costs associated with a planned process. That said, the project looked promising, and not all good ideas work. This work, though unsuccessful, may provide a useful benchmark for other processes with regards to commercial feasibility.
- This project revealed several important insights concerning technical risk in switching feedstocks on a highly engineered industrial production strain. After establishing growth inhibition, assays helped pin down organic acids as the major contributors, and liquid chromatography-mass spectrometry was used to identify specific toxins. This information was successfully used to guide the engineering of strains containing workaround pathways. This data-driven strain engineering was impressive, but it is unfortunate that the TEA estimates that ultimately triggered a "no-go" for the project were not performed at an earlier project phase.
- The assumptions used for the cost of production of farnesene were not sufficiently detailed to show cost sensitivity from higher OPEX and CAPEX for the added unit operations that would be needed for processing of pine hydrolysate and waste treatment required for a stand-alone facility. A more rigorous TEA at the outset may have helped in determining targets for commercial viability.
- Knowing when to kill a project or put a pause on it is as valuable as having a successful outcome. It is great that the PIs are making the decision to stop the project due to the high production costs.
- Amyris has a well-established process for producing farnesene from pure sugars, and the objective of this program is to adapt this process to lignocellulosic feedstocks. One of the main challenges is sensitivity of the strain to impurities in the feedstock. It appears that the magnitude of this problem, compared to conventional ethanol yeast, was not fully appreciated at the start. This issue was partially solved, but farnesene productivity suffered as a result. Both TEA and evaluation of tolerance should have been done much earlier in the project, before a significant amount of money was spent to continue. Although a go-no-go milestone on process economics was not reached, it is doubtful the strain performance metrics would have been reached by the end of the project. However, a number of accomplishments could have general applicability:
  - Characterization of biomass inhibitors
  - Synthetic inhibitor mix to match hydrolysis inhibition
  - Engineering inhibitor consumption into the yeast strain.

The reason economics did not work out was high cost of Outside Battery Limits (OSBL) infrastructure, so a possible solution is to co-locate multiple bioprocessing plants at the same facility. However, this result is rather surprising because it wouldn't seem that OSBL costs should vary too much across all the biochemical conversion projects. Thus, it is suggested that the team works with the biochemical platform analysis team at NREL to check assumptions compared to those used for evaluation of internal projects.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

## IMPROVING TOLERANCE OF YEAST TO LIGNOCELLULOSE-DERIVED FEEDSTOCKS AND PRODUCTS

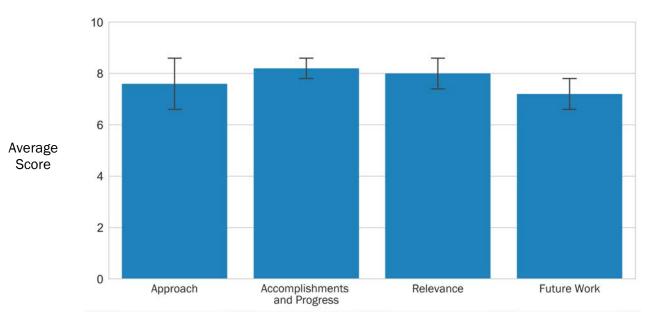
#### Massachusetts Institute of Technology

#### **PROJECT DESCRIPTION**

Combined substrate-product toxicity in microbes is one of the major constraints hampering the scale-up and economic competitiveness of bioprocesses based on lignocellulosic feedstocks. Hydrolytic pretreatments of biomass release numerous compounds impinging on cell viability. The three most significant to yeast (the industrydominant biocatalyst), and common to all plant sources, are furfural, hydroxymethylfurfural, and acetic acid.

| WBS:                      | 2.3.2.208               |
|---------------------------|-------------------------|
| CID:                      | EE0007531               |
| Principal Investigator:   | Dr. Greg Stephanopoulos |
| Period of<br>Performance: | 10/1/2016-9/30/2019     |
| Total DOE Funding:        | \$1,500,000             |
| Project Status:           | Ongoing                 |
|                           |                         |

Furthermore, the desired end product, such as ethanol, typically attacks a multitude of host cellular functions via mechanisms yet to be fully understood. We propose to enhance lignocellulosic fermentations in yeast using nutrient adjustments proven previously to boost alcohol tolerance combined with genetic modifications aimed at alleviating hydrolysate toxicity. Thus far, we have systematically characterized the component toxicities in biomass hydrolysates and quantified their relative impacts on ethanol production. Currently, we are engineering tolerance to these inhibitory compounds using strategies combining enzymatic detoxification with viability-enhancing adjustments of the fermentation medium. Ultimately, we will assess the extent to which these tolerance methods are transferrable beyond ethanol, specifically to yeast processes synthesizing the antifreeze precursor monoethylene glycol.



#### Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

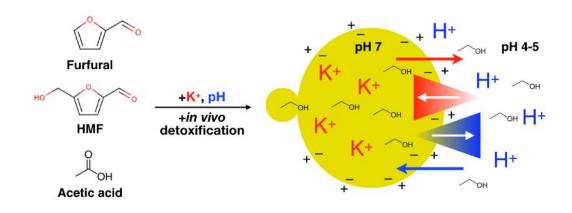


Photo courtesy of Massachusetts Institute of Technology

#### **OVERALL IMPRESSIONS**

- The goal of this project is to improve the tolerance of yeast to inhibitors to lignocellulosic hydrolysate. The team is making excellent progress. The project would be strengthened by the inclusion of competitive benchmarks, as similar work has been completed by many other groups. The team also needs to use real hydrolysates rather than synthetic ones, which they readily acknowledge. Finally, they also need to consider hydrolysate variability, which would improve the impact of the work.
- This team has made compelling progress toward engineering hydrolysate tolerance into *S. cerevisiae* via rational, stepwise metabolic engineering. To do this, they have established a system that uses media with defined composition of inhibitors that appear in feedstocks and have shown nearly complete recovery of ethanol production with their engineered strains. The resulting yeasts have the potential to provide a bridge between benchtop research and platform production systems grown on cellulosic biomass. The group has also demonstrated monoethylene glycol production in yeast and aims to combine these efforts to show production in the presence of inhibitors.
- This project aimed for the development of industrial yeast strains with increased inhibitor tolerance for second generation that can ferment both C5/C6 from biomass hydrolysate. The project also aims to engineer a yeast strain for the production of monoethylene glycol from xylose.
- The project provided sound technical approach, and the described technical approach presented the accomplishments so far and was clear on future work. Adding a go-no-go and more details into the percentage of work done for the last two remaining tasks would make the project even more clear.
- This project aims to engineer *S. cerevisiae* to produce ethylene glycol, then introduce lignocellulosic inhibitor tolerance. Tolerance is assessed by the ability to produce the product in fermentation using hydrolysate, and the targets are based on product titer from this substrate. The product pathway has been introduced to produce ethylene glycol from xylose, and 4 g/L were obtained. The team has also made good progress evaluating toxicity mechanisms and found that nonproductive cells were still alive. Improving tolerance has been the topic of numerous past studies, and some strategies discussed here have already been evaluated (e.g., drug efflux pumps, conversion of aldehydes to alcohols). The results presented here so far show improvement over wild type, but it is unclear how it compares to the current state of technology.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Many thanks to the reviewers for the overall positive feedback and insightful comments. Spurred on by multiple suggestions to validate our approach on real hydrolysates, we are working to secure genuine pretreated biomass through our various BETO contacts. Furthermore, given the relatively high tolerances we have observed with our simulated feedstocks, we are hoping to ultimately source a variety of samples in order to evaluate the robustness of our strains to inhibitor variability. Regarding how our efforts compare to the current state of the art, we acknowledge that the lack of benchmarking against commercial strains is a weakness. However, it is one that remains difficult to address given the proprietary nature of these materials. While we continue seeking the partnerships to gain access to these reagents, the production numbers published in the literature continue to serve as our metric. Lastly, to our knowledge, our plans to make cellulosic monoethylene glycol will continue to be the first demonstration of a non-ethanol product to be fermented directly from un-detoxified hydrolysates.

# ENGINEERING THERMOPHILES TO PRODUCE DROP-IN FUELS FROM SYNGAS

#### Kiverdi

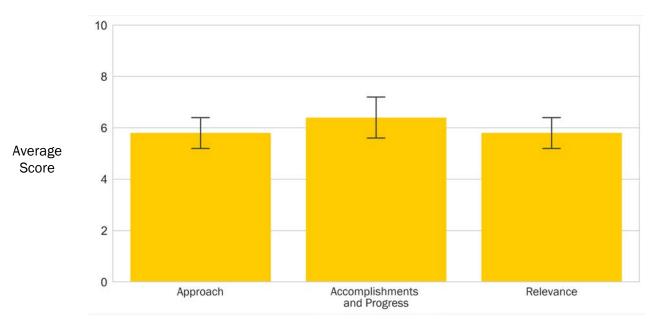
#### **PROJECT DESCRIPTION**

Develop recombinant thermophilic microbial strains capable of metabolizing syngas (carbon monoxide, CO<sub>2</sub>, hydrogen) into monoterpenes to enable industrial production of fuels and solvents.

| WBS:                      | 2.3.4.204          |
|---------------------------|--------------------|
| CID:                      | EE0007008          |
| Principal Investigator:   | Dr. John Reed      |
| Period of<br>Performance: | 9/1/2015-6/30/2018 |
| Total DOE Funding:        | \$886,322          |
| Project Status:           | Sunsetting         |
|                           |                    |

#### Weighted Project Score: 6.1

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- The goal of this project was to develop a thermophilic microorganism capable of converting syngas to monoterpenes. The team was not able to achieve the goals of this ambitious project. They did accomplish most of their intermediate goals. The team was able to produce terpenes from syngas using mesophiles, though not at target titers. Progress was stymied, in part, due to initial strain choice, which did not use syngas despite claims in the literature.
- This team sought to bring monoterpene biosynthesis online from syngas in a new hyperthermophile. The team was able to identify a new production host and to engineer in genes for monoterpene biosynthesis, as well as establish analytical methods for detection. Product was not observed, but the genetic design was validated in a separate mesophilic host. Relevance of targeting hyperthermophiles was not clearly explained, but bioconversion of syngas has clear implications for BETO.
- The basic premise for this project was to establish the growth of thermophilic mixotrophic green nonsulfur bacterium selected on syngas for the production of drop-in fuels from syngas.
- Presentation (with its current format) seems incomplete without clear flow, in a way that makes it look like more information is needed to assess this project. One main comment for the PIs—besides from presentation—is to comment on the scalability and relevance of the Air-Lift Syngas Bioreactor.
- This project is a collaboration between Kiverdi and NREL to develop a thermophilic microbial strain to convert syngas into monoterpenes. Challenges are obtaining a terpene synthase that can function at high temperature, development of genetic tools for the thermophilic strain, and the high demand of adenosine triphosphate for terpene synthesis. The originally chosen thermophile was not able to consume carbon monoxide, so much of the project focused on identifying a new strain that could consume syngas and was transformable. A suitable strain was found, as was a thermostable monoterpene synthase, but production was not obtained. Instead, terpenes were produced from syngas in a mesophilic organism. Anyway, the advantages of using a thermophilic strain are not really convincing.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# DEVELOPMENT OF A SUSTAINABLE GREEN CHEMISTRY PLATFORM FOR PRODUCTION OF ACETONE AND DOWNSTREAM DROP-IN FUEL AND COMMODITY PRODUCTS DIRECTLY FROM BIOMASS SYNGAS VIA A NOVEL ENERGY-CONSERVING ROUTE

#### LanzaTech, Inc.

#### PROJECT DESCRIPTION

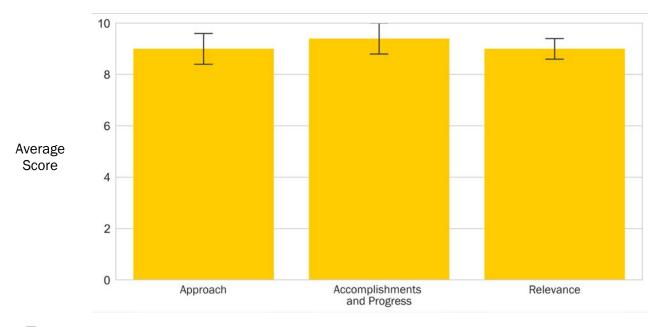
LanzaTech and ORNL have developed and scaled up a process for sustainable production of acetone and downstream drop-in fuel and commodity products directly from biomass syngas via a novel energy-conserving route in engineered acetogenic bacteria. This process offers a safer and more environmentally friendly production method for acetone production than the current phenol-dependent method, and the product has significantly lower GHG emissions. The developed process offers a cost-competitive

| WBS:                       | 2.3.4.205           |
|----------------------------|---------------------|
| CID:                       | EE0007566           |
| Principal<br>Investigator: | Dr. Michael Koepke  |
| Period of<br>Performance:  | 10/1/2016-9/30/2018 |
| Total DOE Funding:         | \$736,544           |
| Project Status:            | Sunsetting          |

route to acetone and enables biofuels at or below DOE's \$3/GGE target. In addition, it also provides an attractive biological alternative to traditional sugar-based acetone-butanol-ethanol fermentation by enabling utilization of non-food biomass resources as fermentation feedstocks.

#### Weighted Project Score: 9.2

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

#### Challenges overcome:

- **Byproducts formation:** Byproduct 2,3-butanediol and 3-hydroxybutyrate reduce yield and stability. Addressed by elimination of both pathways in our chassis acetone production strain.
- **Cost competitiveness:** Addressed by developing an integrated acetone strain and eliminating byproducts to increase yield and stability. Optimized co-selectivity and co-productivity of acetone and ethanol instead of titer, based on TEA.
- Limited enzyme variety: Addressed by genome mining of over 300 industrial strains in the LanzaTech collection, identifying unique enzyme sequences, and refactoring these unique enzyme variants through LanzaTech's engineering platform. Resulted in over 10-times improvement in acetone production from gas.
- **Continuous process (stability):** Identified bottleneck through detailed omics studies, addressed by integration of the acetone pathway on the chromosome.
- Novel process to scale-up: Addressed by demonstrating stable acetone production in 80-L pilot reactor, with acetone productivity and selectivity comparable to those observed under the same condition in 2-L reactors.

We have demonstrated stable acetone production for over seven days at commercial target rate and selectivity in 2-L reactors and have piloted the process.

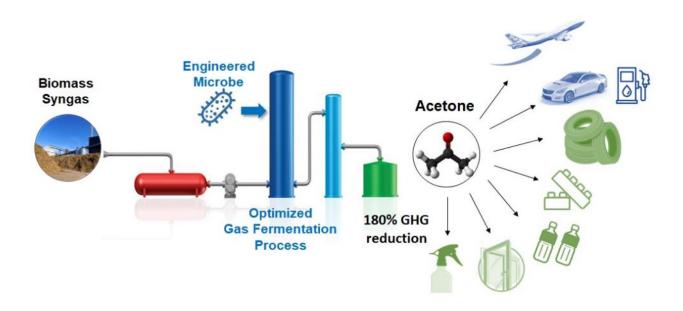


Photo courtesy of LanzaTech, Inc.

#### OVERALL IMPRESSIONS

• The goal of the project was to convert syngas to acetone using a gas-based fermentation process. This works builds on LanzaTech's syngas-to-ethanol process. The team was able to complete all of their technical milestones. A key milestone was engineering a strain with >10-times acetone production. Another key milestone was maintaining acetone productivity during 25-day continuous operations. In

addition, they were able to scale the process up to 80 L. Overall, the project was a success and lays the foundation for a commercial bio-based acetone production process.

- The team has demonstrated a commercially viable system for the production of acetone from syngas.
- An interesting approach to engineering a *Clostridium* strain for acetone production from syngases. There is a misconception about biomass feedstock pricing, supply, and costs. A viable biomass-to-chemical industry will compete as any other commodity in an open market that cannot be completely decoupled from fossil-fuel prices. A robust sensitivity analysis will also reflect this uncertainty.
- Great project that took a concept from lab scale to full product development and a great selection of partner and project allocation between the teams. It was great to see economic/cost analysis as well. Well done.
- This project is intended to develop a process for acetone production from syngas in a continuous bioreactor. An acetone pathway was introduced into an acetogen, then the strain and process were optimized to increase flux. Through a combination of pathway improvement, host modification, and process optimization, the goal of maintaining continuous production was achieved. Good use of modeling and omics analysis. Project is complete, and commercialization is planned. However, as there were no goals defined for rate or yield, it is hard to tell how far they are from commercialization.

- We appreciate the reviewers' concerns. Gasification is able to access biomass on the far end of the supply curve and thus access lower-priced feedstock. There is substantial analysis that negative externalities have been heavily discounted by society in the domain of energy production and use, which undervalues some alternative pathways, like the ones in the project. A competitive market would appropriately price all externalities (positive and negative).
- At the end of this project, we had acetone and ethanol co-productivity and co-selectivity within 5% of the commercial target goal. Exact rate, titer, selectivity, and yield are stated in the progress and public reports (nonpublic information).

# BIOSYNGAS TO FATTY ALCOHOLS (C6-C14) AS A PATHWAY TO **FUELS**

#### **Dow Chemical Company**

#### **PROJECT DESCRIPTION**

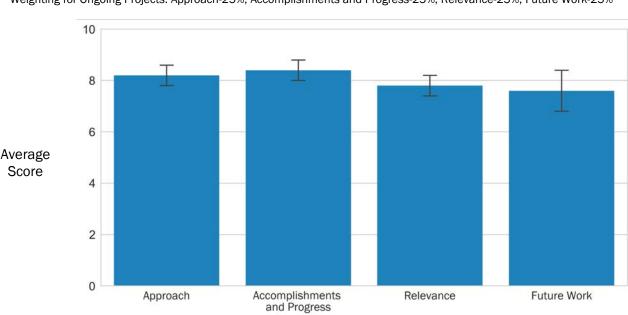
The Dow Chemical Company, in partnership with LanzaTech and Northwestern University, is developing a process for the bioconversion of biomass-derived syngas to fatty alcohols as a pathway to biofuels. The fermentation of biosyngas from lignocellulosic biomass will decouple the biofuel supply chain from the food chain. The production of intermediate fatty alcohols offers a unique opportunity to traverse the "valley of death" for biofuel

| WBS:                      | 2.3.4.207           |
|---------------------------|---------------------|
| CID:                      | EE0007728           |
| Principal Investigator:   | Dr. Devon Rosenfeld |
| Period of<br>Performance: | 1/1/2017-5/31/2019  |
| Total DOE Funding:        | \$1,988,690         |
| Project Status:           | Ongoing             |
|                           |                     |

process and infrastructure development by leveraging the robust chemical markets and high-margin applications of fatty alcohols and their derivatives. The process will change the paradigm for biofuels production, enabling the sale of fuel for less than \$3/GGE while vastly improving sustainability.

Initial laboratory experiments produced fatty alcohols and demonstrated bottlenecks limiting overall alcohol yield. Our research project deploys the syngas fermentation and strain engineering expertise of LanzaTech, the computational modeling capabilities of Northwestern University, and the process development expertise of the Dow Chemical Company to remove bottlenecks discovered in the previously developed metabolic pathway maximizing the production of C6–C14 alcohols for channeling into the chemical derivative and fuel markets. The project team has delivered all of our milestones since the 2017 Project Peer Review, including our go-nogo milestone at the end of budget period two. With the target of completing our project in 2019, we are

#### Weighted Project Score: 8.0



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

One standard deviation of reviewers' scores

focused on overcoming key technical challenges through strain and fermentation optimization and conceptual flowsheet design.

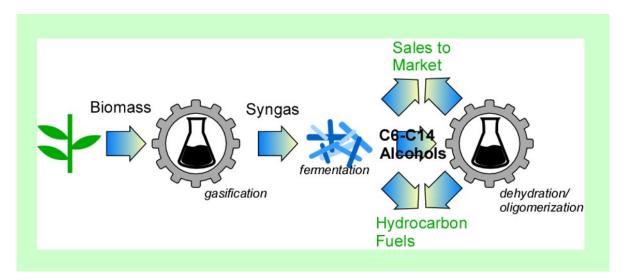


Photo courtesy of Dow Chemical Company

#### OVERALL IMPRESSIONS

- The goal of this project is to produce fatty alcohols from syngas. Fatty alcohols can be upgraded to numerous chemicals. The basic strategy involves producing fatty alcohols using the +1 iterative pathway. This process can potentially produce odd-chained fatty alcohols, which are not currently attainable using current approaches, with linear or branch chains. The team is making excellent progress. They have achieved their titer targets and have developed stable continuous fermentations but are still far away from achieving their productivity targets. Details are vague regarding how they will achieve these final targets.
- Dow presented results of a collaboration with LanzaTech and Northwestern University to produce a variety of fatty alcohols from syngas. The project is not yet complete, but the team has shown promising progress toward industrially relevant levels of bioconversion performance.
- This project aims for the engineering of bacteria for the production of high alcohol from syngas. The proper adaptation and selection of strains is critical to commercial viability. The project is optimistic in its projections for ease of engineering of a production strain with current cost constraints.
- Reallocating the work, when needed, and changing priority is a great approach. The project has a lot of compressed milestones to complete in the next few months; a no-cost extension might be good to consider, as the project is really interesting.
- This collaboration between Dow and LanzaTech is to develop a fermentation process for syngas conversion to intermediate fatty alcohols, produced concomitantly with ethanol. These molecules have a strong market as intermediates that are upgraded to specialty chemicals. The primary challenges of pathway limitations, byproducts, and fermentation stability are well understood, and the team is well suited to address them. Various modeling approaches were used to drive progress, including enzyme kinetics, metabolic network, and thermodynamics; these guided improvement of pathway flux and reduction in byproducts. The project is still far from commercial targets of less than \$3/GGE. The tools are in place to achieve them, but it will be difficult to do so by the end of the project period, even with the extension.

- We appreciate the reviewer's feedback. To address the gap in productivity, we are pursuing multiple parallel paths. We are in the process of carrying out a combinatorial analysis of pathway genes with a large library we constructed to generate optimized strains. We are also carrying out optimization of fermentation parameters to find the optimal balance between titer and productivity guided by targeted metabolomics.
- Our team requested and was granted a six-month no-cost extension, changing the end of our program to November 30, 2019, and a strategy has been worked out to address the remaining gaps within this timeframe.

### **BENCH-SCALE INTEGRATION**

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

Producing renewable fuels and chemicals from biomass at a cost that is competitive with petroleum is the ultimate challenge. With many steps in the process—from feedstock handling, to pretreatment and conversion, to separations and upgrading—each unit operation has its own set of technical barriers to overcome. The technical barriers for the conversion step are many. Specifically, the fermentation step requires high titers, rates, and yields for a cost-competitive biofuel. This is what drives the research direction of the strain engineers and fermentation scientists. For the bench-scale R&D team, we are focused on development and optimization of fermentation processes with the outcome being an optimized, robust,

| WBS:                      | 2.4.1.100           |
|---------------------------|---------------------|
| CID:                      | NL0026683           |
| Principal Investigator:   | Dr. Nancy Dowe      |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$3,752,475         |
| DOE Funding FY16:         | \$1,000,000         |
| DOE Funding FY17:         | \$1,000,000         |
| DOE Funding FY18:         | \$1,002,475         |
| DOE Funding FY19:         | \$750,000           |
| Project Status:           | Ongoing             |
|                           |                     |

and industrially relevant fermentation process. Our approach is to first assess the microorganism, product, and the TEA to determine the R&D approach. Then we apply fermentation science to develop and optimize conditions like aeration levels, feeding strategies, fermentation conditions (pH, temperature, redox), and nutrient management for high titers and production rates. Increasing titer and production rates have a direct impact on capital and operating costs of the conversion and downstream processing equipment.

The project made improvements in lipid and 2,3-BDO production, which directly impacted the TEA. These improvements are captured in yearly SOT reports. Lipids are produced in an aerobic fermentation utilizing the oleaginous yeast *Cryptococcus curvatus*. Because lipid production is not associated with cell growth, growth

#### Weighted Project Score: 8.8

Average Score 4 2 0 Approach Accomplishments and Progress Relevance Future Work

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 $oldsymbol{I}$  One standard deviation of reviewers' scores

and lipid production required separate optimization. Our approach was to manipulate nutrients and employ a fed-batch process for fast growth and high cell density and to limit nitrogen after growth for high lipid production. The type of nitrogen source was also key to high lipid titer; an organic nitrogen source (yeast extract) was preferred over inorganic nitrogen (ammonium sulfate). Lipid titer and productivity increased from 50 to 60 g/L and 0.76 to 0.97 g/L/hour, respectively, during FY 2017, reducing MFSP by \$0.50/GGE.

NREL's BDO process utilizes a different microorganism, a recombinant strain of Zymomonas mobilis developed by the Target Microbial Development (TMD) project. Z. mobilis is an anaerobic bacterium that produces ethanol as the primary product from sugars. TMD strain developers have successfully made a strain of Z. mobilis that no longer produces ethanol, only BDO. However, the modified strain of Z. mobilis suffers from a redox imbalance, which can be alleviated by adding small amounts of air to the process. Optimizing the micro-aeration conditions in the fermenter became the primary focus of the fermentation development research to increase titers. High titers are necessary to reduce the cost of downstream separations and catalytic upgrading. Over the past two years, we have used a fed-batch process using biomass liquor and optimized aeration levels to demonstrate increases in BDO titers by nearly 10 times (10.6 g/L in FY 2016 to 90 g/L in FY 2019). We have also successfully demonstrated scaling of the process from 0.5 L to 100 L. In addition, we have begun the transition from biomass liquor to whole slurry and have demonstrated 55 g/L BDO from whole slurry, which helped reduce the MFSP by \$0.85/GGE. Future work will continue to focus on BDO titer and using biomass whole slurry. Our goal is to produce 125 g/L BDO titer by 2020 to further reduce upgrading costs and incorporate whole slurry to reduce solid-liquid separation costs. We will develop operational parameters and procedures for scaling fermentation so that we can produce pilot-scale quantities of fermentation broth for separations and upgrading R&D and prepare for pilot-sale demonstrations of the conversion process in 2022. As new strains are available, we will incorporate them into the fermentation process.



Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- This project is focused on process development and optimization. The project was initially focused on lipid and BDO production; however, lipid production was dropped due to challenges associated with separations and oxygen transfer. Current work is focused on BDO production. The goal is to develop a process at the ~100-L scale. A key accomplishment is the incorporation of off-gas analysis; this will enable them to close the fermentation mass balance. Overall, the work in this project is central to many activities within NREL and BETO. The team is making excellent progress. The milestones are clear. The impact of the project would greatly improve if they explicitly considered product recovery rather than focusing on fermentation titers. In addition, the team should consider how they can generalize these results for new processes.
- This project has applied process integration to achieve impressive BDO titers from cellulosic biomass and appears to be on track to further increase these numbers. The project also demonstrated new capacities to test commercial enzymes and for off-gas analysis, both of which have general applicability.
- The team has had good successes in fermentation development and improvement and scale-up to the 100-L scale. They have done a very good job in attempting to have better fermentation control and analysis and the development of robust fermentation processes with two different microorganisms.
- This team works on fermentation development and optimization at the small scale from cellulosic sugars, leading towards scaling to the pilot scale. Bench-scale fermentation is a key de-risking step prior to scale-up and provides a standard platform for evaluating strains from different projects. Thus, it clearly plays a critical role in reaching the MYP objectives. The current focus is on 2,3-BDO, though they also collaborate with both internal and external projects in other areas. Historically, the team played a big role in meeting cost targets for cellulosic ethanol and reducing the cost of lipid production. This demonstrates their ability to work in a variety of organisms and inspires confidence in their ability to achieve the same with 2,3-BDO. These expectations were met, exceeding the goal and producing nearly 90 g/L BDO from relevant substrates. The team also works closely with the TMD team so that learnings from one can help to guide the other.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

We thank the reviewers for their positive comments and appreciate their acknowledgment of the importance of the bench scale R&D team's role in developing biofuel fermentation processes at bench scale to facilitate and de-risk scale-up. We recognize the importance of working closely with the strain development groups to evaluate strains in process-relevant conditions and providing important feedback on strain performance. The project has historically been aligned with pretreatment, pilot-scale integration and analysis. With the focus of the project on 2.3-BDO fermentation process development, we have begun to collaborate closely with the Bioprocessing Separations Consortium and the Chemical Catalysis for Bioenergy Consortium to provide material for separations and upgrading research and begin producing fermentation broth that aids the research and development efforts. We continue to maintain a close association with industry by providing information on biocatalyst performance in a process context, which we hope will aid in scale-up. For future work, we agree with the reviewers that developing a scaled-down fermentation model to evaluate new strains would accelerate the screening process, and we have plans to utilize the BioLector micro-fermentation system. We also recognize there are significant challenges in scaling a fermentation process with whole-slurry biomass and agree that engaging industrial fermentation experts on vessel design and micro-aeration would greatly help our development and scale-up efforts.

# CONTINUOUS ENZYMATIC HYDROLYSIS DEVELOPMENT (FORMERLY SEPARATIONS DEVELOPMENT AND APPLICATION)

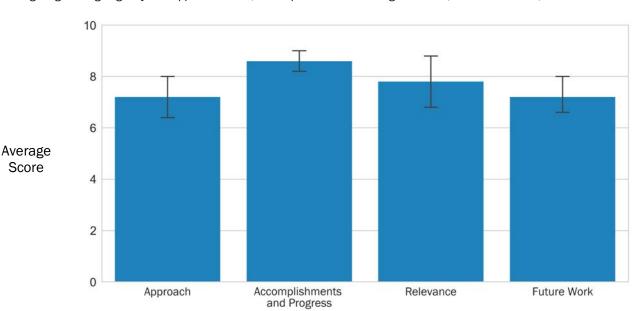
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

This project is focused on developing, demonstrating, and improving continuous enzymatic hydrolysis (CEH) as a transformational, process-intensified, and lower-cost method compared to batch enzymatic hydrolysis (BEH) for producing soluble clarified biomass sugars and insoluble lignin-rich streams—two essential biochemical platform intermediates. The project's goal is to apply combined reaction-separation technology to intensify the production and reduce the cost of producing and recovering these key intermediate streams at or above minimum yield and quality specifications. This scope complements the Bioprocessing Separations Consortium's emphasis on separations to recover upgraded products rather than process intermediates.

| WBS:                      | 2.4.1.101           |
|---------------------------|---------------------|
| CID:                      | NL0026682           |
| Principal Investigator:   | Dr. Jim McMillan    |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$2,774,214         |
| DOE Funding FY16:         | \$750,000           |
| DOE Funding FY17:         | \$750,000           |
| DOE Funding FY18:         | \$774,214           |
| DOE Funding FY19:         | \$500,000           |
| Project Status:           | Ongoing             |
|                           |                     |

Guided by TEA, the project's objective is to prove through a combination of experiments and cost modeling (joint with the biochemical platform analysis project) that CEH can pass relevant technical and economic performance go-no-go criteria (high yield, scalable, with potential to achieve BETO's MFSP [\$/GGE] cost goal). Performance data on CEH are generated to inform and refine process TEAs and LCAs. Ultimately, we



#### Weighted Project Score: 7.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

seek to produce compelling experimental data and descriptive physicochemical models to inform TEA calculations to show that MFSP can be significantly reduced using CEH. The project's stretch goal is to reduce projected MFSP by  $\geq$ \$1/GGE through implementation of CEH.

Current SOT performance levels of BEH and CEH are as follows: For BEH, the 2016 SOT used a starting solids concentration of 20%, which equates to ~12% insoluble solids (IS), and an enzyme loading of 10-mg Novozymes Cellic<sup>®</sup> CTec3 enzymes per gram of cellulose. After 120 hr (5 days), a cellulose conversion yield of 85% is achieved, which after downstream solid-liquid separation losses (required to produce a solids-free sugar stream for upgrading) translates into a BEH SOT process yield to produce clarified biomass sugars of approximately 81%. The required enzymatic hydrolysis reactor size is approximately 720 L/kg insoluble solids fed.

In contrast, CEH is envisioned to be implemented in a multiple continuous stirred-tank reactors (CSTRs)-inseries-type process, although experiments are so far limited to showing proof-of-concept performance of a single CEH stage comprising an CSTR reactor and membrane unit. We have so far operated CEH using IS levels up to 8.5%. At this IS level, using an enzyme loading of 10-mg Novozymes Cellic CTec2 enzymes per gram of cellulose and a mean residence time of 15 hr, a single CEH stage achieved 58% cellulose conversion yield. The total conversion yield approaches 99% in a simulation model of four such CEH reactor stages running in series. After accounting for sugars lost in the spent (residual) solids, the process yield is 90%. Total required CEH reactor size is estimated to be 220 L/kg insoluble solids fed, less than one-third the size required for BEH. While CEH produces a more dilute sugar stream than BEH, both streams require further concentration if fed-batch production using concentrated sugar streams is intended, which it is in the current base case. Thus, additional concentration of a CEH-produced sugar stream to match what is produced in BEH must be included in comparative TEA. Or, conversely, clarification of BEH slurry to remove solids from the product sugar stream must also be included in TEA so that in comparative assessments, the two processes are producing equivalently clarified and concentrated sugar solutions.

The main goal of recent CEH research has been to overcome technical challenges encountered at bench minipilot scale in feeding and recirculating high IS concentration slurries (IS  $\geq$ 10%). In FY 2019, new equipment better suited to higher-IS solids CEH operation is being purchased, installed, and tested. Once a higher IS-capable experimental system has been established, CEH performance at IS levels  $\geq$ 8.5% will be benchmarked and the cost benefit of using CEH over BEH will be assessed through TEA (joint with the biochemical platform analysis project).

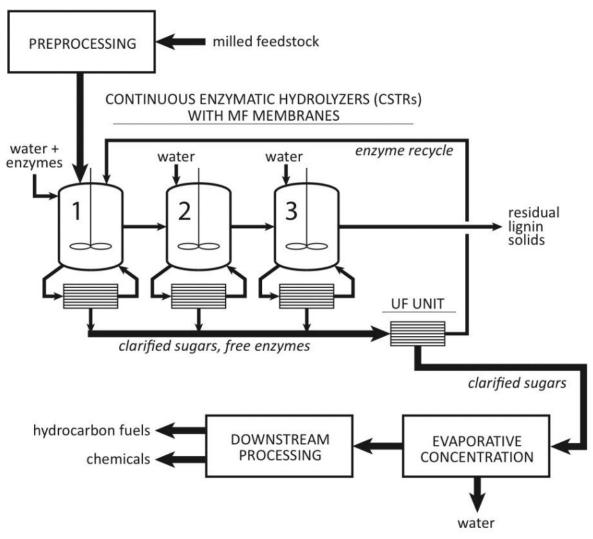


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- The goal of this project is to develop a continuous, multistage enzymatic hydrolysis process. The team is making solid process with regards to their overall goals. The focus on process intensification is especially appealing. One limitation of the project is that the work focuses on single-stage processes and does not address the ultimate goal of developing a multistage process. In addition, it is not clear how well membrane-based separations for enzyme recovery would scale, or whether these operations are economically feasible.
- The group has begun important work toward demonstrating a new method to reduce costs and improve manufacturability of a biomass hydrolysis. A central tenant of the project is to convert to a multistage system, in which residual lignin from each stage is passed to the next, which can, in principle, greatly reduce CAPEX. Thus far, the group has built a benchtop model of a first stage and has tuned and measured its performance. The project has interesting prospects if the performance can be made to match the TEA assumptions, but it has had to confront technical challenges in coping with insoluble solids. It will be important to see the updated TEA results that incorporate the proposed enhancements to the

method, as well as updated modeling predictions that incorporate expected data from simulating stages two and three using their single-stage system.

- On the overall, the project seems to be progressing in spite of some of the limitations in bench-scale equipment that have been identified by the project performers. There are numerous challenges inherent in this work from the choice of pumps, reactors, mixing equipment, and membranes.
- Continuous enzymatic hydrolysis in multiple stages will reduce cost and improve efficiency over the traditional batch process. At this stage of the project, the team is demonstrating using a single stage at insoluble solids that approach 10%. Clear progress has been made towards operating at higher insoluble solids content. The team takes a unique approach, combining TEA and reactor modeling to guide performance improvement. Overall, the team has demonstrated continuous progress in the past two years, and future work is also well positioned for success. Cost modeling indicated MFSP reductions that meet a go-no-go decision point if sustained performance can be achieved. Rather early in the project, they determined that final goals could not be reached with the current facility, so they acquired and tested new equipment for various unit operations. The team appears to have a good understanding of what is needed for success.

- Thank you. We agree that it is not yet clear to what level membrane-based separations for enzyme (and solids) recycle and sugar recovery can be scaled, or how economically competitive they can be. Reducing this knowledge gap is a key objective of this project, albeit it is still at a low technology-readiness level and not focused on scale-up per se for FY 2019–FY 2020, but rather on demonstrating compelling proof of concept that this approach to implementing CEH can be efficacious at high insoluble solid levels where substantial economic benefits can be realized. The experimental portion of the project's focus is constrained by available budget and existing equipment to studying a single CEH reactor stage. However, we are considering approaches to extend experiments to explore system performance in a second or further CEH reactor stage, as this will be key to validating modeling results for later states. Two methods conceived to date are: (1) running at extended mean residence times in the single CEH reactor system to achieve greater extents of reaction, as would occur in subsequent stages; and (2) collecting and storing the first-stage reactor's solids output stream or partially batch enzymatically hydrolyzed material (how to stabilize such materials and for how long they can be stored must also be explored). This partially enzymatically hydrolyzed material could then be used as the input feed into the single CEH reactor in a subsequent experiment to simulate second- or later-stage operation.
- Thank you. We agree, and a key objective of FY 2019–FY 2020 work is to develop performance data at higher insoluble solids levels (10% or higher targeted) that can be used to further validate the kinetic model, as well as to update the TEA. To clarify potential confusion about the model development and validation cycle used to date: the CEH model is developed based on batch kinetics data and model projections are used as input for Aspen Plus software-based TEA, with experimental CEH results used to validate the model.

# TARGETED MICROBIAL DEVELOPMENT

#### National Renewable Energy Laboratory

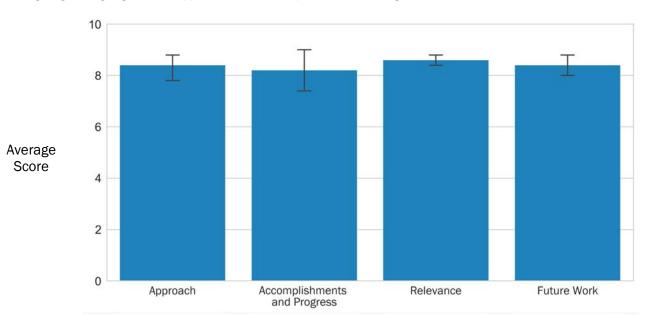
#### **PROJECT DESCRIPTION**

The goal of this project is to develop microbial pathways capable of producing high-carbon-efficiency intermediates amenable to economic separation and catalytic upgrading to hydrocarbon fuels and chemicals. This work will substantially contribute towards achieving BETO's 2022 cost target of \$3/GGE (\$2.50/GGE in 2030). By applying metabolic engineering and synthetic biology tools, we are working to engineer *Zymomonas mobilis* to efficiently utilize sugars for 2,3-BDO production. 2,3-BDO can be chemically upgraded to fuels and other chemicals as coproducts. Moreover, *Z. mobilis* is known for its high specific glucose uptake rate, rapid catabolism, and high ethanol yield. It has been engineered to efficiently convert

| WBS:                      | 2.4.3.102           |
|---------------------------|---------------------|
| CID:                      | NL0026684           |
| Principal Investigator:   | Dr. Min Zhang       |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$6,061,559         |
| DOE Funding FY16:         | \$1,900,000         |
| DOE Funding FY17:         | \$1,900,000         |
| DOE Funding FY18:         | \$1,461,559         |
| DOE Funding FY19:         | \$800,000           |
| Project Status:           | Ongoing             |
|                           |                     |

the second- and third-most abundant plant-derived sugars—xylose and arabinose—to ethanol at high yield. With its ability to utilize most biomass sugars, even in toxic hydrolysate environments, it is now important to enable this microorganism as one of the leading platforms for biomass conversion. It is therefore essential to turn down or knock out the ethanol-producing pathway to redirect carbon flow to other chemical syntheses. We recently demonstrated success in redirecting carbon flow by deleting the ethanol synthesis pathway, which enabled the organism to produce 2,3-BDO exclusively. The outcome of this project will be to provide leading technologies to produce high-carbon-efficiency intermediates suitable for catalytic upgrading to hydrocarbon fuels at reduced cost. We also intend to identify future sugar-upgrading technologies, as well as the critical





 ${\mathbb I}$  One standard deviation of reviewers' scores

knowledge base needed to support the bioenergy industry and research community to further R&D working towards production of third-generation hydrocarbon biofuels from biomass.

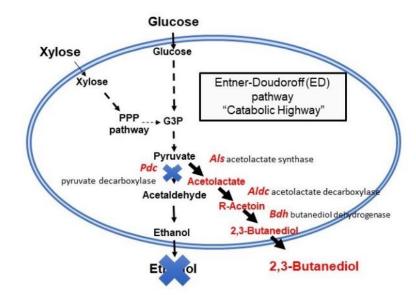


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- The goal of this project is to covert lignocellulosic sugars to 2,3-BDO. The team is accomplishing this task by genetically engineering *Zymomonas mobilis*. Engineering *Z. mobilis* to produce 2,3-BDO and not ethanol is a significant technical achievement. Moreover, they are able to achieve good productivity numbers with their engineered strain. Future work is devoted to improving pentose sugar utilization and addressing issues associated with redox balancing. The plan is compelling and there is no better team capable of achieving these goals. One question concerns the use of *Zymomonas*. Many other microorganisms can produce 2,3-BDO, including yeast. In addition, even though *Zymomonas* is an excellent ethanol producer, it has never displaced yeast. More justification would be useful, especially comparative TEA.
- The team has successfully engineered *Zymomonas* strains to produce industrially relevant titers of BDO from hydrolysate liquor, increasing yields from 20 g/L to 80 g/L.
- The strain development and fermentation groups need to be congratulated on a good effort. They have demonstrated over the past three years that they can improve fermentation titers and strain performance.
- The objective of this program is to develop a biochemical conversion strategy that is carbon efficient. In particular, they are focused on producing 2,3-BDO in *Z. mobilis*. The project originally had three tasks, but one was discontinued because of a low technology-readiness level and the other was spun out as a separate project. The team has focused on solving the key issues of ethanol byproduct and redox balancing, which will reduce manufacturing cost due to easier separations and a lower aeration requirement, respectively. The team works closely with the bench-scale integration team to evaluate their strains in fermentation. Through a combination of strain engineering and process development, significant progress has been made toward reaching commercially relevant metrics. Little work has been done on improving pentose and arabinose utilization, but this work is planned for the coming year.

- We thank the reviewers for the positive comments about the progress the project has made over the past three years with regard to achieving the high 2,3-BDO titers from hydrolysate liquors using engineered *Zymomonas* strains. We appreciate the reviewers' supportive feedback on our future research plan to improve pentose sugar utilization and addressing issues associated with redox balancing. As noted by the reviewer, there are many native and engineered microorganisms, including yeast, that are capable of producing high titers of 2,3-BDO from glucose. However, many of them do not ferment xylose well, including the engineered yeast strains. In addition, to reach high productivity, these organisms usually grow under highly aerobic conditions to produce cell mass in the first stage. Carbon is therefore used for cell mass growth rather than product formation, resulting in overall lower yield. *Zymomonas* has a threefold higher specific sugar uptake rate compared to yeast and it does not have an active TCA cycle; therefore, carbon is mostly directed to product formation, thus achieving high rates. It would be interesting to conduct comparative yeast TEA as suggested.
- Due to resource constraints in FY 2018, we reprioritized our research by downselecting to one pathway focusing on engineering *Z. mobilis* for producing 2,3-BDO. This decision was based, in part, on our success in making 2,3-BDO exclusively from mixed ethanol and BDO products, as well as TEA assessments.

# PROCESS INTENSIFICATION FOR THE REDUCED COMMERCIAL CAPEX OF BIOFUELS PRODUCTION (PRICE CAP) USING DYNAMIC METABOLIC CONTROL

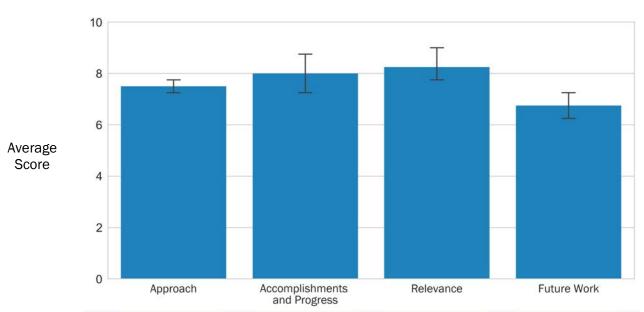
#### **Duke University**

#### **PROJECT DESCRIPTION**

Major barriers currently impede the successful commercialization of integrated biorefineries and largescale industrial bioprocesses for the production of biofuels and value-added chemicals. One of the most challenging barriers is the large capital requirement needed to scale these technologies (CAPEX per plant capacity). These challenges persist despite the numerous advances in strain and pathway engineering that have resulted in attractive

| WBS:2.4.3.200CID:EE0007563Principal Investigator:Dr. Mike LynchPeriod of<br>Performance:10/1/2016-12/31/2020Total DOE Funding:\$1,691,595Project Status:Ongoing |                         |                      |
|---|-------------------------|----------------------|
| Principal Investigator:Dr. Mike LynchPeriod of<br>Performance:10/1/2016-12/31/2020Total DOE Funding:\$1,691,595   | WBS:                    | 2.4.3.200            |
| Period of<br>Performance:         10/1/2016-12/31/2020           Total DOE Funding:         \$1,691,595   | CID:                    | EE0007563            |
| Performance:         10/1/2016-12/31/2020           Total DOE Funding:         \$1,691,595  | Principal Investigator: | Dr. Mike Lynch       |
| <b>C</b>  |                         | 10/1/2016-12/31/2020 |
| Project Status: Ongoing   | Total DOE Funding:      | \$1,691,595          |
|   | Project Status:         | Ongoing              |

product yields using fermentation-based approaches. Large capital costs are a major challenge to the realization of the potential of numerous sustainable bioconversion technologies. The focus of the proposed program will be to develop a first ever semi-continuous fermentation process producing the fuel precursor farnesene from cellulosic sugars at currently unprecedented titers, rates, and yields, resulting in greatly reduced commercial CAPEX requirements. The result will be a technology enabling a commercial-scale bioprocess (100 million gallons of fuel per year) with capital costs less than that of a current demonstration plant (\$40 million). This translates to a cost less than \$0.50 per gallon of fuel production capacity and a step change in capital cost reductions compared to the current state of the art.



#### Weighted Project Score: 7.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- The goal is to produce farnesene with reduced capital expense. The key innovation involves two-stage metabolic control, where cell growth is decoupled from production. One strength of the proposal is that it is motivated by TEA. Reduced CAPEX will be achieved by high-density continuous fermentation. The team has accomplished a lot work. However, it is not clear that the team will meet their final productivity milestones. Nor is it clear how close the team is toward reaching these milestones.
- Duke University presents a compelling case for an innovative approach to cutting production costs by combining process intensification with dynamic metabolic control. The group first validates its approach via TEA, and then pursues intensification technology, strain development, and process integration. The project is not yet complete, but the initial results from these efforts look promising.
- The project outlines the use of a dynamic metabolic control process to reduce the CAPEX of manufacturing biofuels. This process relies on recycling of cellular biomass and the use of stationary cells as the biocatalyst.
- Great basic research project. Adding project management will help the project track progress better.
- This project uses dynamic metabolic control and cell recycle to increase cell density and reduce CAPEX, enabling the construction of smaller plants. Farnesene is the model product. The team has improved C5 utilization by *E. coli*, and reasonable co-utilization was obtained. TEA was used to guide the optimization of process conditions, finding the best biomass concentration that reduces fermenter size without introducing unreasonable heat removal and oxygen transfer problems. This demonstrated that CAPEX of <\$0.50/gal for the product could be achieved if the target metrics could be reached. The team achieved high specific rates of farnesene production and implemented a semi-continuous process. Project management was very loose, which could have had more serious consequences if significant problems had arisen.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

### **BIOCHEMICAL PROCESS MODELING AND SIMULATION**

#### National Renewable Energy Laboratory

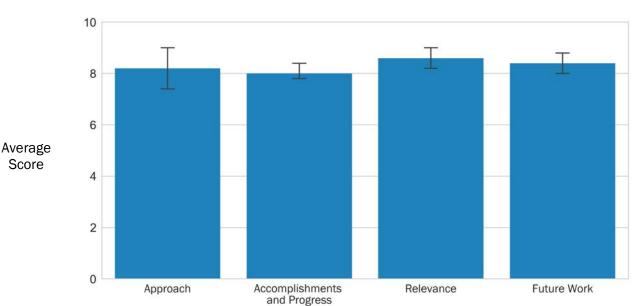
#### **PROJECT DESCRIPTION**

This 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.

| WBS:                      | 2.5.1.100           |
|---------------------------|---------------------|
| CID:                      | NL0013377           |
| Principal Investigator:   | Dr. Mike Crowley    |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$5,432,276         |
| DOE Funding FY16:         | \$1,500,000         |
| DOE Funding FY17:         | \$1,500,000         |
| DOE Funding FY18:         | \$1,382,276         |
| DOE Funding FY19:         | \$1,050,000         |
| Project Status:           | Ongoing             |
|                           |                     |

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 simulation that could otherwise not be solved or would take too long with experiment alone to reach BETO's targets. We have produced solutions that have resulted in determining the most likely fatty-acid derivative for passive transport out of bacteria that upgrade biomass, and we have also designed enzyme mutations for enhanced lignin upgrading. Metabolic models have been developed to tune the activity of BDO production for the 2022 target. A computational method to deliver understanding of how the complex metabolomics and proteomics data can be interpreted in the metabolic pathways of organisms used in the Agile BioFoundry consortium. We have found methods to overcome



#### Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

specific barriers and continue to develop those methods. Our reactor studies have guided the design of both the microbes and reactors for aerobic and microaerobic 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 2022 and 2030 biofuel production targets.

#### OVERALL IMPRESSIONS

- This team uses modeling, theory, and simulation in conjunction with experimental data to examine solution space that cannot be accessible easily by experiment. This enables the projects to downselect targets, pathway options, knockouts, enzymes, fermentation conditions, etc. Three tasks are molecular modeling, metabolic modeling, and mechanistic process modeling, thus spanning scales from molecular to cellular to macroscopic. The team has demonstrated impact on project teams; for example, leveraging models of membrane transport to prevent unproductive research. In the future, the team is using a unique combination of metabolic modeling and computational fluid dynamics to design a microaerobic process for BDO production. This is a well-managed program that has demonstrated very relevant work and will likely continue to do so in the future. It is recommended to increase funding to this effort so they can work on more projects, because this project has demonstrated clear benefits so far.
- The goal of this project is to provide modeling support for various NREL and BETO activities. The activities range from atomistic simulations to fermenter models. A key strength is the connection to experimental work. Most of the progress in the past year was related to membrane permeability and enzyme design. In addition, there has been some work related to aerobic fermenter design. This is the most promising and unique aspect of this project, as it directly supports the goal of commercialization. In other words, it can help de-risk scale-up. More resources should be directed towards these efforts. Overall, the team is productive, supporting key activities within BETO and doing quality work.
- This reviewer especially appreciates the characterization of the role of modeling to help reduce the experimental search space. This team is developing a multiscale portfolio of approaches to address this challenge, including molecular, metabolic, and process-level modeling. They have produced impressive models in all of these areas and have shown that they have a positive impact on experimental outcomes. However, it should be noted that this kind of model validation is very indirect (perhaps out of necessity), which limits the direct feedback available to further refine these models in the future.
- The 2,3-BDO titer and/or increased yield of 10% represents a major milestone and challenge to meet. It is a good test for the use of modeling to drive process improvements by identifying process bottlenecks.
- Bringing together a metabolic model, dynamic process modeling, and reactor design is a great idea and will help reduce the timeline from concept to product. The project will benefit from focusing on one of the three tasks instead of working on all three together.

- We thank the reviewers for all their effort to carefully evaluate this project, its strengths, and its weaknesses. The feedback is valuable and appreciated. It is very clear that these reviewers carefully considered our project and took the time to understand and provide valuable feedback.
- Regarding validation, we agree that validation is essential to the value of modeling and prediction and appreciate the comments of the reviewers. Our work is always connected with an experimental effort and our predictions are always tested in experiments and provide, perhaps not directly, a means of validating our models. Rarely, if ever, are the main takeaways of a modeling effort directly measured in an experiment. We are always using all experimental feedback for improving models in an iterative fashion.
- Our history has shown that the combination of multiple models has been very successful in all three tasks and allows us to provide a multiscale approach to experimental bottlenecks from reaction

mechanism to industrial-scale reactors. Often these scales overlap in a question and require expertise at each scale to work together, such as in the BDO work. This project does not require the direct attention of the PI in all three tasks. Each task lead has the responsibility of concentrating on achieving the goals of each task and collaborating with experimental efforts in BETO.

# ANALYTICAL DEVELOPMENT AND SUPPORT

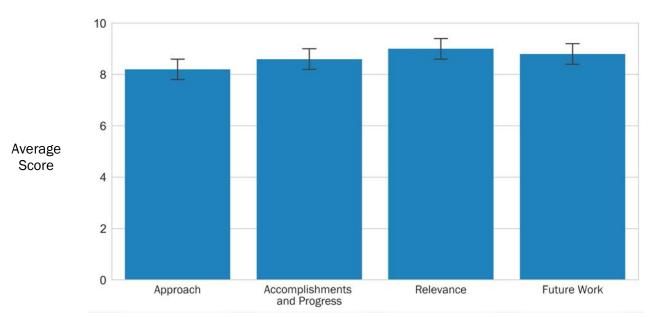
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

The goal of this project is to enable biofuel and bioproducts R&D at NREL by ensuring high-quality analytical data, and to advance the tools available to the wider community through method development and globally adopted procedures. Our project is divided into two tasks: one task to improve existing analytical methods and to develop and implement new methods, and one task to maintain existing analytical facilities at NREL and to provide outreach to external stakeholders. We actively cultivate partnerships with industry, academia, and other government laboratories, based largely on our reputation for excellence in analytical chemistry. This project is best known for our publicly available laboratory analytical

| WBS:                      | 2.5.1.101           |
|---------------------------|---------------------|
| CID:                      | NL0026685           |
| Principal Investigator:   | Dr. Ed Wolfrum      |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$4,396,516         |
| DOE Funding FY16:         | \$1,200,000         |
| DOE Funding FY17:         | \$1,200,000         |
| DOE Funding FY18:         | \$1,246,516         |
| DOE Funding FY19:         | \$750,000           |
| Project Status:           | Ongoing             |
|                           |                     |

procedures, which provide detailed methods for the summative analysis of biomass materials. Our work is relevant to the overall goals of the program because robust, accurate, and precise analytical methods that can be easily and widely implemented directly support and help decrease the costs associated with analytical measurements. This is a critical enabling activity both for other NREL researchers and for the larger biofuels research community.



#### Weighted Project Score: 8.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- This is a necessary project (both from running and keeping labs and developing new methods) and it will provide more predictability to biofuels and bioproducts. It would be great to see a comparison between methods for PI-developed fermentation parameter monitoring and on-the-shelf equipment.
- The goal of this project is to provide analytical services for various NREL and BETO projects, along with a large group of external collaborators. Overall, the project and performance are outstanding. A key strength is that they are posting procedures for biomass analysis and standards. The proposed transition to low-cost near-infrared (NIR) spectroscopy is very promising. The only recommendation is to keep doing what you are doing.
- This project plays a vital role in developing, providing, and standardizing analytical services for the national laboratories and collaborators in academia and industry. They perform tens of thousands of analyses a year, supporting dozens of research groups, and have emerged as an important repository of knowledge regarding laboratory analytical procedures. The greater community increasingly relies on this important resource.
- This project is need driven. NREL should continue to focus on the development of cost-effective methods that can be deployed by research, testing, and industrial labs. More attention should be paid to cost-effective, user-friendly methods that can be successfully implemented by potential industrial end users.
- This project helps ensure the generation of high-quality data for both internal and external stakeholders. The team develops and improves analytical methods that are used across projects and manages sample workflow so that the project teams can operate efficiently without having to wait on data. There is a strong emphasis on standardization, consistency, and quality control. The project team is also developing new methods and has reported development of a low-cost at-line NIR method for real-time analysis of a fermentation broth that is nearly as accurate as a much higher-cost instrument. One gap in their tools is the analysis of intracellular metabolites for metabolomics and 13C metabolic flux analysis applications.

- We thank the reviewers for their comments. We will "keep doing what we are doing" and we will try to improve our performance with closer collaborations with internal and external collaborators.
- We strongly believe that there is substantial value in establishing, supporting, and communicating common analytical procedures to ensure a "common language" among biomass researchers, and this is a unique role that BETO and NREL can play in moving the community forward.
- Analytical method development is core to this project, and we are continually developing methods that will improve the ease of sample analysis and will share these improved methods with the community. However, recent programmatic shifts to focus on a diversity of product pathways has necessitated a shift to an increased breadth of methods over improvement of existing methods. To share method improvements with the community and ensure that methods developed are relevant to industry end users, we collaborate through avenues such as ASTM International standards. We ultimately hope to help implement robust secondary methods, such as NIR partial least squares (PLS) prediction, to provide cost-effective alternatives to more labor-intensive primary methods.

# ADVANCED SCADA FOR BIOCHEMICAL PROCESS INTEGRATION (WITH BEND)

#### **Pacific Northwest National Laboratory**

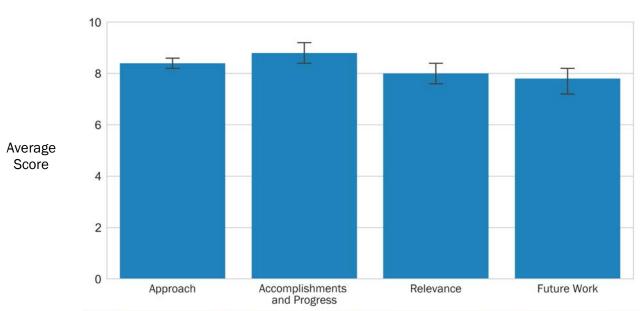
#### **PROJECT DESCRIPTION**

Bioconversion pathways for hydrocarbon fuels and biochemical are expected to deploy fed-batch control systems, systems that can discern sugars, viable cell mass, and products in crude, high-solids hydrolysates. This will require real-time sensor systems that are not yet commercially available for tracking hydrolysate chemical components. PNNL, in collaboration with industrial partners, is advancing process analytical technologies (PAT) for bioreactor control systems to support profitable bioconversion of biomass feedstocks to advanced biofuels and commodity chemicals.

| WBS:                      | 2.5.1.102           |
|---------------------------|---------------------|
| CID:                      | NL0026718           |
| Principal Investigator:   | Dr. Jim Collett     |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$1,177,000         |
| DOE Funding FY16:         | \$300,000           |
| DOE Funding FY17:         | \$300,000           |
| DOE Funding FY18:         | \$327,000           |
| DOE Funding FY19:         | \$250,000           |
| Project Status:           | Ongoing             |

Dielectric, NIR, and Raman spectroscopy tools and

methods are being developed to support fed-batch and chemostat controls that will scale from the lab up to biorefinery supervisory control and data acquisition (SCADA) systems. During the present three-year project cycle, we have demonstrated Raman spectroscopy methods and equipment configurations that enabled prediction of both glucose and xylose concentrations during bioconversion of DMR hydrolysate with respective root mean errors of prediction of 3.39% and 3.77%.



#### Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

Further work during the present project cycle will include development of:

- Raman methods for real-time prediction of bioconversion products within bioreactors
- Multiblock PLS models that fuse data from multiple spectroscopy modes to improve accuracy
- Chemometric data-processing workflows within the free and open-source, web-enabled LabKey database platform to support faster, more efficient development of PLS calibration models
- PAT-enabled chemostat controls to support directed evolution of microbial biocatalysts.

This project responds to industry stakeholder interests and reduces risk in BETO R&D by working with equipment manufacturers to develop efficient, scalable PAT tools for biomass conversion that can be predictably scaled up or down to reliably extrapolate biorefinery unit operation performance from bench- and pilot-scale data.

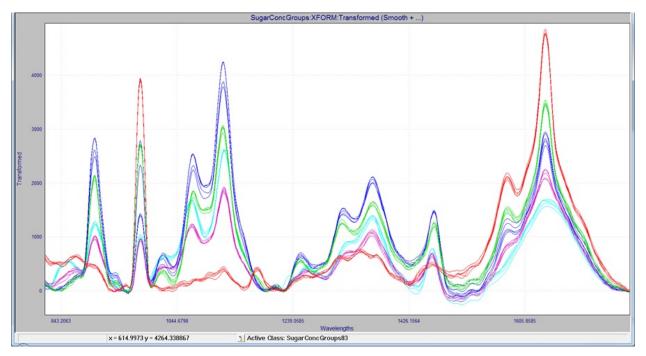


Photo courtesy of Pacific Northwest National Laboratory

#### OVERALL IMPRESSIONS

- Great progress so far (achieved set milestone, clear plan for 2019). Needs to better define how "integrated spectroscopy methods and the LabKey open-source chemometric informatics platform" fits with the overall project and what are the risks and critical success factor for these efforts.
- This team has been developing important new technologies to enable at-line (potentially on-line) monitoring and controls, as well as software to facilitate data integration. Their results in using dielectric spectroscopy to monitor growth and NIR (FY 2017) and Raman (current) techniques to monitor and control glucose levels in hydrolysate with insoluble solids is very promising. Active industry and national laboratory engagement help ensure relevance.
- The goal of this project is to provide process analytic technologies for fermenter control and monitoring. The team is making excellent progress. Much of the work is focused on using Raman spectroscopy to

measure sugar concentrations within DMR hydrolysates. In addition, they propose to develop fusion data models that incorporate multiple measurements. Overall, the team is making excellent progress. This project is well integrated with other BETO projects and external stakeholders. Clear project milestones are provided for the next year. If successful, this project can have real impact with regards to commercialization.

- The overall project has been successful in demonstrating the use of dielectric, infrared, and Raman spectroscopy to monitor and control a fed-batch fermentation process for substrate and biomass production. This has been demonstrated in presence of a high level of lignin that may interfere with spectroscopic analysis. The team approach and involvement of several labs, startups, equipment manufacturers, and end users has provided the framework that enables a good and successful outcome.
- The team is using new spectroscopy tools to support advanced control systems for fed-batch bioreactors. Great progress has been achieved so far using Raman spectroscopy to measure composition of complex fermentation broths, and to integrate all measured data with metadata in a software platform. Use of the data for process control has not yet been demonstrated but is a goal for the end of the project. Also, it is not clear how well the analytical methods will scale to commercial fermentation vessels.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

We appreciate the Peer Review panel's experience and broad perspective on industrial bioconversion operations, and their endorsement of our approach for developing new spectroscopy tools and methods for real-time control of bioreactors. Commercial deployment of such tools requires not only the increasingly affordable spectroscopy hardware that we have adapted for use in biomanufacturing in the course of our project; it will also be necessary to reduce the complexity of joining process sensor, event, and sample analysis data that have different formats and varying timestamp intervals into integrated training data sets for the construction of multivariate calibration models. Moreover, tracking the performance of calibration models over the course of many process runs is necessary to ensure their robustness in predicting concentrations of bioreactor broth components during bioconversion of crude biomass feedstocks that may vary considerably in composition with changes in season and market conditions. As such, we are customizing the open-source LabKey R&D data management system to provide a user-friendly software environment that will support chemometric data integration and calibration model development by relatively skilled biorefinery personnel such as senior operators. Indeed, although we are encouraged by the advances we have made in our laboratory in developing process analytical technologies for the production of advanced biofuels and bioproducts, we are keenly aware that empowering plant personnel to build and maintain calibration models themselves (rather than having to rely on outside vendor specialists) will be critical for cost-effective deployment of these new tools within the biorefinery.

# ENGINEERED REVERSAL OF THE BETA-OXIDATION CYCLE IN CLOSTRIDIA FOR THE SYNTHESIS OF FUELS AND CHEMICALS

#### Northwestern University

#### **PROJECT DESCRIPTION**

Rapid population growth, a rise in global living standards, and economic competitiveness have intensified the need for sustainable, low-cost production of biofuels and bioproducts. Industrial biotechnology using microbial cell factories is one of the most attractive approaches to address this need, particularly when large-scale chemical synthesis is untenable.

| WBS:                      | 2.5.3.206           |
|---------------------------|---------------------|
| CID:                      | EE0008354           |
| Principal Investigator:   | Dr. Michael Koepke  |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$1,600,000         |
| Project Status:           | New                 |
|                           |                     |

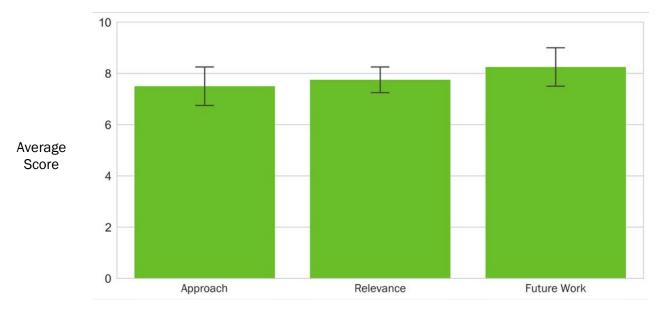
Unfortunately, designing, building, and optimizing

biosynthetic pathways in cells remains a complex and formidable challenge for many reasons. First, Design-Build-Test cycles for optimizing a given biosynthetic pathway can take on the order of weeks to months, requiring hundreds of person-years of R&D time to bring a new bioproduct to market. Second, most high-throughput platforms for testing engineered organisms focus on *Escherichia coli* or yeast, which limits the platform organisms, accessible feedstocks and target molecules, and stable operating environments for development. Third, a focus on linear heterologous pathways limits co-development of multiple products.

With support from DOE, we will address these limitations via unique pathway tools and engineering strategies that enable rapid synthesis of next-generation biofuels and bioproducts from lignocellulosic biomass in *Clostridia*. The core of our unique approach is to reconceptualize complex biological systems engineering by combining *in vitro* and *in vivo* work to advance state-of-the-art pathway design, prospecting, and validation in

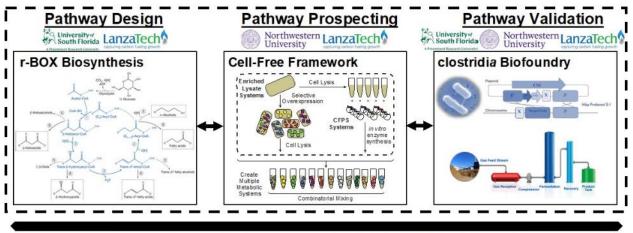
#### Weighted Project Score: 7.9

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

an integrated framework. This framework will diversify the breadth of both products and platform organisms to meet DOE and USDA bio-based industry goals. We specifically aim to develop a new platform for engineering reversal of the  $\beta$ -oxidation cycle (r-BOX) in *Clostridia* for synthesis of advanced fuels and bioproducts from biomass syngas produced by established gasification technologies. The targeted products are worth \$1,600-\$3,000/metric ton and have a multibillion-dollar market, showing the potential economic impact of our proposed technology. The environmental, community, and rural economic development impacts will be assessed for implementation in the Southeast region of the United States, utilizing regionally abundant forestry residues as feedstocks.



# Rural Economic Development & Sustainability Analysis

Photo courtesy of Northwestern University

#### OVERALL IMPRESSIONS

- The goal of this new project is to produce a wide range of value-added chemicals from syngas using a fermentation process. The key step involves reversing the beta-oxidation cycle, which has previously been shown to produce a wide range of valuable chemicals in a sugar-based process. Overall, the project has a strong technical plan. Clear milestones are provided. The work is compelling, though high-risk, as it is not clear how easy it will be to reverse the beta-oxidation cycle in an anaerobic bacterium. That said, this is the best team imaginable to accomplish such a task.
- The team assembled has a good past record of accomplishment. The approach taken is valid.
- This is a relevant project with well-defined project plan and targets. Regardless of having a positive outcome, the approach the PIs are taking is great.
- This project is a collaboration among three academic labs with LanzaTech to convert syngas to a range of advanced bioproducts by *Clostridium* fermentation. This is a highly capable team composed of leaders in their respective fields. Distinct tasks are well outlined, and quantitative goals defined. Most challenges are well understood, and the team has a good plan to address them. However, even in model organisms like *E. coli*, productivity and yield of compounds with more than four carbons via the reverse beta-oxidation pathway has been low to date. Use of a syngas substrate in a non-model organism poses an even greater challenge. There is no specific product selected to achieve milestones. Although this project could address a range of products derived from the TCA cycle, a particular model product should be

chosen to demonstrate that chain-length-specific enzymes can be found. A challenge that is not yet addressed is the need to balance enzyme rates to prevent buildup of intermediates.

#### **RECIPIENT RESPONSE TO REVIEWER COMMENTS**

• We thank the reviewer for this critical evaluation. The specific products we have in mind for the initial testing are not yet public information.

### ENZYME ENGINEERING AND OPTIMIZATION

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

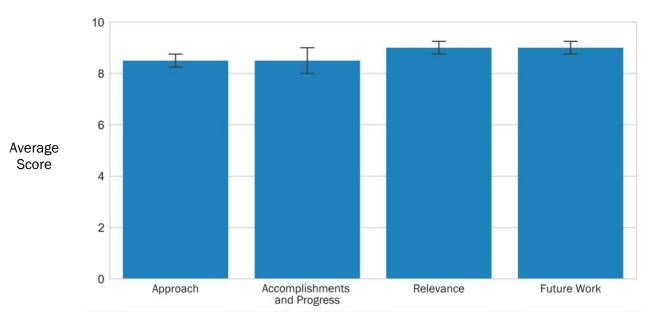
This project continues to be one of the leading research efforts worldwide in understanding and improving cellulases for biomass conversion to fuels, especially in the context of the industrial production host *Trichoderma reesei*. Pivoting from deacetylated dilute acid to DMR pretreatment of corn stover will dramatically improve the lignin quality and pretreatment CAPEX aspects of the biofuels process. However, DMR solids require an improved and differently formulated enzyme blend. In the context of the biochemical platform, cellulase hemicellulose use-related costs account for approximately 10% of the cost to produce advanced fuels and intermediates. As an example, our approach will target

| WBS:                      | 2.5.4.100           |
|---------------------------|---------------------|
| CID:                      | NL0026686           |
| Principal Investigator:   | Dr. Mike Himmel     |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$5,846,452         |
| DOE Funding FY16:         | \$1,600,000         |
| DOE Funding FY17:         | \$1,600,000         |
| DOE Funding FY18:         | \$1,746,452         |
| DOE Funding FY19:         | \$900,000           |
| Project Status:           | Ongoing             |
|                           |                     |

achieving a cost savings of about \$1.20/GGE relative to the 2018 SOT case for 2,3-BDO production. This will be accomplished by meeting very specific enzyme loading and sugar yield (final glucan and xylan conversion) goals. In collaboration with the Low Temperature Advanced Deconstruction and Biochemical Process Modeling and Simulation projects, we propose a two-task project for FY 2019–2021. In Task 1, Cellulase Improvement (CI), we will identify the best cellobiohydrolase (CBH) I enzymes from natural diversity for enhanced digestion of DMR solids (Megatron I). In several Enzyme Engineering and Optimization milestone reports last FY, we noted the discovery of new CBH I enzymes from preliminary diversity studies that have improved kinetics compared to the *T. reesei* enzyme. Note that the co-development of Megatron II, which will

#### Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

deliver improved CBH II enzymes, is based on a separately DOE-funded proposal. In Task 2, Lignin Modifying Enzymes and Xylanases, we will deliver enzymes found to enhance the digestion of DMR feedstocks in the presence of the improved cellobiohydrolases from Task 1. Task 2 will interrogate enzymes from diversity, as well as commercial formulations. To ensure success, we have built the special constitutive and native CBH I delete strains of *T. reesei* needed to quickly produce and test new enzyme candidates. Finally, collaboration with Novozymes will help us achieve our enzyme performance goals by ensuring process relevance and utility into new enzyme formulations.

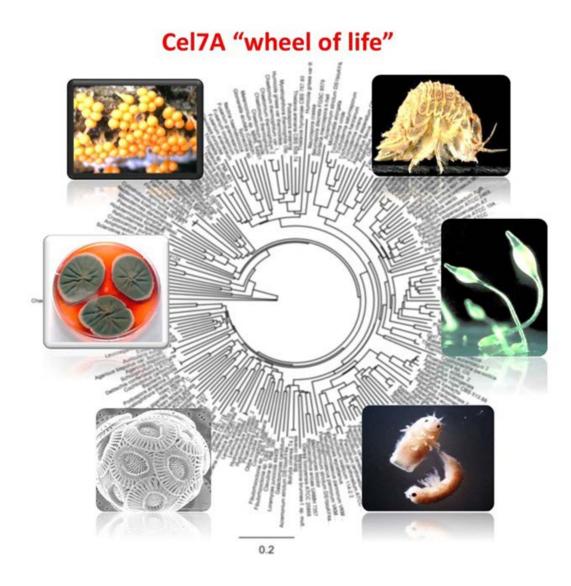


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• The goal of this project is to develop enzyme cocktails for DMR-treated biomass (which is the focus of other BETO-funded projects). The team provides a compelling argument for improving these enzyme cocktails—namely, that these commercial cocktails do not work well on DMR-treated biomass. In addition, this work is central to all sugar-based conversion strategies. Overall, the team is making excellent progress. The raptor-enzyme concept is especially appealing, as is the collaboration with

Novozymes, which highlights the commercial viability of the work. That said, addressing feedstock variability would strengthen this project.

- This team has combined enzymology, enzyme design, genome mining, and strain engineering to produce a comprehensive platform for optimizing enzymatic treatment and saccharification of DMR solids. Key results include identifying critical protein domains, establishing a cell-based production and secretion system, engineering an enzyme with increased activity, and preparing an enzyme library for screening. Although the final results of this project have yet to be fully realized, the enzyme-optimization platform itself is an achievement that can likely be applied to other challenges in the future.
- This an impressive tour de force that combines enzyme discovery and engineering with the development and testing of new cellulase/other hemicellulase/lignin-modifying blends. It brings a credible team of internal and external collaborators together with a key enzyme supplier. Achieving realistic enzyme cost reduction is critical to the success of an industry that aims to commercialize or use these enzymes. A parallel development can be envisioned for algal/oilseed/high-protein feedstocks. BETO should consider broadening the scope of this project and to look for other enzyme conversion opportunities beyond lignocellulosics.
- This team is developing an enzyme formulation that works well on DMR solids, while most traditional formulations are more suited for deacetylated dilute acid solids. They are also developing an improved enzyme expression system. There is clear commercial interest in the outcome of this work, and industrial partners were engaged early in the project. The approach involves a combination of enzyme discovery in nature and enzyme engineering via domain shuffling. The team is encouraged to try additional directed evolution methods in the coming year, as their work transitions from basic R&D to achieving performance targets. In addition, this team could be of use in engineering pathway enzymes that may be bottlenecks in microbial bioconversion processes, so a broadening of scope is encouraged.

- Thank you. The raptor concepts are indeed intriguing and follow an interesting principle from nature you get the best biomass deconstruction performance by bringing all tools to the table. It is true that feedstock variability will impact enzyme formulation. The extent of this impact is not known at this time; however, the Feedstock-Conversion Interface Consortium platform should begin to address these issues and we will certainly assist in any way possible.
- Thank you for your comments. This work is indeed the culmination of years of technical preparation and partnering with industry. Also, knowing the performance targets in the context of a more mature process was very important. Evolutionary methods regarding cellulase performance improvement (specific activity) have always been challenging. One historical problem has been the sometimes-poor connection between activity on surrogate substrates and actual biomass. For this reason, we take a reductionist approach aimed at reducing numbers of candidates quickly and then employing more relevant assays. Of course, when outstandingly superior or inferior enzymes are found, we examine them closely using structural biology. We are involved as a team in supporting some of the pathway projects in the program, including Cell Free Technology (Bomble), Carbonic Anhydrase for Flu Gas Cleanup (Zhang), and Targeted Microbial Development (Zhang).

# **CELL-FREE AND IMMOBILIZATION TECHNOLOGIES**

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

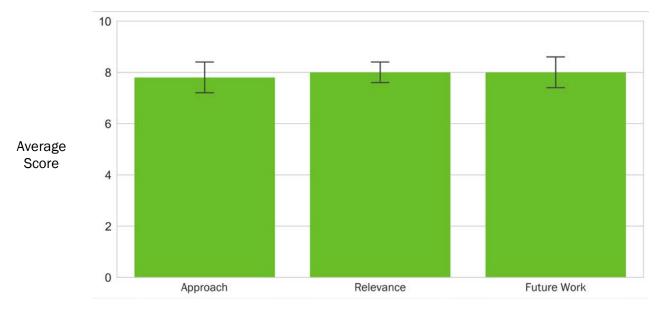
Today, several key factors negatively impact the production of fuels and chemicals from renewable sources. Common hindrances in the biological production of biochemicals are: (1) end-product or intermediate toxicity to the microbial biocatalyst, (2) the diversion of carbon to biomass formation, and (3) 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

| WBS:                      | 2.5.4.101           |
|---------------------------|---------------------|
| CID:                      | NL0034445           |
| Principal Investigator:   | Dr. Yannick Bomble  |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$900,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$900,000           |
| Project Status:           | New                 |
|                           |                     |

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 biological conversion of feedstocks to biochemicals.

#### Weighted Project Score: 8.0

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

More specifically, we will develop new technologies and routes that could be used to produce high-value biochemicals such as 1,3-propanediol, 3-hydroxypropionic acid, 2,3-BDO, or polyhydroxybutyrate 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 lead to new concepts and 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 will also develop basic design principals for constructing synthetic metabolons, using fusion proteins and synthetic protein scaffolds, to promote substrate channeling and stability while conserving peak activity. Additionally, our efforts will 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 will focus on further increasing stability, operating lifetime, and efficiency of the pathway enzymes by immobilization on support surfaces. We will focus on immobilizing pathway enzymes or combinations of enzymes on several different conducting polymers and evaluate 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.

Taken together, these approaches will enable process intensification, continuous operation, lower capital and separations costs, and end-product flexibility, and thus has the potential to contribute significantly to BETO's goals of cost-competitive biofuels and bioproducts.

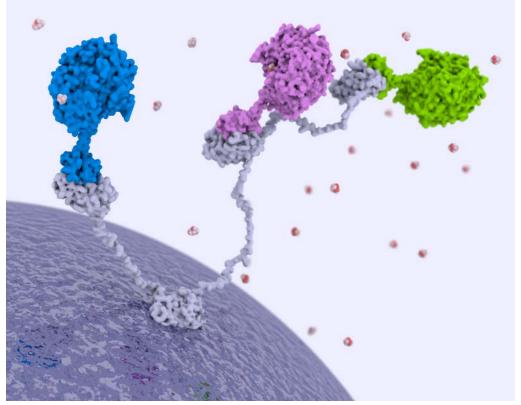


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• The project has a clear focus. The PI is looking into TEA and used that for prioritizing tasks and selecting the main focus for the project, which is a great approach. Manufacturability—especially in

regard to achieving needed stability of the enzyme and the cost associated with making such stable proteins—needs to be addressed.

- This team seeks to demonstrate the potential for bioproduction by applying immobilized cell-free biocatalysts to industrially relevant hydrolysates. If successful, this project could provide an interesting and relevant alternative for products that are toxic or that could benefit from higher reaction densities. Even though the project was only recently initiated, they have already shown cell-free production of 1,3-propanediol.
- The goal of this project is to develop a cell-free process for 2,3-BDO production. While cell-free technologies are promising, it is not clear whether these technologies can be scaled for the production of commodity chemicals. One key challenge will be developing efficient strategies for recycling cofactors. While the team addresses this challenge, the details regarding how they will solve this problem are vague. In addition, the work associated with encapsulation has many potential problems; key among them are the costs associated with using such approaches. Again, the key question is whether these technologies can be applied at scale for the production of a commodity chemical.
- Cell-free manufacturing of a chemical such as 2,3-BDO represents an intriguing possibility with many challenges. Proof of concept and cost effectiveness from continuous operation need to be established for the commercial viability of this approach.
- The project is aimed at developing cell-free processes to enable biochemical and fuel production, which would reduce downstream separation costs. This could facilitate implementation of non-natural pathways with toxic intermediates and allow higher-density reactions. This work is intended to address the major barriers to commercialization of cell-free processes, including enzyme stability and cofactor regeneration. The first task is to engineer enzymes to construct an *in vitro* bioconversion pathway, and the second task focuses on immobilization technology. Initial success has been demonstrated in tethering, immobilization, and cofactor recycling, and about half of a long metabolic pathway has been demonstrated. The team has a good understanding of the risks, and the milestones are oriented around de-risking the approach; however, there is no clear technical plan on how the risks of enzyme production and stability will be addressed. Also, issues with scale-up are not considered. Overall, this is a high-risk project as no cell-free process for a long metabolic pathway has been commercialized. Furthermore, the economics of this process compared to a conventional fermentation are not clear. This will be addressed in the TEA.

- 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.
- There are indeed challenges in scaling up the production of biochemicals using cell-free biocatalysis: (1) enzyme production costs and operating lifetime and (2) cofactor management. However, we believe these can be overcome using either tools that have already been demonstrated for enzymatically driven processes, or increased R&D.
- Enzyme production costs is a risk that can be remediated, as enzyme production can be dramatically improved using dedicated production strains, as is the case for cellulases or other industrial enzymes. We are currently investigating the cost of producing these enzymes at large scale.
- Enhanced enzyme stability can be achieved using several approaches such as immobilization, enzyme engineering, or prospecting. All of these approaches have been successfully used in industry to reduce operating costs of enzymatically driven processes. Additionally, cell-free biocatalysis offers more process flexibility, as they allow for the replacement of less-stable enzymes in the pathway while others

can keep operating for many more production cycles. Reviewers mention issues with encapsulation, which can indeed lead to problems such as enzyme inactivation, limited diffusion, or additional costs. We aim to test several encapsulation and immobilization technologies and assess the most promising for stability and production while also minimizing costs.

• Finally, proper cofactor maintenance can be achieved using balanced pathways for efficient recycling; in this case, cofactor costs only reside in priming the system, allowing easier scale-up. Cofactor costs at scale can also be reduced by creating a market for these cofactors to be mass produced, isolating cofactor mixes from spent cells from other processes, or developing the use of biomimetic cofactors.

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# CARBON DIOXIDE UTILIZATION

TECHNOLOGY AREA

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## INTRODUCTION

The Carbon Dioxide (CO<sub>2</sub>) Utilization Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 11 projects were reviewed in the CO<sub>2</sub> Utilization session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$6,590,000 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 0.8% of the BETO portfolio reviewed during the 2019 Peer Review. During the Project Peer Review meeting, the principal investigator (PI) for each project was given 20 to 30 minutes (depending primarily on the funding level) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the Project Peer Review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the CO<sub>2</sub> Utilization Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. Ian Rowe as the CO<sub>2</sub> Utilization Technology Area Review Lead, with contractor support from Dr. Mark Philbrick (Allegheny Science & Technology). In this capacity, Dr. Rowe was responsible for all aspects of review planning and implementation.

## **CO2 UTILIZATION OVERVIEW**

The CO<sub>2</sub> Utilization Technology Area addresses research and development (R&D) barriers associated with the conversion of CO<sub>2</sub> to fuels and chemicals. To establish this recent addition to the Conversion R&D portfolio, BETO sought to learn from past and ongoing efforts in CO<sub>2</sub> utilization across DOE to determine the research area that best suits BETO capabilities. Notably, efforts exist within BETO's Advanced Algal Systems portfolio, the Office of Fossil Energy, and the Advanced Research Projects Agency–Energy (ARPA–E); BETO communicated closely with individuals in all of these programs when developing its CO<sub>2</sub> utilization strategy in an effort to avoid duplication and learn from previous results.

Traditionally, producing renewable fuels and products relies on biogenic carbon, and this renewable carbon feedstock has been largely limited to terrestrial plants or algal biomass and associated intermediates. In such strategies, plants use solar energy to chemically reduce CO<sub>2</sub> into biomass. This feedstock is then collected and deconstructed into simple intermediates (sugar, syngas, oil, etc.) before being upgraded to fuels and products. In contrast, the majority of this CO<sub>2</sub> Utilization R&D portfolio takes an alternative approach and specifically investigates technologies that perform CO<sub>2</sub> conversion through non-photosynthetic and abiotic means, substituting electricity for solar energy in powering CO<sub>2</sub> reduction. Such pathways generate one-carbon (C1) or two-carbon (C2) products or intermediates that can be further upgraded through biological or catalytic means that are quite similar to existing conversion efforts within the BETO portfolio.

This CO<sub>2</sub> Utilization Technology Area within BETO began in FY 2017; thus, many of the projects discussed below are new and focused on determining what the current state of technology is in the field. Projects generally fall within three categories: (1) non-photosynthetic or nonbiological CO<sub>2</sub> reduction for generating intermediates, (2) biological upgrading of CO<sub>2</sub>-derived intermediates, and 3) enabling analyses to help inform R&D and the life cycle implications of products derived from CO<sub>2</sub>. Given recent trends in renewable energy deployment and carbon capture, utilizing CO<sub>2</sub> as a feedstock is a field of research that is poised to grow, and BETO is well suited to investigate such technologies.

## **CO2 UTILIZATION REVIEW PANEL**

The following external experts served as reviewers for the CO<sub>2</sub> Utilization Technology Area during the 2019 Project Peer Review.

| Name                     | Affiliation          |
|--------------------------|----------------------|
| Alissa Park <sup>a</sup> | Columbia University  |
| Matt Lucas               | Carbon180            |
| Z. Jason Ren             | Princeton University |
| Matthew Kanan            | Stanford University  |
| Igor Bogorad             | Amyris               |

<sup>a</sup> Lead Reviewer

## TECHNOLOGY AREA SCORE RESULTS

| Average Weighte   | d Sco | res by | Project |     |     |    |
|---|-------|--------|---------|-----|-----|----|
| NREL (2.1.0.304): Feasibility Study of Utilizing Electricity to Produce Intermediates from CO2 and Biomass  |       |        |         |     | 8.6 |    |
| NREL (2.3.2.111): Improving Formate Opgrading by Cupriavidus Necator  |       |        |         | 7.  | .7  |    |
| NREL (2.3.2.112): Enhancing Acetogen Formate<br>Utilization to Value-Added Products   |       |        |         | 7.3 |     |    |
| NREL (5.1.3.101): Integration of CO2 Electrolysis with<br>Microbial Syngas; Upgrading to Rewire the Carbon<br>Economy   |       |        |         | 6.9 |     |    |
| NREL (2.3.2.106): CO2 Valorization Via Rewiring Carbon<br>Metabolic Network   |       |        |         | 6.8 |     |    |
| NREL (2.3.2.113): Synthetic C1 Condensation Cycle for<br>Formate-Mediated ElectroSynthesis  |       |        |         | 6.6 |     |    |
| ORNL (2.3.1.317): Hybrid Electro- and Thermo-Catalytic<br>Upgrading of CO2 to Fuels and C2+ Chemicals   |       |        |         | 6.6 |     |    |
| NREL (2.3.1.316): CO2 Utilization: Thermo- and Electro-<br>Catalytic Routes to Fuels and Chemicals  |       |        |         | 6.5 |     |    |
| NREL (5.1.3.103): Novel Cell-Free Enzymatic Systems for<br>CO2 Capture and Utilization: Bio-Energy Based<br>Biologically Carbon Capture and Valorization (BeCC&V) |       |        |         | 5.8 |     |    |
|   | 0     | 2      | 4       | 6   | 8   | 10 |

Sunsetting Ongoing New

## **CO2 UTILIZATION REVIEW PANEL SUMMARY REPORT**

#### Prepared by the CO<sub>2</sub> Review Panel

The CO<sub>2</sub> Utilization program is a new endeavor by BETO to explore the opportunities and potential of converting carbon dioxide into biofuels, bioproducts, and biopower using non-photosynthetic pathways such as electrocatalytic, thermocatalytic, biocatalytic, and hybrid approaches. BETO's recent report, "Rewiring the Carbon Economy: Engineered Carbon Reduction Report," serves as the foundation and guideline of this program, and the panel agrees with the evaluation that "the CO<sub>2</sub> reduction and utilization technologies discussed have significant potential to impact carbon management and provide economic, environmental, and electric grid stability benefits."

The panel reviewed 9 slide decks and 11 presentations, and panelists conducted extensive Q&A and discussions with the PIs, BETO program managers, and other participants. Overall, the panelists were impressed by the organization of the program, the diversity of project topics, and some new findings presented by the groups. There are several areas that can be improved, such as finding synergies among different approaches and groups, collaborating with partners outside of national labs, and better utilizing techno-economic analysis (TEA) and other tools. The panel provides in this report summarized review comments and recommendations on program development.

#### IMPACT

Because this is a new topic that has an intrinsic nature of high risk, high reward, BETO funding is critical to advance the state of technology. Once technologies are advanced to higher technology readiness levels (TRLs) and risks are reduced, private sector investments will likely follow suit.

All projects are aligned with the BETO goals on carbon rewiring, and different pathways were well represented. All but one team presented in this program were from the National Renewable Energy Laboratory (NREL), which has been leading the efforts in helping BETO develop the carbon rewiring initiative. Many scientists and managers were involved in providing technical support, performing feasibility studies, and developing programs. The presentations were grouped in three main categories following a first presentation on TEAs. The three groups each focused on electrocatalytic and/or thermocatalytic pathways, biocatalytic pathways (focused on formate), and the BETO biopower annual operating plan (AOP) call, respectively.

The panel was impressed by the techno-economic analysis presented by NREL and thinks this project is strategically and technically important for carbon rewiring research and program development. The project "Feasibility Study of Utilizing Electricity to Produce Intermediates from CO<sub>2</sub> and Biomass" provided good analysis on state of the art of CO<sub>2</sub> valorization and identified challenges and opportunities to guide and support technology development. The panel suggests in the next period the team consider including more sensitivity analysis and, if possible, benchmarking evaluation metrics for different processes and technologies. However, the panel cautions that the findings should not be used to pick winners and losers. In addition to academic publications, it will be much more impactful for the tools and findings to be publicly available via a website or other platforms.

The projects on electrocatalytic and/or thermocatalytic  $CO_2$  conversions were primarily focused on electrochemical catalysts development. Broadly speaking, the ability to access multi-carbon products through electrocatalytic or thermocatalytic  $CO_2$  conversion is a key capability that must be advanced to make these processes viable. The focus on accessing multi-carbon targets is therefore relevant at a fundamental level to the BETO goals. The presentations reported on different types of catalyst development, but various challenges were reported. While  $C_2$ + products were targets, none of the catalysts have been able to demonstrate efficient conversion toward targeted products, and the conversion efficiency was low. It was not clear whether some of the catalysts such as bimetal cocatalysts would have a high impact on electrochemical  $CO_2$  reduction. While some projects mentioned the plan of a  $CO_2$  electrolyzer and other device development, little results were presented. The development of efficient reactor systems can be as critical as catalysts, and associated challenges including mass transfer and product separation need to be considered in future studies.

The projects on biocatalytic pathways include one project focused on developing the clustered, regularly interspaced short palindromic repeats-associated protein 9 (CRISPR-Cas9) tools for *Clostridium ljungdahlii* to directly convert CO<sub>2</sub>/carbon monoxide (CO)/hydrogen (H<sub>2</sub>) to 3-hydroxybutyrate (3HB). The CRISPR tool development can be very impactful, as such capacity is critical to enable targeted product generation from CO<sub>2</sub>. Three other projects were funded via a formate AOP to convert a key CO<sub>2</sub> reduction intermediate formate to higher-carbon products. This includes using *Cupriavidus necator* to produce polymer precursor  $\beta$ -ketoadipate, using *Escherichia coli* to produce glycolate, and using *Clostridium ljungdahlii* to produce butanol. All these projects were just started with little data presentation. All the projects recognized the value of formate valorization using biological pathways because they can be complementary to the upstream electrochemical pathways, which can be highly efficient in converting CO<sub>2</sub> to formate. However, common areas that need improvement include better rationales and quantitative analyses why the proposed pathway makes sense in both technological and economic means. The project must also consider the potential markets and commercialization pathways for these chemicals.

The last group of projects were funded by the BETO biopower AOP, which focused on converting waste carbon into biopower. All projects were required to have industry partners, which the panel thinks is a very good approach. The projects spanned from CO<sub>2</sub> electrolysis with syngas fermentation to biogas upgrade, and to enzyme-accelerated solvents for waste gas scrubbing. While the panelists think that these projects may have potential in niche applications, a common concern is that the novelty of these projects is not clear. Much of the proposed work seems to have been carried out previously by industrial partners or other entities that the national lab team attempted to replicate to fit into the AOP scope. In addition, partially because of the early stage of these projects, it was difficult to evaluate the economic viability of these pathways. TEA and life cycle assessment (LCA) could be very beneficial.

#### INNOVATION

 $CO_2$  utilization is a new program, and many of the funded projects were recently started without much data generated. However, the panel feels many projects presented innovative ideas and feasible research plans. The TEA project was ranked highly because it showed very interesting data and could provide critical insights in technology development, which may avoid unnecessary efforts and provide guidance on addressing critical barriers. The CRISPR-Cas9 tool development project also received positive feedback, as it can become a powerful in-house capacity to not only develop engineered *Clostridium ljungdahlii* strains but also other bacterial strains that are capable of producing targeted compounds that have never been accomplished before. The development of novel electrochemical catalysts with high conversion efficiency and selectivity can be a major milestone for  $CO_2$  utilization, so even though the projects have not demonstrated success, further investigations will be critical.

#### SYNERGIES

So far, most projects have a focus on individual areas of CO<sub>2</sub> utilization such as catalyst development, strain development, and process engineering. However, there exist significant synergies among the groups with different expertise. The panel highly suggests BETO and researchers explore interdisciplinary collaborations. For example, chemists and material scientists could work together to develop more efficient catalysts for CO<sub>2</sub> reduction; microbiologists could collaborate with electrochemists to develop high-performing conversion systems; and scientists and engineers could work jointly to tackle major barriers such as mass transfer, system integration, and product separation.

Another synergy that should be explored is the collaboration between national lab scientists with university researchers and industry partners. Many university groups have been highly productive in CO<sub>2</sub> valorization R&D and increasing numbers of companies have demonstrated success in CO<sub>2</sub> utilization as well. Such

collaboration will greatly accelerate the advancement of  $CO_2$  research as well as facilitate the development and expansion of BETO's carbon rewiring program.

#### FOCUS

Overall the  $CO_2$  utilization program is well organized, and the portfolio contains diverse and complementary projects that covered most conversion pathways. The panel suggests BETO investigate several focus areas that have not been funded.

The program should consider funding projects that investigate hybrid  $CO_2$  utilization approaches. As discussed in BETO's report, a hybrid approach maybe the most efficient way to realize practical  $CO_2$  utilization with renewable electrons, as it combines the efficient abiotic  $CO_2$  reduction to intermediates (H<sub>2</sub>, syngas, formate, methanol, etc.) followed by biological upgrade of the intermediates to high-value, long-chain products. Thermodynamically, the potential losses can be reduced by focusing on desired intermediate production in a  $CO_2$  electrolyzer and overcoming surface area limitation in the bioreactor; kinetically, multiphase mass transfer can be increased by designing efficient gas production and delivery system in bioreactor; economically, high-purity and high-titer chemicals can be produced by taking advantage of the metabolic engineering tools; and engineeringly, scaleup systems can be relatively easily developed by modulating each unit and streamlining production.

The program could also consider funding projects that address gas solubility issues, mass transfer limitations, product separation, and issues in system development and integration. These are critical barriers in CO<sub>2</sub> utilization development, and the understanding and advancement of these topics will help steer the direction of fundamental science related to BETO goals, and they will help identify major technological and economic barriers that maybe overlooked by TEA.

The early TEA study presented a great opportunity to provide early intervention help for projects struggling with value proposition. Similar work can be supported for LCA as well, because some pathways seem to consume large amounts of energy, chemicals, materials, and water, and generate a significant amount of waste. The environmental benefits will be important to evaluate, considering these conversion processes are largely carbon neutral, yet the life cycle may pose negative environmental impacts.

#### TECHNOLOGY DEVELOPMENT PIPELINE

Given that the majority of the projects are still at low TRLs, it is reasonable for BETO to keep investing in different pathways until they become mature for early technology adoption by industry. The biopower AOP was a good approach that required collaboration between national labs and industry partners, but more guidance and clear expectations could be helpful to identify appropriate project objectives and deliverables. More applied projects on process and reactor development may be valuable to facilitate technology development.

#### RECOMMENDATIONS

**Recommendation 1:** The panel recommends that all projects conduct carbon and energy efficiency calculations as well as TEA, and, if possible, LCA. Such quantitative analysis should be done at the beginning, middle, and end of the project, because it can provide important insights in project development directions, identify critical barriers, and find new opportunities. The panel would recommend TEA-guided milestones and measurable deliverables for project management. The panel also cautions that sensitivity analysis should be included in TEAs, since most of the time assumptions were made to serve rather than check the project goals.

**Recommendation 2:** The panel supports establishing standardized matrices for project evaluation. Standard parameters may include carbon efficiency, energy efficiency, normalized cost, product titer, selectivity, scalability, etc. The calculation methods should be accessible to the public so the project results can be evaluated by using standardized methods. An open-source user interface and data platform will be helpful to achieve such a goal.

**Recommendation 3:** Interdisciplinary collaborations and applied research need to be encouraged and facilitated. Such partnerships will accelerate the translation of science understanding into technology and business development. Success measurements need to include both scientific publications and other accomplishments such as patent filings, technology licenses, and entrepreneurship.

### **CO2 UTILIZATION PROGRAMMATIC RESPONSE**

#### INTRODUCTION/OVERVIEW

The Conversion R&D program would like to thank the entire  $CO_2$  Utilization Panel for their hard work and helpful discussion related to this emerging research area within BETO. As the above summary points out, the panel found the organization of this new program and the variety of projects within it to be commendable and aligned with BETO goals. The technology balance between biological and catalytic options was seen as well balanced. Specifically, the panel found the TEA associated with the "Feasibility Study" to be especially important for the strategic development of this program specifically as well as the broad field of  $CO_2$ utilization.

The reviewers pointed out the synergistic opportunity for combining researchers that work on catalyst development with their counterparts that 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<sub>2</sub> utilization.

The panel pointed toward opportunities in funding projects that integrate hybrid approaches to realize practical  $CO_2$  conversion. This can allow catalysis researchers to specify their output stream for the proper engineering of the relevant bioreactors. Other opportunities in addressing mass transfer limitations, separations, and system integration were mentioned as items BETO should be considering.

The following section specifically addresses the three major recommendations from the review panel.

#### Recommendation 1: All projects are recommended to conduct carbon- and energyefficiency calculations as well as TEA, and, if possible, LCA.

The program agrees with the importance of these assessments. The LCA of any product made from CO<sub>2</sub> is extremely important. We currently have an analysis project that broadly looks at the carbon footprint of various pathways related to CO<sub>2</sub> utilization. While we absolutely agree that initial LCAs should be considered when thinking about the portfolio, it is still quite early in the process for many of these technologies to dive very deeply into specific pathways; however, we are considering having projects explicitly point out what metrics would be needed to hit relevant TEA or LCA values.

## Recommendation 2: The panel supports the establishment of standardized matrices for project evaluation.

The program wholeheartedly agrees with the importance of such assessments and metrics and this has been a point of regular discussion. The program is actively considering the specific metrics outlined by the panel as possible metrics for further work. One opportunity we are examining to get uniformity across the portfolio is to leverage the "Feasibility Study" as well as recent TEA/LCA guidelines from the National Energy Technology Library and The Global  $CO_2$  Initiative.

## Recommendation 3: Interdisciplinary collaborations and applied research need to be encouraged and facilitated.

BETO agrees with the importance of this integration. Of note is the FY 2018 BETO Funding Opportunity Announcement, which included a topic area titled "Rewiring Carbon Utilization" that specifically sought to connect catalytic experts and biologists to ensure that they are developing technologies that complement one another. This resulted in three awards that connected electrochemists and biologists. The projects did not begin in time to be presented to the review panel; however, they have since commenced. In general, this specific recommendation is well received and BETO considers the connection of interdisciplinary efforts to be essential to advancing CO<sub>2</sub> conversion technologies.

## FEASIBILITY STUDY OF UTILIZING ELECTRICITY TO PRODUCE INTERMEDIATES FROM CO<sub>2</sub> AND BIOMASS

#### National Renewable Energy Laboratory

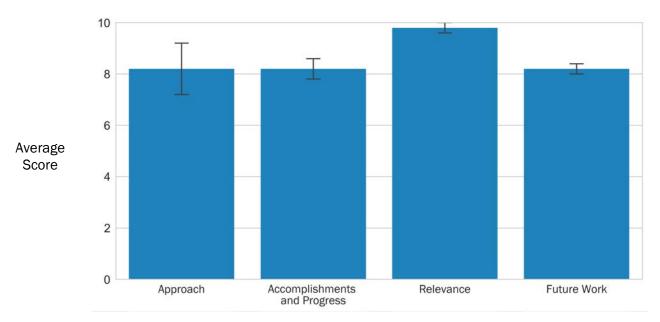
#### **PROJECT DESCRIPTION**

The primary objective of this project is to assess the technical and economic feasibility of utilizing electricity for (1) the reduction of CO<sub>2</sub> to C1–C3 intermediates and (2) the generation and upgrading of biomass-derived intermediates. Through critical literature review, subject matter expert interviews, collaboration with experimental projects, and both high-level comparative and detailed TEA coupled with biorefinery integration, this project will develop a roadmap for the effective utilization of electricity within existing and emerging biorefinery designs that can guide ongoing R&D activities towards cost reductions and carbon energy efficiency improvements.

| WBS:                      | 2.1.0.304           |
|---------------------------|---------------------|
| CID:                      | NL0033391           |
| Principal Investigator:   | Dr. Josh Schaidle   |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$800,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$400,000           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

#### Weighted Project Score: 8.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

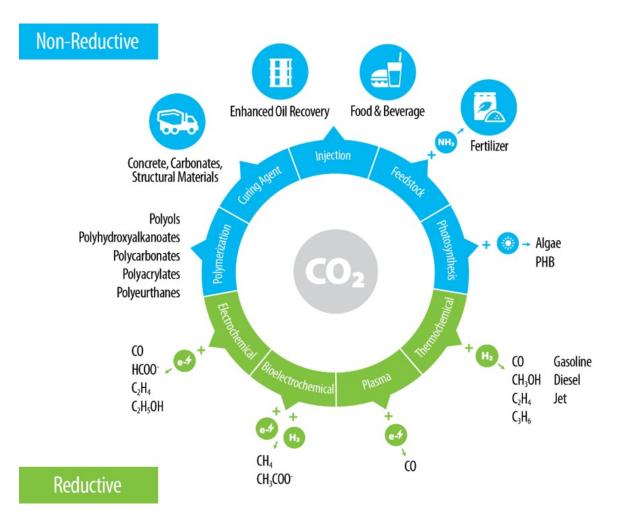


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- This is an important study that can set the important logical pathway toward the future technological development for CO<sub>2</sub> utilization. The team has developed a good platform to analyze different pathways to identify their challenges and opportunities. This project can be expanded to provide a better assessment platform for a broader user group.
- This project is timely and strategically important. The performers did a very good job organizing the project and delivering critical findings. The findings will be very valuable in understanding the challenges and opportunities in carbon rewiring R&D. Quantitative metrics will be desired for standardized evaluation. Uncertainty analysis and mitigation strategies will be helpful when making assumptions.
- This project evaluates the technical and economic feasibility of using CO<sub>2</sub> or biomass feedstocks and creating C1–C3 chemicals from them. This work could help identify targets for R&D.
- The project provides essential analysis to underpin BETO's goal of employing CO<sub>2</sub> utilization to improve the economic competitiveness of biofuels. The team has identified the critical success factors. Further depth on some of the technical issues will be necessary to clarify the research challenges.

• The performers have proposed to do an in-depth analysis of various technologies to upgrade CO<sub>2</sub>, including electrochemical, thermochemical, and biological. The performers are covering a very wide space with many built-in assumptions to what the current state of technology is and potential for future improvements. During the presentation, the performers focused on electrochemical, which appears to be most in line with their expertise. The performers are encouraged to narrow the scope of their study to just electrochemical upgrading, which is already a challenging endeavor. Extending the analysis to biological upgrading may lose focus for the study and would be extremely challenging. For example, many potential bioproducts could be made such as *n*-butanol, fatty acids, ketoadipate, polyhydroxybutyrate, etc. Publishing their results early on would be very helpful for the other BETO teams, who also will be performing their own TEA on each project.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We greatly appreciate the thoughtful analysis and constructive feedback provided by the reviewers. We have sought to assess the technical and economic feasibility of utilizing electricity to reduce CO<sub>2</sub> into C1–C3 intermediates, with the end goal of providing guidance to the R&D community. To that end, we agree with the reviewers that further depth is needed in specific technical areas and that the results need to be broadly disseminated through peer-reviewed publications; we are working diligently to address these comments. While we acknowledge that the scope of the study is fairly broad (spanning across five different direct and indirect CO<sub>2</sub> reduction technologies), we believe that the cross-cutting nature of this analysis is critical to its value creation for the research community. Due to the time allocated to the peer-review presentation, we decided to use electrochemical conversion as an example case; we have similar detailed studies and cost analyses for all five reduction technologies. Since the start of this project, we have engaged with subject matter experts across these included technologies, and our project team members have diverse technical backgrounds. In out-years, we plan to dive deeper into specific technologies, especially in regard to integration of these technologies with existing biorefinery designs.

# CO<sub>2</sub> UTILIZATION: THERMOCATALYTIC AND ELECTROCATALYTIC ROUTES TO FUELS AND CHEMICALS

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

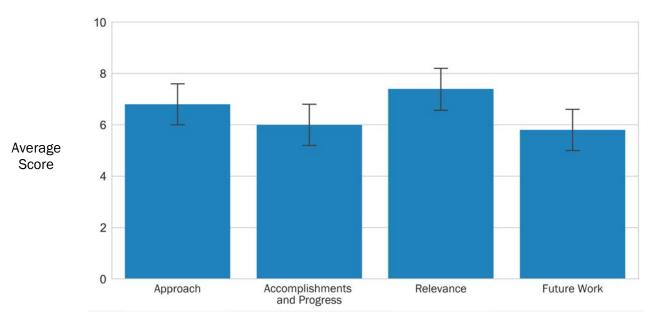
Over the past several years, it has become clear that the emergence of inexpensive and intermittent electricity provides an opportunity for electron-enabled conversions of  $CO_2$ . In this project, both direct electrochemical and thermochemical conversions of  $CO_2$  are being investigated. Electricity provides the driving force for chemical reaction in the electrochemical pathway, while  $CO_2$  is reacted with hydrogen (which can be produced from the electrolysis of water) in the thermochemical pathway. While the thermochemical pathway is the most developed for conversion of  $CO_2$  (e.g., the production and utilization of syngas), these existing processes operate at a scale that is too large to match distributed  $CO_2$  sources.

| WBS:                      | 2.3.1.316           |
|---------------------------|---------------------|
| CID:                      | NL0033403           |
| Principal Investigator:   | Dr. Jack Ferrell    |
| Period of<br>Performance: | 11/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,000,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$500,000           |
| DOE Funding FY19:         | \$500,000           |
| Project Status:           | Ongoing             |
|                           |                     |

Consequently, process intensification and scale-down is needed to enable distributed thermochemical CO<sub>2</sub> utilization. Development is needed to produce catalysts combining reverse water gas shift (RWGS) and C-C coupling functionalities. Over the past year, we have shown that bulk molybdenum carbide is a promising candidate to enable direct formation of C2+ products from CO<sub>2</sub>. Subsequently, we have experimentally baselined existing molybdenum carbide catalysts, and synthesized and tested nanoscale molybdenum carbide catalysts that have achieved increased performance, including increased selectivity to desired C2+ products.

#### Weighted Project Score: 6.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

For the electrochemical conversion pathway, we are focused on low-temperature (generally less than  $100^{\circ}$ C) electrochemical technologies. Copper remains the state-of-the-art catalyst and is the only catalyst that can produce C2+ products. However, catalyst development is needed to reduce overpotential and increase selectivity to individual C2+ products. We have begun the investigation of metal phosphide catalysts for electrochemical CO<sub>2</sub> conversion. These are tunable materials that have recently shown promise for CO<sub>2</sub> conversion and have produced novel C3 and C4 products. Beyond electrochemical CO<sub>2</sub> conversion has been heavily studied, most of the work has been performed in aqueous solutions, where the low solubility of CO<sub>2</sub> prevents high-enough currents for scale-up. Therefore, it is widely held that electrolyzer configurations are needed where gas-phase CO<sub>2</sub> is used. While several different membrane-electrode assemblies have been tested, there remains no consensus on the best electrolyzer configuration. Furthermore, relevant electrolyzer setups are needed for catalyst evaluation in a relevant environment, as results obtained in aqueous solutions may not clearly translate to the electrolyzer environment. Overall, we aim to advance the state of the art for both electrochemical CO<sub>2</sub> conversion and help to enable the effective processing of this large biorefinery waste stream.

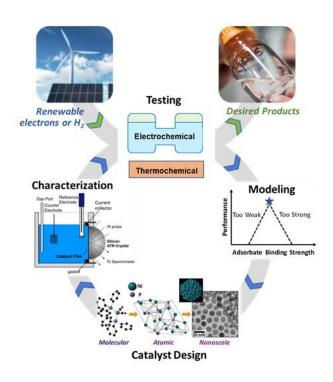


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project aims to benchmark and then further develop both electrochemical and thermochemical catalysts for the conversion of CO<sub>2</sub>.
- This is a comprehensive project, and advancements were made in catalyst development. System design results can help demonstrate the variability of the approach. The connections between electrochemical and thermochemical pathways can be articulated to identify the synergies, and the linkage between the identified BETO barriers and deliverables can help shape future priorities.
- This is a great team leveraging the Chemical Catalysis for Bioenergy Consortium efforts and has active collaborations with other expert groups. Thus, the team has a great potential to significantly advance the

thermochemical and electrochemical catalysts for  $CO_2$  conversion to C2+. The consideration of using a wide range of  $CO_2$  sources (e.g., ambient to industrial sources beyond ethanol plants) and the investigation of challenges associated with different  $CO_2$  waste streams would further improve the potential impact of this study.

- While the thematic goals are highly relevant to the BETO mission, the project has presented insufficient evidence to show that specific efforts in this project have a good chance of advancing the state of the art.
- The performers have proposed to improve both electrochemical and thermochemical conversion of CO<sub>2</sub> to C2+ products. The performers will be collaborating with the Feasibility Study from NREL. We suggest the performers focus on one of the two approaches (likely electrochemical) to maximize chance of success. The performers should also more clearly list out the metrics of success and the rationale for choosing those targets.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewer for the feedback and agree that there are clear synergies between the CO<sub>2</sub> conversion routes such as the synthesis of catalyst materials that are being leveraged across both pathways and characterization efforts that focus on key intermediates that are similar in both cases. Future deliverables will have metrics that directly address BETO Multi-Year Plan barriers through the incorporation of TEA in upcoming years.
- We thank the reviewer for their positive comments and agree that the investigation of realistic CO<sub>2</sub> sources will bring additional value to the project. In the initial two years of the project we focused on developing a synthetic platform of catalyst materials and an understanding of the corresponding reactivity. Additionally, we have developed capabilities for the testing of different membrane-electrode assemblies that are required for performing relevant research (including the screening of different CO<sub>2</sub> sources).
- On the thermochemical side, we sought to develop a synthetic strategy for a tunable catalyst system to develop a fundamental understanding of the impact of catalyst features on the resulting product slate. We acknowledge that the metal carbide system is only one type of catalyst system used for CO<sub>2</sub> reduction, but we believe that it affords the ability to rationally tune the catalyst structure and advance the state of the art over industrial materials. On the electrochemical side, our catalyst development efforts have yet to find a material that can outperform the state-of-the-art copper catalyst. However, electrocatalyst development with a tunable materials platform (transition metal phosphides) have been useful for studying electrochemical CO<sub>2</sub> reduction, and we are actively exploring new materials systems. Additionally, much work has been spent developing capabilities for catalyst testing in the relevant environment (in a membrane-electrode assembly), and these capabilities are required to advance the current state of the art.
- In the future, we will more closely align metrics of success for the project with BETO Multi-Year Plan barriers, which will be facilitated with ongoing TEA efforts to compare electrochemical and thermochemical approaches.

## HYBRID ELECTROCATALYTIC AND THERMOCATALYTIC UPGRADING OF CO<sub>2</sub> TO FUELS AND C2+ CHEMICALS

#### **Oak Ridge National Laboratory**

#### **PROJECT DESCRIPTION**

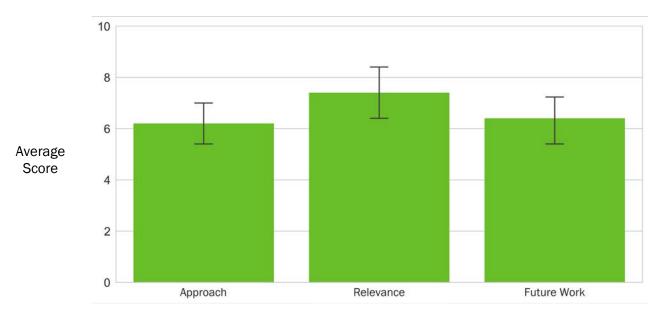
Electrocatalytic reduction of  $CO_2$  to useful products is a possible pathway towards higher rates of  $CO_2$  recycling and lower rates of fossil carbon utilization. It is also a means of using electrical energy to convert or reduce (in the chemical sense)  $CO_2$  to useful products. In this approach, an electrochemical catalyst acts as a cathode in an electrochemical cell. Energy in the form of electricity removes oxygen from the carbon and replaces it with hydrogen or other elements, moving the carbon from a low energy state ( $CO_2$ ) to a higher energy state (alkane, oxygenates). This strategy will become critically important in the future as an alternative to fossil carbon sources and as renewable electricity becomes more available. To fully

| WBS:                      | 2.3.1.317           |
|---------------------------|---------------------|
| CID:                      | NL0034400           |
| Principal Investigator:   | Dr. Adam Rondinone  |
| Period of<br>Performance: | 10/1/2018-10/1/2020 |
| Total DOE Funding:        | \$250,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$250,000           |
| Project Status:           | New                 |
|                           |                     |

utilize renewable electricity, we will need to develop appropriate catalysts and processes for the conversion of  $CO_2$  to a variety of important industrial chemicals and fuels. Previous major R&D efforts in  $CO_2$  electrocatalytic reduction have been targeting C1 products, such as CO, methane, and formate. There are strong interests and motivations to convert  $CO_2$  to heavier (C2+) alcohols (e.g., ethanol and 1-propanol) and hydrocarbons (e.g., olefins) as a critical approach to directly produce liquid fuels.

#### Weighted Project Score: 6.6

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

Recently, the Oak Ridge National Laboratory has developed a novel and efficient copper nanoparticle carbon nanospike (CNS) electrocatalyst to convert CO<sub>2</sub> to ethanol with high selectivity of 84% and high Faradaic efficiency (63% at -1.2 V versus reversible hydrogen electrode) that operates in water and at ambient temperature and pressure. Based on this groundbreaking technology, we propose to develop new bimetallic electrocatalysts supported on the carbon nanospike to further reduce the overpotentials and improve Faradaic efficiency and C2+ product selectivity. While there are only limited works on bimetallic approach for CO2 conversion to C2+ products, a bimetallic catalyst has been computationally shown to break the linear relationship between the binding energies of CO and carboxyl groups (COOH) on the electrode surface. The addition of the second metal could modify both the electronic property and the geometry of the Cu metallic nanoparticle, which will impact the adsorption of reaction intermediates and potentially improve the Faradaic efficiency of C2+ products. In addition to the promise of a bimetallic cocatalyst for promoting C2+ products formation, we also expect a synergistic effect between the high localized electric fields of the carbon nanospikes and the bimetallic nanoparticle cocatalysts. The carbon nanospikes generate high localized electric fields that effectively convert CO<sub>2</sub> to CO, providing abundant CO for further oligomerization on the bimetallic cocatalyst. All of these suggest bimetallic nanoparticles coupled with CNS could offer a great solution to advance the current state of technology on CO<sub>2</sub> conversion.

In this proposed work, we aim at improving the selectivity of C2+ products at lower overpotential, especially alcohols and olefins, which can be either used as fuels or be converted to fuels and value-added products. Ethanol and 1-propanol, for example, can be used as fuels or fuel additives, or converted to produce other hydrocarbon fuels and important precursors for carbon fiber or polymers. Other products (ethylene, acetaldehyde, acetone, hydrogen, etc.) from the proposed electrocatalytic process can be further thermocatalytically upgraded to produce high-quality gasoline, jet diesel, or precursors for polymers, rubbers, detergents, plasticizers, or lubricants. If successful, this hybrid integrated pathway provides significant advantages compared with the current state of technology on  $CO_2$  conversion.

#### **OVERALL IMPRESSIONS**

- The performers have proposed to electrochemically reduce CO<sub>2</sub> to C2+ products. The performers have developed new copper "nanospikes" that convert CO<sub>2</sub> to ethanol in favorable conditions. The performers aim to test other catalysts to reduce overpotential and produce molecules larger than ethanol. TEA will be extremely important for this work and the performers should determine ease of scalability of their new nanoparticle catalysts. Overall, the project is very promising and aligned with BETO's goals.
- Electrochemical conversion of CO<sub>2</sub> to C2+ chemicals is an important technical goal for making CO<sub>2</sub> utilization viable. The justification for the specific approach in this project is a speculative mechanistic hypothesis. Data at high current density is needed to properly assess the promise of the core technology.
- This project will use a carbon nanospike platform that previously showed interesting activity for CO<sub>2</sub>-toethanol conversion to investigate electrochemical synthesis of new C2+ products.
- This is an interesting project combining carbon nanospikes with bimetal cocatalysts to produce C2+ products from CO<sub>2</sub>. The catalyst development for the electrochemical conversion of CO<sub>2</sub> is a very important research field.
- The performers developed the unique structure of catalysts with nanospikes to convert CO<sub>2</sub> into alcohol. The science is interesting and technical approach is sound. Clear strategies on how cocatalysts will be synthesized can help guide future development. Identifying meaningful products and understanding the economic viability of the potential products will be helpful too.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

## **CO2 VALORIZATION VIA REWIRING CARBON METABOLIC NETWORK**

#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

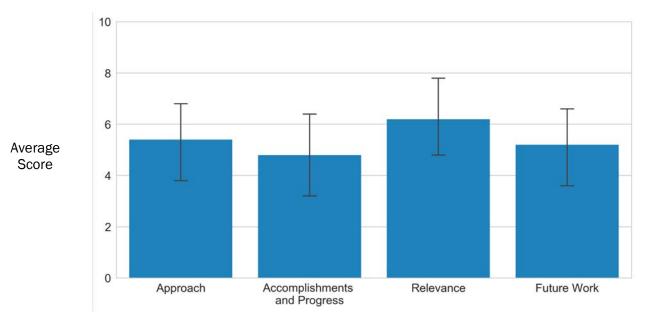
The overarching goal of this project is to perform strain development and preliminary TEA on a process valorizing  $CO_2$  to high-value hydrocarbon products, including 3HB, using the renewable electrons from H<sub>2</sub>. *Clostridium ljungdahlii* is the model CO<sub>2</sub>-fixing autotrophic microbe to realize this goal. A BETO assessment report has concluded that gaseous waste streams represent a significant and underutilized set of carbon-based feedstocks for biofuels and bioproducts. We aim to develop a microbial-based strategy to upgrade CO<sub>2</sub> gaseous waste streams with its successful outcome, paving the way to a new waste-based bioeconomy. With the foreseeable abundance of renewable electrons in the form of H<sub>2</sub> generated from electrolysis,

| WBS:                      | 2.3.2.106            |
|---------------------------|----------------------|
| CID:                      | NL0033406            |
| Principal Investigator:   | Ms. Pin-Ching Maness |
| Period of<br>Performance: | 10/1/2017-9/30/2020  |
| Total DOE Funding:        | \$650,000            |
| DOE Funding FY16:         | \$0                  |
| DOE Funding FY17:         | \$0                  |
| DOE Funding FY18:         | \$325,000            |
| DOE Funding FY19:         | \$325,000            |
| Project Status:           | Ongoing              |
|                           |                      |

progress of this project aligns well with DOE BETO programmatic goals. Choosing the H<sub>2</sub>-supported CO<sub>2</sub>fixing *C. ljungdahlii* microbe is another merit because it is genetically tractable with the highest rates of growth in syngas (H<sub>2</sub> CO) reported in the literature. NREL already has the genetic toolbox and further improvement is an ongoing research plan. A detailed 13C-metabolic flux analysis including under the autotrophic growth mode has not been conducted. This NREL project will provide more detailed insights to guide genetic engineering efforts and probe the strategies cells employed to manage its carbon and energy flow under autotrophic conditions, leading to high titer and yield of the targeted products in a more robust microbe.

#### Weighted Project Score: 6.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

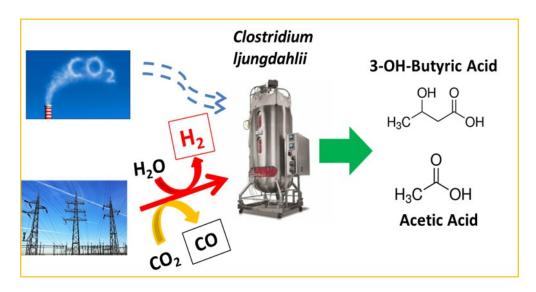


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project aims to produce 3HB, a platform chemical, using CO<sub>2</sub>/CO and hydrogen. Initial data were taken under growth with sugar and have demonstrated small but increasing titers of the desired product.
- The concept is interesting, and the team has the appropriate expertise. The results with C1 co-fed with sugar are promising, but the performance with C1 only is critical moving forward.
- This study focuses on engineering *Clostridia ljungdahlii* to convert a CO<sub>2</sub> and H<sub>2</sub> to 3HB. The project is well aligned with the BETO goals and has a great potential to be high impact, although the overall economics of this process are not clear.
- The performers have proposed to engineer *Clostridia ljungdahlii* to convert a CO<sub>2</sub> and H<sub>2</sub> to 3HB. The performers have developed the CRISPR-Cas9 system and demonstrated a phosphate acetyltransferase knockout can increase titers. The performers are encouraged to carefully do all titer benchmarking in autotrophic conditions, not mixotrophic conditions. Also, it is unclear what the value is of performing 13C fluxomics work in mixotrophic conditions. The performers are encouraged to explore multiplexing with Cas9 to enable faster engineering and to maintain genome-integrated copies of all overexpressions. TEA should be very valuable to direct the performers to the market size of 3HB, and what the necessary titer/productivities should be in order to commercialize. The project has great potential, aligned with BETO's mission, and has a high chance of success to reach the goal of 2 g/L 3HB titers.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree with the reviewers that performance with a C1-only substrate is critical moving forward.
- The project is well integrated with a TEA to evaluate the overall economics, which sets research targets and guides future research directions.
- We thank the reviewers for recognizing the great potential of this project, its alignment with BETO's mission, and the high chance of success to reach the goal of 2 g/L 3HB titers. Developing the CRISPR-Cas9 tool is the critical first step toward its multiplexing, aimed to modify microbial genome with higher throughput and efficiency, for which we are in full agreement with the reviewers. Thus far, genome integration has not been reported in this microbe and is a research goal of the project team. We also agree that the goal is to obtain final 3HB titers under autotrophic conditions. Current work conducted

under mixotrophic conditions including the initial 13C-fluxomics work is solely to obtain baseline information. We plan to systematically probe and gain insights as to how this microbe manages carbon, energy, and electron flux under varying growth conditions. The outcomes will help guide the design of microbial pathways to maximize growth and product titers under autotrophic conditions. TEA is already an integral component of the research to determine market size, the needed titers/productivity, and coproducts to attain techno-economic feasibility. Indeed, the preliminary TEA has revealed a 3HB minimum selling price of \$1.90/kg, provided a titer of 10 g/L and a productivity of 0.2 g/L/h can be achieved. This can set research targets. A minimum selling price for coproducts like acetate and 2,3-butanediol are \$1.80 and \$2.20/kg, respectively. The major cost drivers are H<sub>2</sub> and CO<sub>2</sub> feedstock cost and capital expenditure of biological conversion. The former can be addressed through improving the production yield to near theoretical maximums and the latter through increasing productivity and product titers. These findings guide R&D efforts carried out by the project team.

## IMPROVING FORMATE UPGRADING BY CUPRIAVIDUS NECATOR

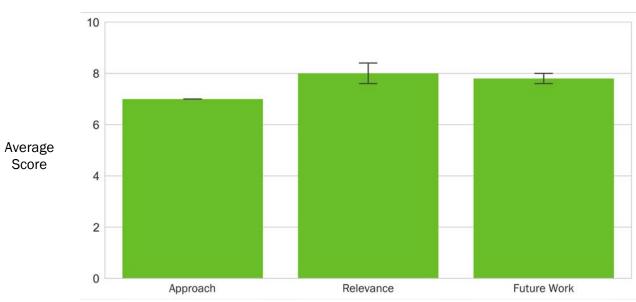
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

In support of BETO's interest in capturing and converting  $CO_2$  into value-added products using low-cost electricity, this project aims to develop the natural formatotroph, *Cupriavidus necator*, as a robust microbial chassis for efficient production of value-added products from formate, which can be produced by electrocatalytic reduction of  $CO_2$ . To date, we have demonstrated and baselined growth of *C. necator* on formate as its sole source of carbon and energy in a format consistent with high-throughput evaluation. In future work, a combination of rational metabolic engineering and evolutionary approaches will be employed to improve *C. necator*'s ability to assimilate formate. Improved strains will be further engineered to

| 2.3.2.111               |
|-------------------------|
| NL0034713               |
| Dr. Christopher Johnson |
| 10/1/2018-9/30/2021     |
| \$310,000               |
| \$0                     |
| \$0                     |
| \$0                     |
| \$310,000               |
| New                     |
|                         |

convert formate to the polymer precursor  $\beta$ -ketoadipate as an exemplary product. Data from this project will be used to generate TEA and LCA that can inform the foci and direction of this and related technologies for biological formate conversion.



#### Weighted Project Score: 7.7

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 ${\mathbb I}$  One standard deviation of reviewers' scores

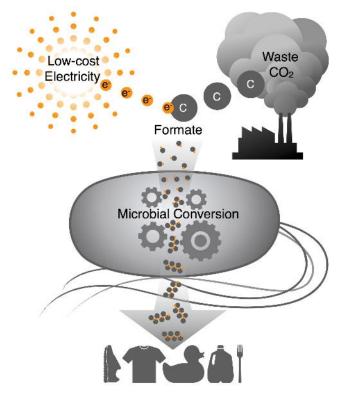


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- The performers have proposed to convert formate to beta-ketoadipate using engineered *Cupriavidus necator*. Though engineering the beta-ketoadipate pathway is promising, the performers seem too optimistic to improve the host's Calvin-Benson-Bassham (CBB) cycle, given this has been attempted for decades with little success. Additionally, the formolase will likely carry very little metabolic flux due to its extremely slow kinetics and should be reconsidered. The performers should consider setting higher milestone titers than 2 g/L of beta-ketoadipate given previous work showing 1.5 g/L of a branched alcohol. TEA will also be extremely important to validate the market size of beta-ketoadipate and what the titer/productivity levels should be for scale-up. Industrial fermentations typically have titers >50 g/L with productivities about 1 g/L/hr.
- The project is well designed and will generate useful baseline data to evaluate the feasibility of using *C*. *necator* for formate upgrading. More attention to the feasibility of operating at high formate utilization is needed to determine whether the overall approach is viable.
- This project aims to use a genetically engineered microbe to convert formate into beta-ketoadipic acid, a potentially performance-advantaged monomer for the production of nylons.
- This project is designed to convert formate to beta-ketoadipate using *Cupriavidus necator*. Formate is one of the target intermediates that can be produced through chemical synthesis, and beta-ketoadipate seems to be higher in value compared to other target products being considered. Thus, there seems to be a high potential for this project in terms of CO<sub>2</sub> to value-added products.
- This is a well-organized project. The performers clearly identified the project goals and approaches, as well as their relevance to BETO interests. The tasks are well defined, and the milestones are quantitative

and clear. More considerations can be given on understanding and improving formate tolerance and improving carbon and energy efficiencies.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

This project aims to improve formate conversion by *Cupriavidus necator* using a combination of rational engineering, including increasing expression of the CBB cycle components and introducing the formolase pathway and evolutionary approaches aimed at enhancing assimilation of formate. We acknowledge that improving the CBB cycle has been a major focus of research for many years. Improved CO<sub>2</sub> fixation has been demonstrated in other organisms by merely overexpressing Rubisco and/or other pathway components, however, and this is the main focus of our rational engineering related to this pathway. In addition, it is likely that laboratory evolution may improve formate conversion without improving assimilation pathways themselves. For instance, it has been shown that higher concentrations of formate do not necessarily lead to higher biomass yields, likely because withstanding higher concentrations requires additional energy. Thus, improved tolerance to formate resulting from laboratory evolution could improve conversion of formate.  $\beta$ -ketoadipate is an exemplary product for formate conversion and is being investigated in other projects in the BETO portfolio as a performanceadvantaged alternative to the incumbent petroleum-derived polymer precursor, adipic acid. TEA is an integral component of this project and will be employed to define titer, rate, yield, and downstream processing goals. We anticipate the need for higher titers, rates, and yields of products for economic viability but the main focus of this project is to improve formate conversion.

# ENHANCING ACETOGEN FORMATE UTILIZATION TO VALUE-ADDED PRODUCTS

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

Electricity from a diversity of sources is increasingly utilized due to its low cost. However, since much of this energy is intermittently generated, there is a mismatch between energy demand and supply. Cheap intermittent energy offers opportunities to utilize this energy and generate value-added chemicals. Low-cost electricity can be used to electrochemically reduce CO<sub>2</sub> to formate, which then can be upgraded to useful chemicals. To utilize formate for production of valuable chemicals, we decided to focus on *Clostridium ljungdahlii* as our host organism due to several advantages: it can already utilize formate under some conditions, it has the most developed genetic system for acetogens, and is a model organism for the

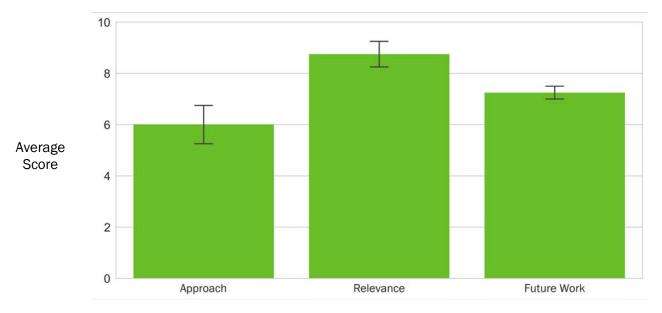
| WBS:                      | 2.3.2.112           |
|---------------------------|---------------------|
| CID:                      | NL0034714           |
| Principal Investigator:   | Dr. Jonathan Lo     |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$280,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$280,000           |
| Project Status:           | New                 |
|                           |                     |

Wood-Ljungdahl pathway, the most efficient anaerobic carbon fixation pathway.

Formate is a feedstock for a variety of bacteria and has several advantages to gaseous electrochemical products, including ease of storage and miscibility in liquid. Acetogens naturally take C1 compounds and convert them to higher-chain products through acetyl coenzyme A (acetyl-CoA), which is a precursor to many valuable products including carboxylic acids and alcohols. For this project, as a proof of concept, we are focusing on converting formate to butanol. This task primarily relies on two parts: improving formate

#### Weighted Project Score: 7.3

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

utilization and installing a butanol pathway. First, we characterized the conditions of native formate utilization in *C. ljungdahlii*. We also have begun working on genetic tools to delete and express genes.

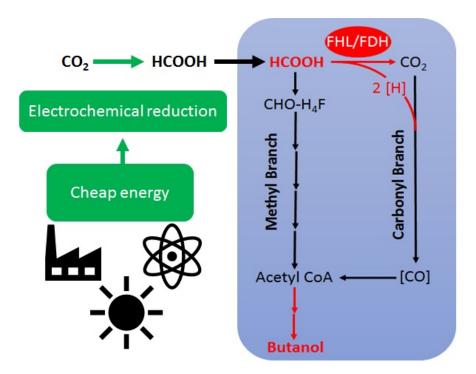


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- The performers have proposed to convert formate to butanol using *Clostridia ljungdahlii*. The performers have set a goal of 2 g/L titer and 0.18 g/L/hr productivity. The performers are encouraged to improve genetic tools in the organism to enable multiplex CRISPR-Cas9 engineering. It will also be important to integrate all overexpressed enzymes because plasmid-based systems are unstable during production. It is also unclear how 13C fluxomics in mixotrophic conditions (sugar and C1) will help the performers improve production in autotrophic conditions. Overall, the project aligns well with BETO's mission to upgrade C1 carbon sources.
- The project is investigating an interesting concept for hybrid electro-bio CO<sub>2</sub> conversion. The use of formate as a soluble reducing equivalent and CO<sub>2</sub> carrier for biological upgrading is conceptually appealing. However, the project would benefit from greater effort on system-level analysis to understand the key drivers of formate-based processes.
- This project uses a genetically engineered microbe to convert formate into butanol.
- This project aims to convert formate to butanol using *Clostridia ljungdahlii*. Formate is one of the target intermediates that can be produced via chemical synthesis. It is not clear whether butanol is the best target product considering their value and subsequent separation issues, etc. Thus, a better system engineering should be incorporated to fully evaluate the proposed technology.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We are working on new strategies to improve transformation efficiency and hopefully bring rapid genome editing to *C. ljungdahlii*. Because formate is not natively completely growth supportive in *C. ljungdahlii*, it cannot be used alone to understand formate-related growth. However, it can be used in conjunction with other energy sources and 13C labeling helps identify how the organism is using formate. There has been one 13C formate study of a formatotrophic acetogen that shows that formate is utilized by both branches of the Wood-Ljungdahl pathway, when grown with CO. Our preliminary study shows that in contrast, formate is used by only one branch of the Wood-Ljungdahl pathway when grown with CO, showing a clear difference between an organism that can use formate only, versus our organism which can only use formate complementary.
- TEA/LCA is being utilized to examine drivers of formate-based processes and may be integrated into a larger "electrons to molecules" concept at NREL.
- The TEA analysis is utilized to evaluate which products could best be made from formate. In our system, formate is first converted into acetyl-CoA, which is a precursor to many other products that could be made instead of formate, including ethanol, butyrate, and mevalonate, which could be made instead of butanol.

## SYNTHETIC C1 CONDENSATION CYCLE FOR FORMATE-MEDIATED ELECTROSYNTHESIS

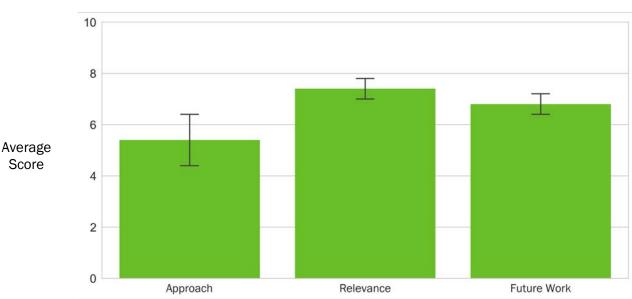
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

The innovative hybrid of biology and electrochemistry provides the potential to develop excelling bioenergy technologies. For instance, Formate-Mediated Electrosynthesis (FMES) offers a promising approach: excess electricity may reduce  $CO_2$  to formate electrochemically and the latter could then serve as the feedstock for the cultivation of microbes and production of value-added chemicals. To facilitate the novel technology, this project leverages *E. coli* as a model organism, engineering its metabolism and enabling it to convert formate and  $CO_2$  into C2 carboxylic acids. A synthetic pathway termed as the C1 Condensation Cycle will be constructed. Specifically, the cycle will achieve C1-to-C2

| WBS:                      | 2.3.2.113           |
|---------------------------|---------------------|
| CID:                      | NL0034715           |
| Principal Investigator:   | Dr. Wei Xiong       |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$300,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | New                 |
|                           |                     |

condensation and have three procedures. In net, it realizes a stoichiometry: formate  $(C1) + CO_2(C1) =$  glyoxylate (C2) by engineering two heterologous enzymes: malate thiokinase (MTK) and malyl-CoA lyase (MCL). We will further engineer a glyoxylate reductase to convert glyoxylate to glycolate as a representative value-added chemical. This technical route has many apparent merits, such as bioenergetics feasibility, pathway simplicity, and production of industrially important chemicals.



#### Weighted Project Score: 6.6

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 $oldsymbol{I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- The performers have proposed a novel pathway to convert formate to glycolate using engineered *E. coli*. A key reaction in their pathway is pyruvate formate lyase (PFL). The performers hope to utilize this enzyme in the reverse direction. Their pathway requires a constant source of adenosine triphosphate (ATP), which can be provided only in respiratory conditions. However, the PFL enzyme is very oxygen sensitive and may likely not function even in microaerobic conditions. The performers should fully evaluate the activity of this enzyme and determine if anaerobic respiration can be industrially scalable. Additionally, the performers have set low productivity targets (0.04 g/L/hr), which should be reevaluated based on their TEA. Most industrial fermentations run at productivities >1 g/L/hr. Electrochemical formate production will likely be a significant cost, and overall success will depend on high titers and productivity of any downstream upgrading.
- Leveraging selective CO<sub>2</sub>-to-formate electrochemical conversion for biosynthesis is an interesting new strategy. *E coli* is appealing from the perspective of the availability of metabolic engineering tools, but the feasibility of engineering pathways that allow *E. coli* to thrive on formate alone has not been established.
- The project endeavors to engineer *E. coli* to use formate as a substrate and produce acetate and/or glycolate.
- The use of *E. coli* to convert formate and CO<sub>2</sub> to glycolate is an interesting approach and very challenging. Unfortunately, this project is still in the early stages and does not have enough data to prove the concept yet.
- The performers provide a straightforward approach to modify model strains for formate upgrading. The technical approach is clear, and the proposed tasks are relevant to BETO's goals. More thoughts could be given on which pathways to be prioritized and techno-economic feasibility.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thanks for reviewers' comments. (1) The PFL enzyme can work in microaerobic conditions. Our 13Cformate labeling data has confirmed its activity in both microaerobic and anaerobic conditions. When we use 13C formate and unlabeled glucose as the carbon sources for microaerobically growing *E. coli*, the carboxylic group of pyruvate is significantly 13C labeled, which aligns with strong PFL activity. The PFL activity in microaerobic conditions was also supported in literature.<sup>1,2</sup> (2) The entire pathway is not ATP expensive as it only costs one ATP for producing a glyoxylate/glycolate from formate and CO<sub>2</sub>. We agree more ATP will be produced in the presence of oxygen. But there is still ATP generation in microaerobic and anaerobic conditions. In our case, it's too early to state that ATP is in shortage. We will investigate this in the study. (3) Down the road, we will do detailed TEA to guide experimental work. Currently, the productivity target is based on our protein cost analysis, which represents the biological expense for formate upgrading.
- We agree with the reviewer's statements of purpose.

<sup>&</sup>lt;sup>1</sup> Alexeeva, Svetlana, Bart de Kort, Gary Sawers, Gary, Klass J. Hellingwerf, and M. Joost Teixeira de Mattos. 2000. "Effects of Limited Aeration and of the ArcAB System on Intermediary Pyruvate Catabolism in *Escherichia coli*." *Journal of Bacteriology* 182, 4934–4940. http://doi.org/10.1128/JB.182.17.4934-4940.2000.

<sup>&</sup>lt;sup>2</sup> Zhu, Jiangfeng, Sagit Shalel-Levanon, George Bennett, and Ka-Yiu San. 2007. "The YfiD Protein Contributes to the Pyruvate Formate-Lyase Flux in an *Escherichia coli arcA* Mutant Strain." *Biotechnology and Bioengineering* 97 (1): 138–143. https://doi.org/10.1002/bit.21219.

- We agree that the project is still in a very early stage, as we have just begun project work in FY 2019. Our project will have more outcomes to share in future reviews.
- Two primary tasks for this project are pathway design/engineering and TEA, which will inform the pathways to prioritize and provide insight into TEA feasibility.

## INTEGRATION OF CO<sub>2</sub> ELECTROLYSIS WITH MICROBIAL SYNGAS; UPGRADING TO REWIRE THE CARBON ECONOMY

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

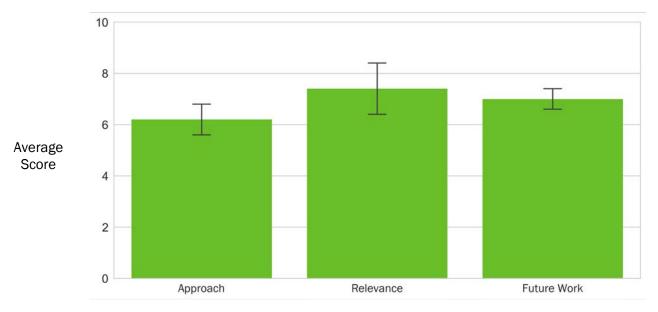
This project will work toward maximizing the carbon efficiencies and incentivizing carbon capture from industrial biopower processes and electricity generation technologies, where our bolt-on technology will produce valuable products from CO<sub>2</sub>. In response to the lab call for biopower: topic area 5, this technology will incentivize bioenergy with CO<sub>2</sub> capture and sequestration through the integration of downstream electrolytic and biocatalytic upgrading of flue gases into fuels and chemical intermediates. The production of valuable products from flue gas-derived CO<sub>2</sub> will reduce the net cost of conventional carbon-capture technologies, leading to a more economically favorable and sustainable process. Two

| WBS:                      | 5.1.3.101           |
|---------------------------|---------------------|
| CID:                      | NL0034004           |
| Principal Investigator:   | Dr. Michael Resch   |
| Period of<br>Performance: | 6/30/2018-3/31/2021 |
| Total DOE Funding:        | \$1,500,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$1,500,000         |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | New                 |
|                           |                     |

core technologies will be employed to demonstrate a novel process integration approach: electrolytic CO<sub>2</sub> conversion and biocatalytic syngas upgrading. Industrial partners 3M and Dioxide Materials have recently demonstrated electrolytic conversion of CO<sub>2</sub> and water to syngas using inexpensive renewable energy under an active ARPA-E subcontract. Concurrently, supporting partner LanzaTech has demonstrated industrial-scale CO fermentation using steel mill off-gas as a substrate. We will leverage these two technologies to examine integrated conversion of several industrial CO<sub>2</sub>-rich flue gases from biopower sources to fuel and/or chemical intermediates such as alcohols, butanediol, acetate, or jet fuel. At scale, we envision this system would be co-

#### Weighted Project Score: 6.9

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

located at an industrial biopower facility and could either use CO<sub>2</sub> from conventional carbon capture and utilization (CCU) sources or avoid the large CCU capital expense and directly use flue gas.

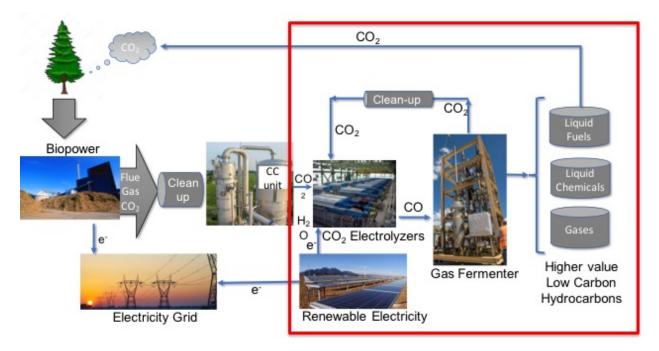


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project aims to demonstrate the integration of a CO<sub>2</sub>-to-CO electrolyzer with a microbial gas fermenter using industrial flue gas.
- The performers have proposed to integrate electrolysis with biological upgrading. The performers aim to convert CO<sub>2</sub> to syngas (electrolyzer by 3M/Dioxide Materials) using electrolysis, which will then be fed to LanzaTech's *Clostridia* for upgrading to a product. NREL will focus on the integration of various parts that work independently but have not been tested together. The project will evaluate the effect of various CO<sub>2</sub> flue gases on the electrolyzer performance and perform strain engineering to adapt strains to the new syngas source. This work is very relevant to BETO's mission and displays a great example of industry/government collaboration. The performers are encouraged to list clear goals of what titer/productivity they hope to achieve using the new syngas stream.
- The system under investigation is potentially a promising strategy to valorize fermentation flue gas. It is not clear, however, how the system would make biopower plants more impactful or economic because the energy demand of converting the emissions to fuel is greater than the output of the biopower plant. The team is likely to generate sufficient data to address the project goals.
- The project demonstrates clear goals and technical approaches to integrate CO<sub>2</sub> electrolysis with microbial syngas upgrading to ethanol. It contributes to BETO objectives, and the partnership with industry improves the potential of applicability. The project can be improved with more quantitative milestone measures, such as product yields, rates, and conversion efficiencies. The low-value products can be better justified. TEA and LCA should be done very carefully to justify why this approach is advantageous compared to mature alternatives such as fermentation. The novelty of the approach is not clear, as the industry partners have already demonstrated similar systems and published results.

• This project aims to capture CO<sub>2</sub> from a biopower plant and convert that into value-added products via the combination of electrolysis and gas fermentation. Two already proven technologies are being integrated and the main findings will be focused around the process integration. It is not clear whether this technology is best suited for CO<sub>2</sub> capture and conversion for biopower plants, but the combination of two technologies does have a great potential for a wide range of CO<sub>2</sub> sources.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- If successful, we feel that this system will be able to utilize a variety of CO<sub>2</sub> feedstocks and renewable energy sources.
- We appreciate the reviewers' supportive comments on how this meets BETO objectives and industrial partnerships. We agree that the milestones could be more quantitative. We are using the native product(s) as a proxy for diverse microbial syngas conversion product suites. A variety of biocatalysts from our industrial partner, LanzaTech, can be substituted and produce a variety of fuels and high-value chemicals. However, the primary goal of this project is to evaluate the potential impact of flue toxins to the electrocatalysts and the biocatalysts. Notably, previous work by our partners has exclusively evaluated pure CO<sub>2</sub>. We will determine how the flue gas components effect selectivity when low concentrations of impure CO<sub>2</sub> are utilized, and how do these varied gas streams propagate downstream to effect fermentation. There is a need for catalysts that are more tolerant of lower-quality feedstocks. Ultimately, what methods might be used for mitigation (filtration or other)—this project will lead to understanding of what is tolerable and not-and costs associated with cleaning gases can be determined. This should have been made clearer in the presentation. We have worked with our industrial partners on building the detailed (although preliminary) TEA models, as some of their data came from vendors' quotations or previous demonstrations. We agree that TEA and LCA should be done very carefully, as this process is much different from terrestrial lignocellulose conversion or water-splitting  $H_2$  electrolysis. We have a Q3 FY 2019 milestone to update the TEA metrics needed for TEA under varying electricity availability and potential CO storage and gas cleanup.

## NOVEL CELL-FREE ENZYMATIC SYSTEMS FOR CO<sub>2</sub> CAPTURE AND UTILIZATION: BIOENERGY-BASED BIOLOGICAL CARBON CAPTURE AND VALORIZATION (BECC&V)

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

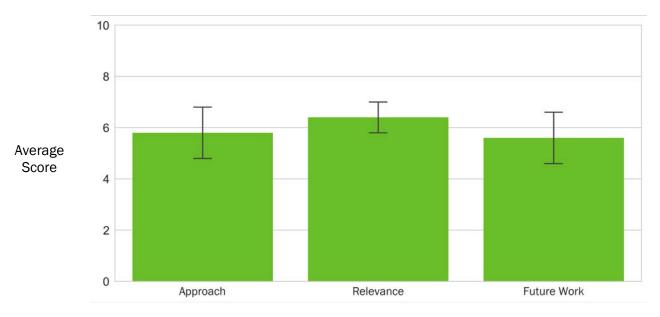
The goal of this project is to develop a novel biological, sustainable, and low-energy CO<sub>2</sub> waste gas scrubbing technology applicable to waste gases using enzymeaccelerated solvents with low regeneration energy. Fastreacting CO<sub>2</sub> absorption solvents such as monoethanolamine (MEA) require high regeneration energy due to high heats of absorption. Alternatively, more benign and sustainable solvents have lower heats of absorption but react more slowly. Bench-scale and pilot testing has proven the ability of carbonic anhydrase to accelerate CO<sub>2</sub> absorption in alternative solvents in both dissolved-enzyme and immobilized-enzyme forms. However, process improvements are still needed to achieve

| 5.1.3.103          |
|--------------------|
| NL0034006          |
| Dr. Min Zhang      |
| 5/1/2018-4/30/2021 |
| \$1,500,000        |
| \$0                |
| \$0                |
| \$1,500,000        |
| \$0                |
| New                |
|                    |

energy reduction versus benchmark MEA. We aim to develop a low-energy CO<sub>2</sub> waste gas scrubbing technology using improved, immobilized thermotolerant carbonic anhydrases and enzyme-accelerated solvents operating at low-regeneration energy. This project will demonstrate a new technology at bench scale that supports TEA and LCA enabling 20% energy reduction compared to the MEA reference case (~90% CO<sub>2</sub> capture). Our process also generates a favorable sustainability profile and potential for capital savings due to

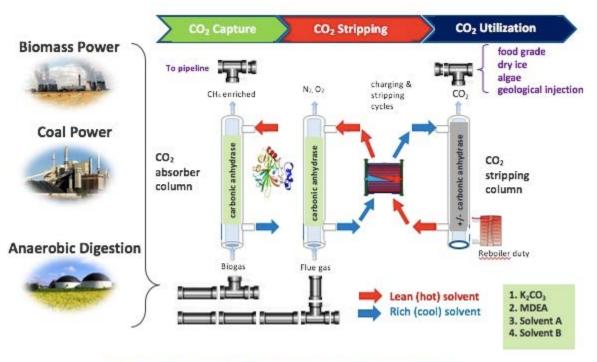
#### Weighted Project Score: 5.8

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

use of benign solvents. This technology can be deployed to many industries that generate waste gases to capture  $CO_2$  from biopower, fossil-based power plants, and biogas productions, thus upgrading natural gas, biogas, and  $CO_2$  for revenues.



#### Flexible solutions for CO<sub>2</sub> mitigation from waste gas

Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project aims to use carbonic anhydrase enzymes to create a bio-inspired carbon-capture system for point sources.
- The performers propose to replace the current CO<sub>2</sub>-scrubbing solvent MEA with another nontoxic solvent that works with an engineering carbonic anhydrase. The goal of the overall process is to reduce energy requirement compared to the MEA case. The performers will need to ensure that their enzyme is cheap, highly active in the new solvent conditions, and scalable. Though this project does not strictly upgrade CO<sub>2</sub> to another product, reducing the energy footprint of CO<sub>2</sub> scrubbing is still of importance to the DOE. The performers are encouraged to describe in more detail how they plan to perform the enzyme engineering, what their screening capacity is, and what the basal level of activity is of various enzymes in the solvents of interest. More focus on TEA should be placed early in the program to ensure that this technology, if successful, will outcompete the MEA process.
- The researchers have crafted a thoughtful plan based on good preliminary results to advance the performance of an interesting technological concept for CO<sub>2</sub> capture. More analysis of the cost of enzyme production is needed to determine feasibility.

- This project aims at using carbonic anhydrase to accelerate CO<sub>2</sub> capture by solvents with lower regeneration energies. Carbonic anhydrase is immobilized to improve its long-term stability. The overall approach is interesting, and the team is well equipped to carry out this study.
- While the project has scientific merit in terms of enzyme development, the focus of using expensive and delicate enzymes to scrub CO<sub>2</sub> from high-temperature and often toxic biogas/flue gas with the goal of reducing 20% energy consumption requires serious evaluations and justification. The commercialization pathway can be better justified. The team could have provided better state of the art, as there have been similar products on the market.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the review panel for their positive comments and helpful critiques. Our goal is to develop a high-performance, robust, scalable, economical, enzyme-catalyzed, solvent-based CO<sub>2</sub> scrubbing system with low energy penalty and low Environment, Health, and Safety (EHS) impacts as an alternative to MEA. Uniquely, in this project we will start by comparing top carbonic anhydrases from published sources and private industry in selected solvents to verify the state of the art and guide our engineering of new, more active, and highly stable enzymes through structure analysis and targeted mutations. These improvements, together with a novel immobilization strategy, will enhance enzyme longevity in desirable solvents at relevant process conditions. High enzyme longevity is a key strategy to minimize enzyme cost. TEA analysis is planned both in early and late stages of the project.
- A previous National Energy Technology Laboratory (NETL) project, led by Novozymes together with the University of Kentucky, Pacific Northwest National Laboratory, and Doosan, reported that improving enzyme longevity is a critical element in reducing operating costs. Thus, by achieving sufficiently high enzyme longevity, concerns around enzyme production cost can be overcome.
- We are excited to move this technology forward with new aspects that build on important previous work.
- Enzyme-based CO<sub>2</sub>-scrubbing technology has been actively developing over time. Supported by federal funding (NETL, ARPA-E), initial promising field tests and feasibility assessments were reported by Akermin (NCCC), Codexis (NCCC) and CO<sub>2</sub> Solutions (with Husky Energy). Additional federally funded projects led by Akermin, Codexis, University of Illinois Urbana-Champaign, Novozymes, and others have outlined the opportunities and challenges of the technology. Building on these prior works, the current project aims to close gaps in enzyme catalyst longevity and improve understanding of enzyme-solvent interactions that will lead to more robust, cost-effective, lower-energy CO<sub>2</sub>-scrubbing process options for the research and industrial community.

# **CATALYTIC UPGRADING**

(#

(1)

TECHNOLOGY AREA

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## INTRODUCTION

The Catalytic Upgrading Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 27 projects were reviewed in the Catalytic Upgrading session by six external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$53,638,660 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 6.2% of the BETO portfolio reviewed during the 2019 Peer Review. During the project peer review meeting, the principal investigator (PI) for each project was given 15–45 minutes (depending primarily on the funding level) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the Catalytic Upgrading Technology Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. Jeremy Leong as the Catalytic Upgrading Technology Area Review Lead, with contractor support from Mr. Trevor Smith (Allegheny Science & Technology). In this capacity, Dr. Leong was responsible for all aspects of review planning and implementation.

## CATALYTIC UPGRADING OVERVIEW

The Conversion Research and Development (R&D) Program Area focuses on technologies and processes that break down biologically derived feedstocks and reassemble them into useful products. BETO's current strategy reflects an approach that more broadly enables a wide variety of potential processes by performing early-stage, applied R&D to overcome technology barriers. The associated processes and steps are grouped into the broader categories of deconstruction, fractionation, synthesis, and upgrading.

The Catalytic Upgrading session included projects focused on overcoming the various challenges and barriers associated with synthesis and upgrading. Specific challenges include improving catalyst lifetime, increasing yields from catalytic processes, and decreasing the time and cost to develop novel, industrially relevant catalysts. These projects address these challenges through a combination of specific, pathway-focused projects with industry, universities, and at individual national laboratories, as well as consortia that combine the unique capabilities of several national laboratories in collaboration with industry via technical advisory groups and joint projects.

The Catalytic Upgrading session covered projects addressing challenges related to the catalytic upgrading of intermediates from both high- and low-temperature processes. Core catalytic technology development projects include upgrading of lignin, carbohydrates, and other biologically derived intermediates (e.g., lignocellulosic ethanol), upgrading of synthesis gas and synthesis-gas-derived intermediates (e.g., C1/C2 oxygenated intermediates), and hydroprocessing and upgrading of catalytic fast pyrolysis (CFP) bio-oils and electrocatalytic and thermocatalytic carbon dioxide (CO<sub>2</sub>) utilization. Enabling capabilities and cross-cutting projects included those related to analysis, modeling, characterization, and other guiding R&D.

The bulk of the session featured projects that are part of the Chemical Catalysis for Bioenergy Consortium (ChemCatBio). ChemCatBio is a national lab-led R&D consortium dedicated to identifying and overcoming catalysis challenges for the conversion of biomass and waste resources into fuels, chemicals, and materials.

The second-largest part of this session included projects with industry partnerships through directed funding awards (DFAs). DFA projects mirror the ChemCatBio but include industrial partners that were funded to specifically address their needs by utilizing world-class national laboratory capabilities which they could not otherwise access.

The final component of the session featured four competitive funding opportunity projects within the Conversion R&D portfolio that aim to enable the bioeconomy more broadly where their technology focus utilized catalytic upgrading processes.

## CATALYTIC UPGRADING REVIEW PANEL

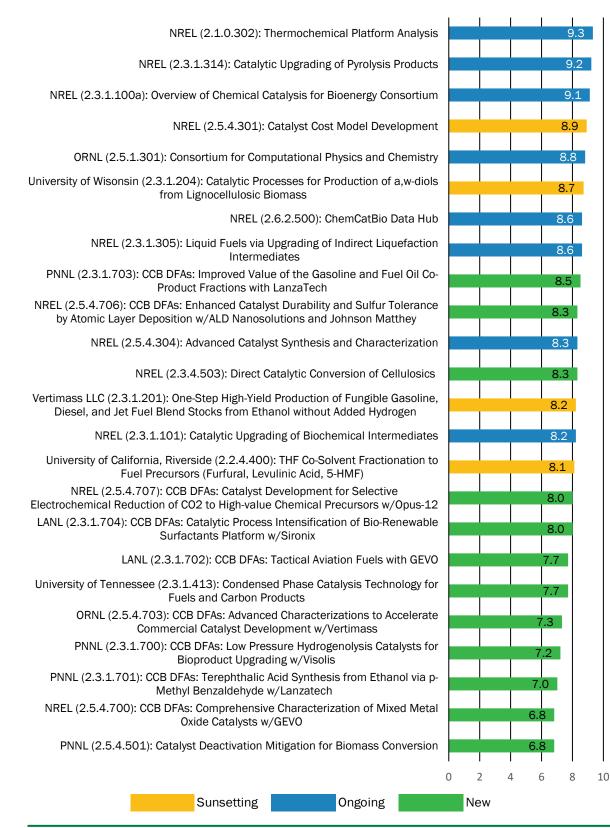
The following external experts served as reviewers for the Catalytic Upgrading Technology Area during the 2019 Project Peer Review.

| Name             | Affiliation                                   |
|------------------|---|
| Lorenz Bauer*    | LJB Chemical Consulting                       |
| Cory Phillips    | Phillips 66                                   |
| Jesse Bond       | Syracuse University                           |
| John Regalbuto   | University of South Carolina                  |
| Viviane Schwartz | U.S. Department of Energy - Office of Science |
| Chris Bradley    | U.S. Department of Energy - Office of Science |
| *Lead reviewer   |   |

CATALYTIC UPGRADING

## **TECHNOLOGY AREA SCORE RESULTS**

#### Average Weighted Scores by Project



## CATALYTIC UPGRADING REVIEW PANEL SUMMARY REPORT

#### Prepared by the Catalytic Upgrading Review Panel

Our efforts in reviewing the catalytic upgrading portfolio and summarizing the outcomes of projects therein are dedicated to the memory of Dr. Lorenz (Larry) Bauer. His leadership, clear thinking, technical depth, and private-sector experience sharpened our focus, and working with him improved our understanding of the challenges facing commercial deployment of bioenergy technologies. Perhaps most importantly, his boundless enthusiasm for renewable energy was an inspiration to all. The words are ours, but the vision is Larry's.

The catalytic upgrading session summarized progress within the portion of the BETO research portfolio focused on enhancing the economic potential of catalytic technologies for converting biogenic carbon into fuels and chemicals. Projects in this portfolio include those within BETO's Annual Operating Plan (AOP), which are led by the national laboratories; those awarded to external investigators through competitive Funding Opportunity Announcements (FOAs); and those awarded through DFA programs, which partner private-sector ventures with national laboratories to accelerate commercial development.

Research within this portfolio has made a significant impact on bioenergy technologies by demonstrating clear reductions in minimum fuel selling price (MFSP), accelerating catalyst design cycles, delivering a new suite of bio-based fuels and chemicals, and advancing bioenergy R&D. Innovations herein are numerous and have resulted in novel material designs and catalyst formulations, both of which are serving to enhance selectivity and decrease costs associated with catalytic processing. Further, research efforts have generated scientific insights that will impact other programs in BETO. More broadly, these insights advance the field, which benefits academic and industrial stakeholders working in similar areas. Synergies are apparent throughout this portfolio. Research projects leverage national laboratory capabilities as well as those of external partners from academia and industry. Project teams are collaborating effectively to accelerate material and process design. These efforts combine to support the overarching focus of this program, which is to enable commercially viable production of bio-based fuels and chemicals. This central theme is appropriate to the goal of increasing the market share of renewable carbon, and the commercialization potential of projects within this portfolio is strong. For example, Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates and Catalytic Upgrading of Pyrolysis Products are both rapidly approaching the 2022 BETO target of producing biofuels at \$3/gasoline gallon equivalent (GGE). High-value coproducts in particular have the best near-term commercial potential, and they are emerging as enabling technologies to facilitate cost-effective biofuels.

#### IMPACT

From a technical perspective, impacts within the catalytic upgrading portfolio arise from accelerating catalyst design cycles and enhancing commercial potential for bio-based fuels and chemicals. These are evidenced by new catalysts with improved activity, stability, and cost; continuous reductions in MFSP for core technologies; and demonstration of new pathways to high-value coproducts to enable near-term commercialization. From a general perspective, this unique, well-executed portfolio is impactful in that it provides a model architecture for cross-cutting, consortium-based research. In many respects, the catalytic upgrading program defines best practices in facilitating commercial deployment of integrated biorefineries. Specifically, this portfolio includes programs in techno-economic analysis (TEA), advanced catalyst synthesis and characterization (ACSC), and computational physics and chemistry, all of which enable the comprehensive set of individual, technology-oriented core research projects.

#### Advancing the Industrial State of Technology

Current research efforts are responsive to guidance from an external industrial advisory board. This has ensured that all projects prioritize work-breakdown structure and take active steps toward addressing existing hurdles to industrial deployment. By doing so, research within this portfolio is advancing the industrial state of technology. Projects have accelerated the catalyst design cycle by identifying material properties that positively impact reactor performance and reduce operating costs. Advances have driven MFSP estimates close to 2022 BETO targets primarily by focusing research on mitigating cost drivers and expanding the suite of accessible coproducts within an integrated biorefinery.

Two clear examples of improved MFSP estimates are the projects Catalytic Upgrading of Pyrolysis Products and Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates. Both have identified novel catalyst formulations relative to benchmark materials. Their new materials improve stability, enhance selectivity, reduce cost, and/or deliver high-value coproducts, thereby bringing MFSP estimates in line with targets of roughly \$3/GGE.

Another outstanding example of advances in the state of technology is the Catalytic Upgrading of Biochemical Intermediates (CUBI) project, which continues to push the boundaries in synthesis and applications for biobased platform molecules, such as furfural, 2,3-butanediol (2,3-BDO), and hydroxymethylfurfural (HMF), which are all produced by selective fractionation of biomass. The CUBI program has also highlighted the importance of lignin valorization in achieving cost targets. In doing so, the CUBI project is responding to guidance from past program reviews—specifically, that BETO should focus on technologies that fractionate biomass to maximally leverage each component instead of relying only on thermochemical front-end technologies for single-stage deconstruction of whole biomass.

It is also worth highlighting DFA projects in this discussion. They provide commercial ventures access to the powerful tools and domain expertise available within BETO. In this way, they directly impact the current state of industry, and they advance technologies along the development pipeline. This is a nice synergy because nascent ventures lack in-house access to the suite of analytical tools accessible to a national laboratory. Further, startups may be unable to dedicate resources, personnel, and time to elucidating the scientific insights necessary to accelerate catalyst and reactor design. At the same time, industrial partners provide crucial access to industrial catalyst formulations and commercial structures (e.g., extrudates and engineered materials), as well as data generated in pilot and/or demonstration-scale facilities.

DFA projects leverage strengths from all partners in moving technologies toward commercial deployment, and they represent one of the clearest demonstrations of how research within BETO is helping to advance the industrial state of the art. A good example of such a partnership is the project Enhanced Catalyst Durability and Sulfur Tolerance by Atomic Layer Deposition (ALD). Catalyst instability is a grand challenge in biomass upgrading, particularly in liquid media. Issues like metal leaching, sulfur tolerance, and particle sintering remain largely unresolved, and they continue to hinder the economic viability of catalytic upgrading process technologies. This project is a collaboration between the National Renewable Energy Laboratory (NREL) and commercial catalyst manufacturers ALD NanoSolutions and Johnson Matthey, and it has allowed the team to rapidly deploy ALD to design a more robust, sulfur-tolerant catalyst for selective hydrogenation of muconic acid. The resultant platform is versatile, and it can be easily adapted for broad applications in biomass processing.

In another example, the Improved Value of the Gasoline and Fuel Oil Coproduct Fractions with LanzaTech project highlights the productive and rewarding partnership between Pacific Northwest National Laboratory (PNNL) and LanzaTech. This collaboration has been successful in generating technologically viable bio-based aviation fuels, ultimately delivering a demonstration flight with Virgin Atlantic. Presently, they are focused on producing higher-value fractions, namely high-octane gasoline additives and lubricants, from ethanol. This will enhance their economic potential and move the field closer toward practical, bio-based aviation fuels.

#### Focus in Light of Private-Sector Investments

In terms of technology readiness level (TRL), research in this portfolio ranges from early to middle levels. At the lower end, projects include bench-scale research to explore novel catalysts and upgrading technologies. At the higher end, projects aim to reduce MFSP estimates by improving catalyst stability, decreasing noble metal loadings, and optimizing coproduct synthesis. As a whole, BETO projects are moving successful proof-of-

concept demonstrations down the development pipeline, and they are aiding industrial partners in resolving hurdles to commercial deployment.

At lower TRLs, private-sector investments are unlikely to support the early-stage, basic research necessary to discover new materials, chemistries, and technologies, nor will the private sector support efforts to elucidate the fundamental origins of catalyst or reactor performance. These steps are crucial to accelerating the design of catalytic materials and catalytic processes, and BETO support at this TRL is accordingly justified. At higher TRLs, one finds mature projects, such as Catalytic Upgrading of Pyrolysis Products, Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates, and CUBI. While their core technologies are capable of delivering a range of biofuels and/or biochemicals, they are as yet unable to generate profits alongside oil and natural gas. This makes it difficult to attract private-sector investment to transition these processes to pilot, demonstration, and/or commercial scales. Continued support from BETO is thus critical to ensuring continued development of technologies that have long-term promise but face a presently unfavorable investment climate.

#### **Standout Projects**

Several projects stand out for bringing their MFSP estimates in line with 2022 BETO targets. Catalytic Upgrading of Pyrolysis Products has appropriately leveraged TEA to direct research toward reducing the primary cost drivers in pyrolysis-based fuels. For example, to decrease catalyst costs associated with pyrolysis oil upgrading, the project team designed an active, low-metal platinum (Pt)/titanium dioxide (TiO<sub>2</sub>) catalyst. This was a major improvement to the first-generation materials synthesized at the outset of the project. To address the issue of a low selling price for commercially available, paraffin-rich fuels, the team optimized coproduction of higher-value aromatic oxygenates like phenol and catechol. These efforts have the potential to reduce MFSP to \$2.50–\$3/GGE, and the work has largely set the current state of technology for pyrolysis-based transportation fuels.

The Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates project leverages a robust liquefaction frontend for biomass deconstruction and offers a suite of downstream upgrading options that improve upon well-known catalytic chemistries (methanol synthesis, methanol to hydrocarbons, and alkene oligomerization). In this way, the project offers flexible fuel production from a range of biomass or waste feedstocks. The indirect liquefication (IDL) team has demonstrated a process development trajectory allowing for a near-continuous decrease in their MFSP estimates. While it may be difficult to commercialize an IDL-based biofuel facility in the near term due to oil and natural gas availability, this platform will almost certainly play a role in the long-term production of alkane fuels, and it remains a vital part of the catalytic upgrading portfolio.

The CUBI project plays a key role in advancing fractionation-based strategies to target production and upgrading of well-defined platform chemicals, such as furans or carboxylic acids, as opposed to the heterogeneous bio-oils sourced from pyrolysis and liquefaction. The CUBI project continues to enhance the commercial potential for bio-based platform chemicals, and the team has highlighted the importance of lignin valorization in achieving cost targets.

Some of the most important impacts of the catalytic upgrading portfolio come from the cross-cutting programs that enable other research projects. TEA is tightly integrated with laboratory research efforts across this portfolio. Formally, this is enabled by the Thermochemical Platform Analysis project. Throughout the biomass-processing community, their work has set an important, best-practice standard of using TEA to guide future research. The ability of TEA to identify primary cost drivers and its ubiquity in the catalytic upgrading program has been instrumental in expanding efforts in lignin valorization and production of high-value coproducts. These new directions have driven the rapid progress toward 2022 BETO dollar-per-GGE targets made by the Pyrolysis, IDL, and CUBI teams.

The Consortium for Computational Physics and Chemistry (CCPC) provides insights about fundamental physical and/or chemical phenomena that underlie the inherent performance of catalytic materials as well as the physicochemical dynamics of catalytic reaction engineering. The CCPC is a mature and well-coordinated

team that has made tangible and impactful contributions within the catalytic upgrading group and across the BETO portfolio. It should serve as a model structure for future consortia launches and subsequent development. The ACSC team provides the synthesis capabilities necessary to deliver well-defined, active, and stable materials, as well as the characterization tools and expertise necessary to understand how catalyst structures evolve under working conditions. These consortia are effective at reducing redundancies across BETO. At the same time, they ensure that adequate technical depth exists to support core technology projects while also generating significant scientific impact. All technology-focused projects effectively leverage these programs. This is a powerful, cross-cutting approach to the complex and multidisciplinary research necessary to advance commercialization of biofuels and biochemicals.

In addition to the projects cited above, the Catalyst Cost Model Development project and the ChemCatBio Data Hub are noteworthy for their far-reaching impact, both internal to and outside of BETO. The former is a robust tool that facilitates estimation of commercial catalyst cost to inform TEA. This tool is therefore able to guide early-stage catalyst design toward utilization of lower-cost and earth-abundant materials as well as less-complex synthesis methods. The developers have demonstrated that this tool is secure, accessible, and sufficiently robust to allow new users to generate realistic cost estimates. Further, they provide tutorials and case studies, and they have undertaken a broad outreach effort within the catalysis community through webinars and workshops at the American Chemical Society (ACS) and American Institute of Chemical Engineers (AIChE) national meetings. These efforts have yielded a quantifiable increase in this tool's use over the past year.

The ChemCatBio Data Hub is a relatively new project, but it shows incredible potential, especially in light of recent and pending advances in data science, machine learning, and artificial intelligence. The Data Hub will serve as a centralized repository for sharing characterization and performance data about materials designed, developed, and tested within BETO consortia. Further, the team aims to develop a catalyst design engine, which will allow users to leverage computational tools to explore the material design space for targeted reactions. Although an early-stage project, the Data Hub is headed in the right direction. In the short term, it will facilitate data sharing as a means to eliminate redundancies across the consortium. It will also allow machine-learning algorithms to leverage a massive set of data in order to improve predictive capabilities in material design. In addition to providing useful support within BETO, these projects will have far-reaching impact as they are intended for distribution to a broad audience, and they should see widespread adoption in the catalysis community.

#### **INNOVATION**

Innovations within this portfolio take many forms. We highlight projects that have resulted in new catalytic materials, new high-value fuel or chemical targets, or new fundamental insights into catalyst and reactor performance.

FOA projects are a clear source of innovation. They focus on lower TRLs and technologies that are as yet unproven; thus, BETO support is pushing the boundaries of known strategies for the production of bio-based fuels and chemicals. A good example is the project Catalytic Processes for Production of  $\alpha$ , $\omega$ -diols from Lignocellulosic Biomass. 1,6-Hexanediol and 1,5-pentanediol are high value, have good market potential as polymer precursors, and are expensive to source in a petrochemical facility. These factors combine to make them attractive for near-term commercial development. Another example is the Tetrahydrofuran (THF) Co-Solvent Fractionation to Fuel Precursors (Furfural, Levulinic Acid, 5-HMF) project, which has delivered a novel approach to the long-standing challenge of biomass fractionation and upgrading. This technology achieves impressively high yields of C5 and C6 sugar dehydration products in an intensified process.

Projects supported through BETO's AOP continue to innovate, primarily through catalyst design and enabling production of high-value coproducts. For example, the Catalytic Upgrading of Pyrolysis Products team has developed a Pt/TiO<sub>2</sub> catalyst that offers improved activity and reduced cost. This effort toward a traditional, thermochemical approach to fuel production is balanced by efforts within the CUBI program, which is

advancing a route toward production of bio-based butadiene that leverages a hybrid biochemical and catalytic technology. In addition, several of the DFAs pursue new and exciting directions:

- Tactical Aviation Fuels with Gevo employs photo-initiated dimerization to produce targeted cyclobutane derivatives that have improved energy density and are appropriate for use in aviation fuels
- Catalyst Development for Selective Electrochemical Reduction of CO<sub>2</sub> to High-Value Chemical Precursors with Opus 12 is designing catalysts to facilitate electrochemical conversion of CO<sub>2</sub> into chemical targets
- Catalytic Process Intensification of Bio-Renewable Surfactants Platform with Sironix is commercializing an entirely new class of furan-derived surfactants that offer a number of performance benefits relative to conventional surfactants.

Overall, the portfolio is well balanced. It includes relatively mature technologies, such as upgrading oils generated through pyrolysis and liquefaction, while also pursuing new directions aimed at the production of high-value coproducts to support near-term commercialization. While the span of projects within the catalytic upgrading program is appropriate, the commercial success of efforts therein depend heavily on two efforts that do not fall within the core of the catalytic upgrading portfolio: lignin valorization and separations. TEAs consistently indicate that lignin valorization is a crucial component of an economically feasible technology, and it will be necessary to incorporate higher-value applications for lignin across the catalytic upgrading portfolio. Analogously, separations contribute substantially to capital and operating expenses, and their efficacy impacts impurity carryover, catalyst lifetime, and product quality. There are clear synergies with lignin valorization and separations consortia within BETO, and efforts therein are vital to decreasing MFSP estimates for technologies in the catalytic upgrading portfolio. Project summaries in the 2019 panel review only hinted at the scope of work in these partner consortia, and their impacts were not clearly quantified in TEA. We encourage continuing and strengthening interactions between catalytic upgrading, lignin valorization, and separations programs and highlighting synergies more clearly during reporting. This is particularly important in the discussion of TEA for individual projects. This will ensure that catalysts are developed with realistic purity specifications in mind and that critical separation stages are detailed in TEA.

#### **SYNERGIES**

The portfolio has many synergies that are effectively leveraged to benefit all stakeholders. A clear example is the critical need for TEA in all projects, which has resulted in the Thermochemical Platform Analysis team providing TEA support across the portfolio and driving research in appropriate directions. Similarly, the capabilities of the ACSC team impact nearly every project. They have the tools and expertise necessary to prepare well-defined materials and to characterize their working state, which is essential to understanding how structure determines function. The ACSC team thus enables a rational and scientific approach to accelerating the catalyst design cycle. Expertise in catalyst synthesis within the portfolio additionally leads to creation of the Catalyst Cost Estimation Tool, which is a nice synergy between TEA and the ACSC.

In terms of deepening scientific understanding, the Consortium for Computational Physics and Chemistry explores physical and chemical phenomena that dictate the performance of catalysts and reactors at micro-, meso-, and macroscales. In doing so, they both advance the state of knowledge and provide the hierarchical modeling that is critical at all stages of the development pipeline. At the atomic scale, electronic structure calculations confer understanding of reaction mechanisms and how the structure of a catalyst determines its activity, stability, and selectivity. At the macroscale, computational fluid dynamics simulations help to capture mass- and heat-transfer impacts on reactor performance, which become increasingly important in industrial processes. Finally, the ChemCatBio Data Hub centralizes data generated across the consortium in a single, searchable repository. This is essential to avoiding redundancy and ensuring that measurements and experiments have maximum impact. Projects supported through FOAs and DFAs exploit synergies between national laboratories, academic institutions, and the private sector. A good example is the pair of Gevo-

affiliated projects that are pursuing different strategies to enhance the value proposition of cellulosic ethanol by offering new, high-value products (cyclobutane derivatives) and by upgrading low-value byproducts (fusel oil). These two projects benefit from Gevo's expertise in cellulosic ethanol production, while also leveraging expertise in catalyst and process design at the national laboratories.

There are strong synergies with groups elsewhere in BETO, such as those working in lignin valorization and those working in separations. Lignin valorization and efficient, effective separations are critical components of a commercially viable technology; thus, outcomes from these partner consortia will directly impact the MFSP estimate for catalytic upgrading technologies. The catalytic upgrading portfolio should continue to leverage these programs to the maximum extent possible. This will generate process models that more accurately anticipate yields of lignin coproducts, feed compositions, impurity carryover, and product quality levels that are attainable at scale.

By partnering national laboratories with industry, DFA projects provide a unique opportunity for the catalytic upgrading program to access commercial catalysts and pilot facilities. BETO should seize these opportunities to research industrial catalysts and to enhance TEA models by incorporating data from industrial pilot or demonstration facilities. At the same time, industrial partners in DFA projects would clearly benefit from leveraging TEA capabilities in the Thermochemical Platform Analysis project as well as the modeling and simulations capabilities within the CCPC. DFA projects should additionally take advantage of the BETO industrial advisory board to help guide technology development.

A major strength of the catalytic upgrading portfolio is cross-cutting assets like the Advanced Catalyst Synthesis and Characterization, Thermochemical Platform Analysis, the Consortium for Computational Physics and Chemistry, the Catalyst Cost Estimation Tool, and the ChemCatBio Data Hub and its forthcoming Catalyst Design Engine. These programs are having significant impact within the catalytic upgrading portfolio and, more broadly, across BETO. They are further poised to have a longstanding impact on the field. It is important to maintain and support these initiatives such that they can continue to evolve and reflect both the state of the art and the needs of the field.

#### FOCUS

The focus on developing pathways that produce fungible transportation fuel components from biomass is appropriate. Although the portfolio supports a range of projects that consider diverse technologies, they share a goal of making integrated biorefineries commercially viable. Projects geared toward decreasing the MFSP estimate of biofuels toward the \$3/GGE target align with the mandate to increase utilization of renewable carbon in the transportation sector. At the same time, the program also acknowledges the challenge in commercializing biofuels alongside inexpensive fossil carbon. The portfolio is smartly balanced by including technologies that pursue higher-margin commodities, such as select fuel additives or higher-value chemicals, which may be more commercially relevant in the near term. It is worth noting that this is responsive to recommendations raised in the 2017 BETO Peer Review of the Thermochemical Conversion program. Finally, this portfolio leverages experimental and computational research in material discovery. This is an appropriate focus considering the programmatic goal of accelerating the catalyst design cycle.

The majority of projects target hydrocarbon production, with fewer focusing on organic compounds functionalized by one or more heteroatoms (oxygen, nitrogen, etc.). Heteroatom-bearing chemicals are useful as fuel additives, solvents, chemical intermediates, and polymer precursors, which are all high value relative to alkanes. Further, they represent a class of chemical commodities where biomass may have a competitive advantage relative to oil or natural gas. Selective activation of alkanes to produce functionalized hydrocarbons is challenging, and it may be possible to leverage the inherent oxygen and/or nitrogen content of biomass for mild, selective production of functional intermediates. Although the markets for heteroatom-containing chemicals are small relative to transportation fuels, they may offer better near-term commercial potential, motivating additional focus in this area. As the consortium continues to leverage the synthesis capabilities within ACSC to accelerate the catalyst design cycle, it is important to address the transition from lab-scale

formulations (powdered catalysts, colloidal nanoparticles, etc.) to extrudates and pellets that are more characteristic of the commercially engineered materials used in industrial-scale reactors. Finally, the ChemCatBio Data Hub is poised for considerable impact. Additional emphasis should be placed on developing the Data Hub such that it is accessible to and can accept input from external users, such as other Energy Materials Network consortia or researchers in industry or academic institutions. A straightforward, computational Catalyst Design Engine would have a tremendous impact on the field, and additional efforts in this direction should be emphasized.

The 2017 BETO Peer Review raised concerns about continued reliance on pyrolysis to deconstruct whole biomass. This yields a low-grade crude that has, to date, struggled to find a commercially viable application. A major challenge with this approach is its reliance on hydrotreating, hydrodeoxygenation, and hydrogenation to stabilize low-grade bio-oils and promote oxygen removal. Because of their hydrogen demand, they remain too costly to deliver a commercially viable fuel. It is unclear whether continued research into catalyst and reactor designs for pyrolysis oil upgrading is improving the process sufficiently to enable commercialization; rather, it appears that the most dramatic improvements in MFSP estimates are coming from coproducts and lignin valorization. It may be possible that additional work in the area of catalyst and process design for pyrolysis oil upgrading will help to improve the state of technology, but the case should be clearly motivated by TEA.

It is critical that assessment and mitigation of catalyst deactivation comprise a central part of each research project that relies on catalytic chemistry. In general, each project currently appears cognizant of the need for this, and all appear well equipped to address catalyst stability in the course of their research. Although the standalone catalyst deactivation project could potentially serve as an enabling technology, it is unclear whether it will be able to provide the type of consortium-wide support envisioned at modest funding levels. Because catalyst deactivation is so complex and technology specific, it may be more appropriate to emphasize catalyst deactivation within individual research pathway projects rather than to outsource to a supporting consortium.

While exploratory work in catalyst design can have significant impact in terms of demonstrating the synthesis of a new material, having a rationale for new material selection is important to ensuring that catalyst design and synthesis efforts align with BETO's mission. For example, the ACSC is expanding its portfolio to include metal-organic frameworks (MOFs); however, it was not made clear which challenges MOF structures are intended to address, nor how this class of materials will uniquely enable commercial development.

#### TECHNOLOGY DEVELOPMENT PIPELINE

Projects span from early- to midscale TRLs, which seems appropriate to the organization's mandate. BETO's support for relatively early-stage research helps to transition projects away from bench scale and toward TRLs that generate intellectual property, leverage intellectual property through licensing agreements, and launch startups that accelerate commercial deployment. Although technologies at higher TRLs are relatively mature, BETO funding remains appropriate. Biofuel technologies based on liquefaction, pyrolysis, and syngas upgrading are established with respect to their technical art; however, they have struggled to gain a commercial foothold because of the large upfront capital investments required and the difficulty of competing in the lowmargin transportation sector. There are clear ways that additional targeted research will benefit their economic potential. For example, the DFA project Terephthalic Acid Synthesis from Ethanol via p-Methyl Benzaldehyde provides LanzaTech with the capacity to convert a portion of their ethanol product to aromatic aldehydes. Although LanzaTech is an established venture, this targeted effort facilitates Guerbet condensation and shape selectivity to enable production of bio-based para-methyl benzaldehyde, which is a valuable coproduct. Success in this project will dramatically improve near-term economic potential. Further, by diverting a portion of their ethanol product to chemicals manufacture, this technology could help to mitigate the blend wall currently facing increased production of cellulosic ethanol. By funding research at these relatively mature TRLs, BETO occupies a critical niche in the technology development pipeline. Specifically, BETO supports projects that are too applied to be competitive in programs oriented toward basic science research (e.g., National Science Foundation or DOE's Basic Energy Science program). At the same time, these technologies have not yet achieved adequate economic potential to attract investment from the private sector. By supporting

mid-scale TRL projects, BETO is helping relatively mature processes to identify (through TEA) and resolve or mitigate the major cost drivers in their technology.

The integration of TEA throughout the ChemCatBio portfolio is clearly working to identify major cost drivers. There is pressure to meet dollar-per-GGE targets, and most technologies that are approaching these targets rely heavily on projected sales of high-value coproducts; however, details on higher-value coproducts were often sparse in project reports, particularly for those products sourced through lignin valorization. Based on summaries during the program review, it was not clear if robust markets exist for these coproducts, which may be problematic if a low MFSP estimate depends on producing these coproducts at scales commensurate with transportation fuels.

The panel accordingly raised the question of whether TEA estimates are sufficiently conservative, or if they reflect an overly optimistic forecast at the conceptual process design level. TEA is appropriate as a relative gauge of whether the economics of the process are improving, but it may not be representative of actual production costs incurred upon initial commercial-scale deployment. Although dollar-per-GGE estimates will look less attractive, it may be helpful to consider the economics of the standalone process (i.e., without coproducts) and to separately highlight the scale and impact of valorized coproducts. This would make clear the extent to which achieving dollar-per-GGE targets for a given process will depend on, for example, lignin valorization, which has been historically challenging. Along these lines, many technologies within the portfolio are bio-based analogs of mature industrial processes. For example, Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates relies on syngas upgrading, and the economic potential of those technologies using methane or coal are well established. Similarly, the Improved Value of the Gasoline and Fuel Oil Coproduct Fractions with LanzaTech project appears to rely heavily on olefin oligomerization for the production of high-octane gasoline. These projects (and others within the portfolio that are relying on technologies with a clear fossil carbon analog) would benefit from a more thorough consideration of the history of these technologies, their MFSP estimates, and their commercial potential. This would be helpful in benchmarking the bio-based technology against fossil-upgrading processes to inform and de-risk commercial deployment.

Catalyst improvements have advanced two pathways—CFP and IDL—and are approaching MFSP estimates at or below \$3/GGE, which stands as an example of helping to orient technologies toward successful adoption by industry.

#### RECOMMENDATIONS

The panel's most important recommendations that would strengthen the portfolio in the near to medium term include:

- 1. The Thermochemical Platform Analysis project is providing critical support across the catalytic upgrading portfolio. It should be formally considered as an enabling technology within ChemCatBio, similar to the ACSC and CCPC, and it should continue to be refined and expanded as necessary to support research across BETO.
- 2. The ChemCatBio Data Hub will play an important role in accelerating the catalyst design cycle, particularly as the role of data science continues to evolve. This effort should be further emphasized and expanded to support the development of more tools, such as the Catalyst Design Engine, and to accept data input from external users, as well as interface with other Energy Materials Network consortia or stakeholders from industry and academia.
- 3. BETO should increase focus on technologies that deliver higher-value products to benefit near-term commercialization. All high-value products are of interest, and TEA indicates that lignin valorization is particularly critical to achieving dollar-per-GGE targets.

## CATALYTIC UPGRADING PROGRAMMATIC RESPONSE

#### INTRODUCTION/OVERVIEW

The Conversion R&D Program would like to take the opportunity to thank the six Catalytic Upgrading session reviewers for their time and careful review of the projects presented in this session. We recognize that this was a challenging review process where other presentations/sessions were difficult to attend due to scheduling and time constraints. BETO is committed to continuous improvement of the peer review such that all reviewers have opportunities to engage other areas within BETO to further their understanding related to specific areas they have been asked to review.

BETO appreciates the review panel's recognition of the successes of consortium-based research, acceleration of the catalyst design cycle, and tight integration of TEA throughout the portfolio. Additionally, the review panel recognized the program's continued efforts in addressing previous recommendations to focus on technologies that fractionate biomass to maximally leverage each component towards higher-value fuels and coproducts, as well as leveraging strengths from consortium and industrial partners in moving technologies towards commercialization. BETO intends to continue to support industry partners by leveraging national lab capabilities through the various consortium national laboratory-led projects, DFAs, and competitive funding opportunities.

The review panel specifically noted the appearance of fewer projects focusing on organic compounds functionalized by one or more heteroatoms (oxygen, nitrogen, etc.) as an area that could benefit from more emphasis within the portfolio. While the majority of projects reviewed within this session are focused on hydrocarbon production, the Performance Advantaged Bioproducts Consortium is in its second year of activities and has the stated mission of exploiting biomass properties for higher-value chemicals that could support near-term commercialization efforts. Similarly, the Advanced Development and Optimization Program has begun an early effort to address the transition from lab-scale catalyst formulations (powdered catalysts, colloidal nanoparticles, etc.) to extrudates and pellets that are commonly used at larger scales. Both of these areas were reviewed in different sessions of this peer review due to time constraints. These efforts will continue to be supported by BETO and results will be tightly integrated through TEA activities and guided R&D.

The review panel noted that continued R&D associated with "low-grade" pyrolysis oil upgrading and the reliance on hydrotreating, hydrodeoxygenation, and hydrogenation (and the associated high hydrogen demand) do not appear as impactful as coproduct and lignin valorization efforts (and associated separations impacts) on overall TEA outcomes. Specifically, they noted that it was unclear that continued research into catalyst and reactor designs for pyrolysis oil upgrading is improving the process sufficiently to enable commercialization. BETO is currently focused on higher-quality bio-oils and will continue to leverage TEA activities to target the most impactful areas for future R&D. For example, in pursuit of the larger goal of achieving a \$3/GGE cost target by 2022, the Catalytic Fast Pyrolysis project will evaluate impacts of lower-cost feedstocks, extending catalyst time on stream, maximizing carbon yield to the oil phase, and capturing and purifying individual components from the light oxygenate stream to generate coproducts, as well as evaluating the potential to couple remaining light oxygenates to increase octane/cetane ratings of fuel blendstocks generated from hydrotreating of the CFP oil. While focus on future catalyst development has already been deemphasized within this project, critical tradeoffs remain between multiple variables within these complex systems, where iterative catalyst development may be required. BETO recognizes the limitations of pyrolysis oil upgrading but remains committed to the thermochemical pathways that can deliver high yields to both fuels and products.

The review panel noted the critical importance that assessment and mitigation of catalyst deactivation play within each individual project reliant on catalytic chemistries, and that each project appears well aware of these factors. The review panel questioned the ability of the standalone Catalyst Deactivation project to provide sufficient support to an entire portfolio at modest funding levels. BETO recognizes that all projects involving catalytic research must include deactivation and mitigation components that are tailored to the individual technologies and will continue to require milestones that target these areas. BETO's support of this new project was intended to develop a broader framework of tools and capabilities that could support new technology approaches that use similar catalyst systems, as well as produce more general publicly available tools and publications to assist researchers who work with biomass but do not use the catalyst systems currently funded by BETO. Initial focus for the project will be on a small suite of catalysts and pathways to determine if similar deactivation research can be applied to alternate approaches.

The review panel noted the potential impact of catalyst development efforts but questioned the specific challenges the ACSC intends to address with MOFs. BETO recognizes the lack of a clear pathway to overcome specific commercial challenges associated with MOFs at this time. While not emphasized in the review presentation, this specific activity was funded as a seed project and will be retired in FY 2020.

The following sections specifically address the three top recommendations from the review panel:

## Recommendation 1: Expansion of the Thermochemical Platform Analysis project as an enabling technology within ChemCatBio.

The review panel recognizes BETO's commitment to using TEA to guide future R&D, but it was noted that the reliance on coproducts and associated details were not well presented and raised questions about assumptions related to markets, pricing, and impacts of required scale-up efforts. The panel suggests a more "level playing field," where a standalone process without coproducts is evaluated through TEA with separate assessments for scale and coproducts, especially where a technology approach is intended to compete with an analogous commercial process.

BETO agrees that better communication of TEA assumptions and results, specifically separate consideration of the relative impact of coproducts, would provide a more transparent assessment of a particular technology. For all new-starts, an initial TEA is already required to demonstrate proof of concept, compare various process assumptions (e.g., inclusion of coproducts vs. standalone), and assess near-term research objectives. Additionally, TEA activities are included as specific tasks/goals within every technology project. The Thermochemical Platform Analysis project is funded based on joint milestones within those projects and BETO will continue to support TEA activities in all phases of research within the portfolio. BETO will discuss and consider ways to "level the playing field" through more uniform presentation of TEA assumptions and coproduct integration for future peer reviews.

#### Recommendation 2: Expanded support of the ChemCatBio Data Hub.

BETO agrees that the ChemCatBio Data Hub project will play an important role in accelerating the catalyst design cycle, especially as data science continues to evolve. The Data Hub project is in its first year of activities and began with the expectation that efforts could expand with demonstrated results. The development of additional tools, such as the Catalyst Design Engine (that can leverage materials R&D data), represents excellent stretch goals for the near term and will be considered in future strategy development. BETO has also committed additional resources to more high-performance computing power in future fiscal years and anticipates that projects like the ChemCatBio Data Hub will greatly benefit from increased access to these resources.

#### Recommendation 3: Focus on higher-value products.

BETO appreciates this recommendation and recognizes the potential for higher-value products to overcome barriers to commercialization. The Biochemical Conversion technology area (including lignin valorization), Performance Advantaged Bioproducts, and Bioprocessing Separations Consortia have specific goals targeting the identification and synthesis of high-value products, and these efforts are expected to continue. Each of these areas had separate peer-review sessions, and while some crosscutting efforts (Biochemical Platform Analysis project and  $CO_2$  Utilization: Thermo- and Electro-Catalytic Routes to Fuels and Chemicals) were presented in the Catalytic Upgrading session, BETO will consider additional means to communicate those impacts at future reviews.

## THERMOCHEMICAL PLATFORM ANALYSIS

#### National Renewable Energy Laboratory

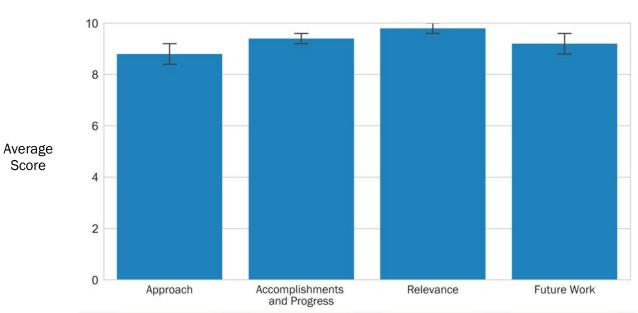
#### PROJECT DESCRIPTION

The objective of this project is to inform and guide R&D priorities for thermal and catalytic conversion processes by providing process design and TEA. This is achieved through close collaboration with researchers and external experts, along with the use of both commercially available modeling tools and the development or use of partnerdeveloped and domain-specific tools and resources, such as refinery integration, kinetic and reactor models, phase equilibrium models, and pertinent bioproduct market studies.

This project is directly aligned with BETO goals—this includes the reduction of projected conversion costs for biomass-derived fuels and products by enabling research

| WBS:                      | 2.1.0.302           |
|---------------------------|---------------------|
| CID:                      | NL0008191           |
| Principal Investigator:   | Dr. Abhijit Dutta   |
| Period of<br>Performance: | 10/1/2016-10/1/2019 |
| Total DOE Funding:        | \$5,250,000         |
| DOE Funding FY16:         | \$1,900,000         |
| DOE Funding FY17:         | \$1,950,000         |
| DOE Funding FY18:         | \$700,000           |
| DOE Funding FY19:         | \$700,000           |
| Project Status:           | Ongoing             |
|                           |                     |

advancements. TEA-guided research has helped achieve significant modeled cost reductions for the *ex situ* CFP pathway since the previous 2017 Peer Review and we have identified specific research steps to help reduce the modeled MFSP to less than \$3/GGE by 2022. Further cost reduction through refinery integration, development of valuable coproducts, and other options are being identified for future research to help reduce the modeled MFSP to \$2.50/GGE by 2030. Additional priorities anticipated in the future, such as the use of renewable electricity for liquid fuels and products, as well as emphasis on waste utilization, are also being explored in conjunction with research on catalytic utilization of syngas and other gases. Industry-relevant

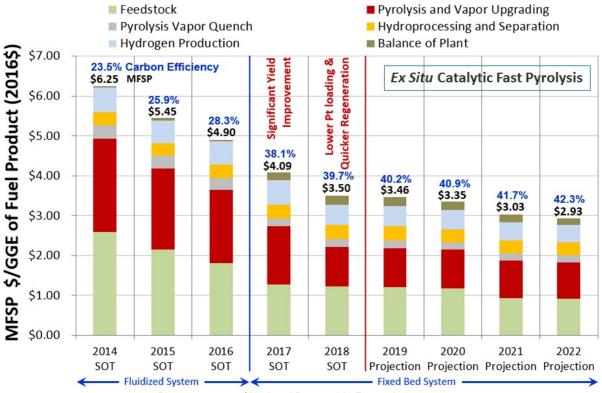


#### Weighted Project Score: 9.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

parameters are given deliberate attention as part of the work done under this project to help answer questions important for future commercialization.





#### OVERALL IMPRESSIONS

- This is a very critical component to the activities of ChemCatBio as a whole. Milestones were met throughout the prior funding periods and the near- and long-term milestone planning seems appropriate.
- Overall, this is a very important enabling technology for emerging biomass-processing technologies. My only concern based on past exposure to TEA is that they are based on a large number of assumptions and often may invoke the most optimistic case rather than most likely cases. The team may want to consider that attainable yields, selectivities, and rates are probably uncertain and should forecast that impact (e.g., Monte Carlo-based TEA to consider uncertainty).
- Overall, this is a strong, well-managed project with solid deliverables thus far. The TEA work is probably the most impactful work to BETO because of its influence on R&D direction. It is extremely important to get this right. I would encourage the project team not to settle on the current tools and continue to explore ways of enhancing the modeling capability that allows multiple scales to be incorporated into the analysis. Please continue to harmonize this work with the Biochemical Platform Analysis project. The less-severe conditions and shape-selective catalyst pivot away from methanol-togasoline is small and the premise is still the same: small alcohol conversion over modified zeolites. This is a winning formula.
- The thermochemical conversion team has produced significant advances over the past two years and now appears to be on target to meet BETO cost and sustainability objectives. The new process scheme and catalysts have performed as predicted. The next steps would be to address operability issues that have plagued other efforts. A detailed feasibility study by an independent outside group would confirm these results. The project shows great synergy with other groups such as Idaho National Laboratory (INL),

Argonne National Laboratory (ANL), National Institute of Standards and Technology, and others. The outputs included technical metrics, life cycle assessment (LCA), MFSP, reports, and journal articles. The TEA shows a path for biomass to fuel of less than \$2.50/GGE, however, it should be noted that this is a comparative number valid for comparing DOE projects. The initial costs of the fuel produced by early plants is likely to be significantly higher. The progress made by this project is impressive; the thermochemical conversion team addressed many of the comments from the 2017 Peer Review and has found new catalysts and other improvements that greatly improve the likelihood of success.

- The TEA and LCA specialty of this work has an application to all BETO processes. One wonders if the CCPC can subsume its modeling efforts on the sunset of the project. This superb work must be continued not only for the CFP platform, but across ChemCatBio projects.
- This is a central effort supporting the technical programs within the consortium. TEA has proved to be a powerful resource to guide research and is undoubtedly a key asset that should continue throughout the years. LCA provided by the collaboration with ANL is also a key portion of this effort and should continue, as it seems to work well. It is important that they keep up with the emerging technologies as described by their presentation. The feedback loop between this effort and the technical efforts are an important approach, and examples presented show the value of TEA providing alternative R&D pathways. CFP timeline and accomplishments presented are impressive examples of how well this effort interacts and is synergistic with the technical projects.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the feedback.
- The projections for future research, presented in design reports, are based on researchers' and reviewers' feedback about attainable performance goals. We include sensitivity analysis to show the impacts of various parameters and the effects of overperformance and underperformance compared to the baseline analysis. The state-of-technology assessments are based on experimental data, but at smaller scales compared to the conceptual designs. We thank the reviewer for the comment and will continue to emphasize and expand on areas where we need to assess uncertainty (Monte Carlo analysis may be helpful at times but may not always help develop additional insights as compared to single-point sensitivities).
- We work with the CCPC, which does multiscale modeling. We will continue to pay attention to their work and include any tools that are useful for TEA into our work. An example of such a collaboration is the development of a one-dimensional entrained reactor model compatible with the TEA modeling framework. We will continue to harmonize with the Biochemical Platform Analysis project; please note that we use the same set of assumptions and modeling frameworks as the work done under that project, and our tools and methods have the same genesis.
- We appreciate the comments and agree with the reviewer about operability issues, which we plan to address through pilot-scale tests. Although higher costs and problems associated with pioneer plants are not explicitly mentioned, we are working closely with other groups, including the Feedstock-Conversion Interface Consortium, to understand and address those uncertainties.
- We will continue to work with the CCPC to find synergy between that work and the TEA modeling under this project.
- We will continue to address emerging technologies under the broad scope of the analysis of catalytic conversion under this project.

# THF COSOLVENT FRACTIONATION TO FUEL PRECURSORS (FURFURAL, LEVULINIC ACID, 5-HMF)

#### University of California, Riverside

#### **PROJECT DESCRIPTION**

The goal of this research project is to advance transformative cosolvent-enhanced lignocellulosic fractionation (CELF) to first achieve high yields of fuel precursors (FPs) such as furfural (FF), 5hydroxymethylfurfural (5-HMF), and levulinic acid (LA) from hardwood poplar biomass, and to further convert the FPs to fungible fuel blendstocks (methylated furans).

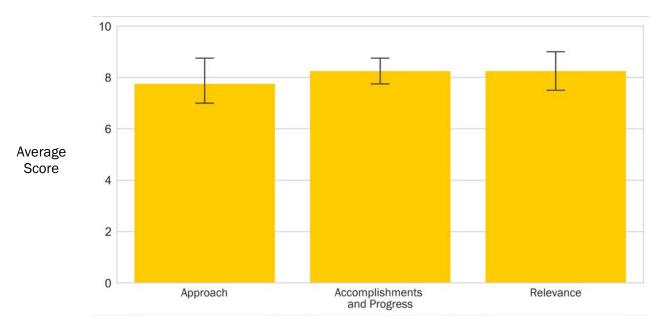
Concurrently, we aim to capitalize on CELF's extremely

| WBS:                      | 2.2.4.400           |
|---------------------------|---------------------|
| CID:                      | EE0007006           |
| Principal Investigator:   | Dr. Charles Wyman   |
| Period of<br>Performance: | 10/1/2015-9/30/2018 |
| Total DOE Funding:        | \$1,060,000         |
| Project Status:           | Sunsetting          |
|                           |                     |

high lignin extraction to produce aromatic platform chemicals to increase process revenues. TEA analysis will inform process design to reduce fuel costs.

#### Weighted Project Score: 8.1

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- This project focused on developing a simple, intensified process for biomass deconstruction and upgrading into methylfuran and dimethylfuran, as well as converting lignin into high alkanes that might blend into jet fuel. Achieving <\$2/GGE for conversion of biomass into fuels is impressive.
- This was a nice, tight project with well-defined objectives and division of labor. It appears that all but the fourth task was ably completed. The reviewer does not know, despite the fine success of the first three tasks, if the process met the goal of <\$3/GGE.
- The THF cosolvent to fuel precursors was a hard project to review. On face value, it describes an integrated process to produce low-cost fuels. However, it is difficult to follow the TEA analysis, which is critical for evaluating the process. The MFSP was calculated to \$1.50/GGE, which would exceed the BETO target. An independent evaluation by the DOE TEA team would provide a more systematic approach. Typically, solvent and chemical cost of multistep processes like the CELF process have been found to produce products with higher costs than other approaches. Organic solvent extraction processes have been shown to work technically but have not been commercialized due to the complexity and requirements of multiple conversion and recovery steps. The products obtained, particular LA, may themselves have value as products, if the costs are lower than the current approaches. The PI reported commercial interest by at least four companies. If this is confirmed, the project can be viewed as a success.
- The project is divided in four sequential tasks that are clearly complementary, and the group has made significant progress with their process. In general, it is well outlined; however, the presentation could have benefited from a greater focus on addressing the use of THF as the solvent in the process while also providing more details regarding the economic analyses.
- The value of the project is clear for the BETO mission, as the aim is to develop a new process that is also evaluated economically to convert lignin fractions. Patents and a license have resulted from this project. TEA using the BETO-derived tool is a plus.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

## OVERVIEW OF CHEMICAL CATALYSIS FOR BIOENERGY CONSORTIUM

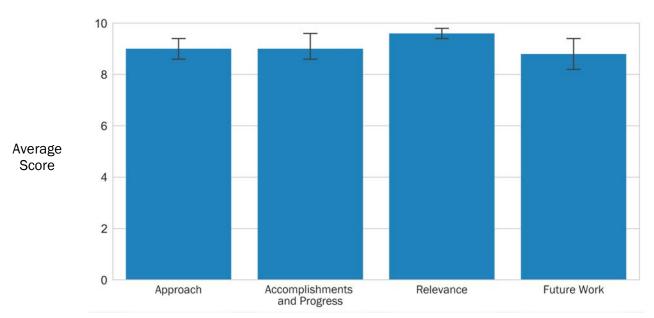
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

Catalysis plays a central role in converting biomass and carbon-rich waste feedstocks into fuels and chemicals; however, critical catalysis challenges exist that are limiting commercialization of emerging bioenergy technologies. By leveraging unique DOE national laboratory capabilities and expertise, the Chemical Catalysis for Bioenergy Consortium (ChemCatBio) seeks to overcome these catalysis challenges and accelerate the catalyst and process-development cycle. The foundation of the consortium consists of an integrated and collaborative portfolio of catalytic and enabling technologies, which positions ChemCatBio to address both technology-specific and overarching catalysis challenges across the development cycle from discovery to scale-up. The core

| WBS:                      | 2.3.1.100a          |
|---------------------------|---------------------|
| CID:                      | NL0024509a          |
| Principal Investigator:   | Dr. Josh Schaidle   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$300,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$150,000           |
| DOE Funding FY19:         | \$150,000           |
| Project Status:           | Ongoing             |
|                           |                     |

catalysis projects target technological advancements for specific conversion processes, such as catalytic upgrading of biochemical process intermediates, CFP, indirect liquefaction, and CO<sub>2</sub> upgrading, while the enabling technologies provide access to world-class capabilities and expertise in computational modeling, materials synthesis, advanced *in situ* and *in operando* catalyst characterization, and catalyst design tools.



#### Weighted Project Score: 9.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores



Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- This presentation provides proper context for the ChemCatBio consortium as a whole. The structure, overall objectives, and future directions provide an excellent framework for the collective and provides the ability for interfacing between labs and researchers in the basic science, applied, and industrial areas. Opportunities to better demonstrate the ChemCatBio synergy and expand the impact of the center to university settings should be considered.
- This is an overview of the ChemCatBio consortium, and it provides a snapshot of outcomes in individual research thrusts. Overall, this is a nice consortium that was established with direct guidance from industrial partners. It broadly unites DOE labs, academic partners, and industrial partners, and it has a pretty impressive footprint with respect to the breadth of research. I think the heavy reliance on TEA for guidance is a strength; however, when assessing an individual technology, it would be beneficial to me to see less focus on leveraging coproducts to achieve DOE cost targets and more focus on how the specific research on a given conversion chemistry is impacting the bottom line. It would also be informative to have a more detailed consideration of carbon economy, as it was unclear in certain technologies like BDO synthesis.
- ChemCatBio was launched in 2017 after following up on the BETO 2015 Peer Review feedback similar to these comments on the need to "establish an experimental catalysis consortium." The consortium should be proud of themselves and deserve to be congratulated for conceiving such a multi-lab collaboration, successfully launching it, and now reaping tangible deliverables as a result. This is a highly intelligent, productive, and capable consortium for the bioenergy community. The leadership is strong, and the members are talented. I strongly recommend continued funding, and everyone involved in 2015 reviews that helped make the feedback clear to BETO should celebrate this achievement. ChemCatBio is an incredible BETO success story and should be celebrated. A sophisticated level of teamwork and technical collaboration was demonstrated here that should be highlighted at the DOE level. It is impressive how the stakeholder feedback was actually used along with other programmatic drivers at the DOE level to inspire the formation of ChemCatBio. The same model can be used for data, separations, engines, infrastructure, etc. It takes organizations of people to do this properly and sometimes making the right partnerships is more important than the early technical achievements. The catalyst design engine coming out of the computational group will be a major deal, especially when the proper back casting is incorporated into the analysis.
- The ChemCatBio consortium is a successful cross-government lab project. The consortium works on problems that are of critical importance. For example, the CFP change in catalyst, coupled with process design facilitated by changes, are making it conceivable to obtain less than \$3/GGE in the near future. The consortium can access a vast amount of expertise and equipment acquired by the national labs and allows them to focus on these critical challenges across sites. Involvement of commercial groups provides an outlet for commercialization. The presentation cites that catalyst costs are 10% of the

production costs of biofuels. This number understates the impact of catalysts, which also are major determinants of yields, product selectivity, required feedstock properties, and overall throughput and operational times. The projects use realistic feeds and are TEA driven. They have kept the project overhead low while coordinating the projects between sites with regular meetings. The project has successfully incorporated industry input by involving an industrial advisory board. While the TEAs reported are internally consistent, they can give an impression the product costs are lower than they would be for initial projects. In part, this may be due to overstating the estimated operational time, which is not included in the TEA. Also, the TEAs and catalyst cost models do not include a projection of potential market changes due to increase supply of product versus demand and possible effect of increased metal use versus the global supply.

- In this age of shale oil, gas, and global warming, it is a delight to see such a comprehensive and deep research consortium as ChemCatBio. I can't imagine another consortium in the world that is working as hard and effectively on bio-based fuels and chemicals. I certainly don't know of one. This stokes my pride at being an American researcher involved in this effort. Decades of management experience at DOE must explain how the whole thing can operate so effectively. Virtually every project sets difficult goals and has made substantive progress. What's working: good structure of the ChemCatBio consortium, an effective matrix of catalytic technologies, enabling capabilities, and industry partnerships underpinned by cross-cutting support. What's not working: TEA may not be utilized to a sufficiently broad extent.
- The goal of this project is to overcome catalysis challenges for the conversion of biomass and waste resources into fuels, chemicals, and materials by leveraging unique DOE national laboratory capabilities. It is a collaborative, lab-led project. It also aims to facilitate industry access to national laboratory capabilities and expertise. The overview is clear and carries a large umbrella. The overarching goal is highly meritorious as it tries to tackle an important and emergent technology of high-energy impact. The effort is impressive and well coordinated with a solid management plan. Cross-cutting support is adequate to help with management and coordination of such a big effort. Cross communication among the different projects is highly encouraged and a formal mechanism to improve, encourage, and measure collaboration among the groups should be pursued. The work involves realistic bioprocess streams but there is no indication of coordination with groups involved with the R&D of feedstocks, which would also be beneficial. It is good to see the industrial partners utilizing unique national laboratory capabilities and the new research directions that can result from these new partnerships. Evidence of high demand for industrial partnerships is another relevance of the impact and relevance of the work. The reviewer only wonders if some of these industrial partnerships/projects could be done as effectively with the utilization of Small Business Innovation Research program resources. ChemCatBio should continue to look for opportunities to demonstrate the consortium's synergy and strategic alliances with university researchers who can augment the existing strengths and capabilities of the consortium.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We would like to express our appreciation to the reviewers for their thoughtful analysis and constructive feedback. Moving forward, we will continue to build upon the collaborative foundation of the consortium and our early-stage technical successes by (1) maintaining our responsiveness to stakeholder feedback; (2) emphasizing carbon utilization as a key metric for all catalytic conversion technologies; (3) strengthening existing partnerships and developing new partnerships, especially with universities; and (4) developing tools that broadly enable the research community to accelerate the catalyst and process-development cycle for bioenergy technologies.

## CATALYTIC UPGRADING OF BIOCHEMICAL INTERMEDIATES

#### National Renewable Energy Laboratory

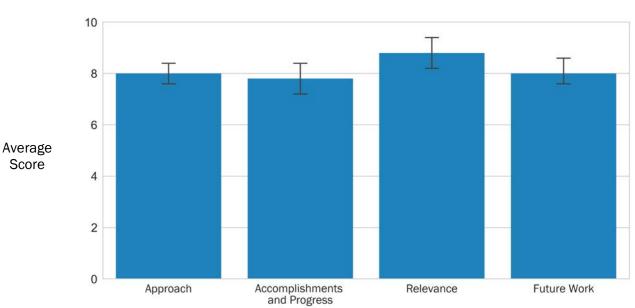
#### **PROJECT DESCRIPTION**

The CUBI project is a multi-lab effort within ChemCatBio that is specifically focused on catalytic upgrading of sugarrelated intermediates from biochemical deconstruction and/or biologically derived (i.e., fermentation) intermediates to hydrocarbon fuels. As several companies are developing catalytic upgrading routes from clean sugars, this project will help facilitate a transition to catalytic upgrading of such intermediates by providing a quantitative performance and economic assessment of several catalytic-upgrading approaches using biochemical deconstruction fermentation intermediates. While there are strong reasons for use of biochemical conversionappropriate feedstocks and deconstruction methods,

| WBS:                      | 2.3.1.101           |
|---------------------------|---------------------|
| CID:                      | NL0026681           |
| Principal Investigator:   | Dr. Richard Elander |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$5,410,593         |
| DOE Funding FY16:         | \$1,200,000         |
| DOE Funding FY17:         | \$1,381,000         |
| DOE Funding FY18:         | \$1,529,593         |
| DOE Funding FY19:         | \$1,300,000         |
| Project Status:           | Ongoing             |
|                           |                     |

numerous challenges exist, including integration of biochemical upstream and catalytic downstream operations; understanding inhibitory impacts on upstream and downstream operations; developing specifications for biochemically derived feed streams to catalytic processes; and quantifying impacts of such feed streams on catalyst durability, lifetime, efficiency, and selectivity.

Specific catalytic upgrading routes are being investigated within the CUBI project, including: (1) catalytic upgrading of fermentation-derived 2,3-BDO; (2) catalytic upgrading of fermentation-derived carboxylic acids; and (3) catalytic upgrading of lignocellulosic sugar-derived sugars and associated intermediates, including



#### Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

furfural and 5-HMF. These routes represent key technology pathways being investigated within BETO's biochemical conversion portfolio. The CUBI project is closely linked to numerous projects within that portfolio, most of which are being reviewed in the "Biochemical Conversion" session of the 2019 Peer Review. Additionally, as one of the core catalytic technology projects within ChemCatBio, the CUBI project interacts with ChemCatBio-enabling projects by utilizing analysis, characterization, modeling, and economic tools to develop improved catalysts and understand reaction and inhibition mechanisms associated with these specific catalytic-upgrading routes.

Driven by the findings from a mid-project go-no-go milestone that identified key areas for R&D focus in order to achieve commercial-scale economic viability (defined as the ability to achieve an MFSP of  $\leq$ \$3/GGE), key technical approaches for each process route being investigated within the CUBI project are briefly summarized below. Yield and selectivity data for each route have been generated, along with a fuel property characterization for generated samples.

**Catalytic Upgrading of 2,3-BDO:** Catalytic upgrading approaches via (1) Cu-zeolite core-shell catalysis to C3+ mixed olefins (primarily butenes), followed by oligomerization and hydrogenation; (2)  $ZnZrO_x$  catalysts for olefins production via methyl ethyl ketone (MEK) condensation and decomposition; (3)  $In_2O_3$  catalysis to methyl vinyl carbinol (MVC) and acid catalysis to butadiene; and (4) single-step conversion to butadiene using CsH<sub>2</sub>PO<sub>4</sub> SiO<sub>2</sub> catalysts.

**Catalytic Upgrading of Carboxylic Acids:** Mixed (C2–C4) and single (C4) conversion of fermentationderived carboxylic acids via ketonization, condensation, and hydrodeoxygenation (HDO) to generate branched fuel-range hydrocarbons.

**Catalytic Upgrading of Sugars and Derived Intermediates:** Aldol condensation of furfural and HMF from mixed C5–C6 sugars followed by HDO to produce C14–C16 hydrocarbons. Additionally, HDO optimization in continuous-flow systems (for this route and other routes involving HDO reactions) is being developed.

Upon the completion of this project, the main outcome will be to quantify the catalytic upgrading performance of these routes using biochemical process-derived intermediates (including an inhibition mechanism assessment) in a fully integrated TEA model, with the identification of further R&D needed to achieve a modeled commercial-scale MFSP of  $\leq$  3/GGE.

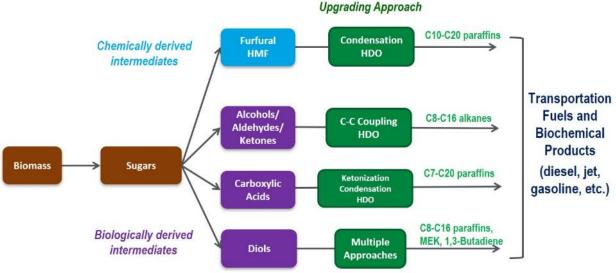


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project successfully assembles a range of projects and integrates them in a very logical way. The structure provides for a cohesive effort. Significant progress appears to have occurred across tasks, and future work has clear metrics established across the portfolio. The relevance to BETO and potential for this technology is clear.
- This program has been very productive, with several routes being identified and promising catalystupgrading results achieved by the team. The comments involving lignin valorization requirements to reach a \$4-\$5/GGE offset cost were honest and revealed how challenging "pathway work" can be. Overall, CUBI has been a solid, successful program taking information from TEA, creating highly organized tasks, operating cross-functionally, taking advantage of resources from several laboratories, focusing on using BETO-derived feedstocks and not model compounds, innovating new catalysts (e.g., Zr, Zn, In) with promising performance, and sound and practical organic chemistry.
- Catalytic upgrading of biochemical intermediates derived from sugars is aligned with BETO's goal of producing lower-cost biofuels with dependency on success of the lignin valorization project. The chemical conversion route provides an alternative to fermentation that has the potential to produce hydrocarbons directly, as compared with other routes that are focused on ethanol as the main cellulose conversion product. Comparison of the competing routes for the catalytic upgrading of biochemical intermediates will provide useful guidance to developers in the future. The project is guided by TEA and looks at several alternative routes that maximize the chances of success. However, the initial MFSP and relative importance of the lignin conversion process are not quantified. The team should consider switching the goal to producing value-added chemicals in place of fuels; as long as these products replace fossil fuel-derived products they will contribute to greenhouse gas (GHG) reduction and increase the cost effectiveness of the process.
- This project summarizes a broad effort in moving a family of technologies for fuel and coproduct production toward commercial development and is driven by TEA-informed decisions that steer the work toward dollar-per-GGE targets. The suite of technologies seems very appropriate to the types of feedstocks available. While TEA is helpful for assessing progress toward dollar-per-GGE targets, the impact of specific catalytic technologies may be somewhat obscured. Such heavy reliance on coproducts may be of concern: it isn't clear if the technologies have been demonstrated yet, and it isn't clear if, for example, lignin coproduct markets are commensurate in size with fuel markets. It would be helpful to make the case for producing fuels plus coproducts, versus fuels alone, versus coproducts alone.
- This is a quintessential ChemCatBio project, taking in biochemically derived intermediates and further converting them with chemical catalysis, all under the watchful eyes of the TEA team. The bar appears to be set high in all the tasks and the overall impact of the project will be commensurately high at sunset later this year. What's not working: while TEA has been used to indicate that each of the main four pathways has potential to reach the goal of <\$3/GGE, the actual current value of the dollar-per-GGE has not been presented. This would provide valuable information.
- This is a large effort involving many labs and four different tasks around a very important topic and many different processes. It is very comprehensive work involving many skills and resources, and one of the backbones of the consortium. It would be beneficial to have a clear definition of the range of products that are being targeted and the state of the art in many of these processes. Routes are being evaluated with comprehensive TEA. It is necessary to relate costs not only to catalyst performance but also to other factors, such as solvent selection and downstream separation process. The relevance to BETO and potential for technology development is clear.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the comment on producing value-added chemicals to enable biofuels production. We are aware of the market volume challenges for specific coproducts. Envisioning the future bioeconomy, there will many coproducts via sugars, along with fuel production. The initial MFSP and importance of the lignin conversion process has been determined and presented in the biochemical conversion session presentations. We will also include more TEA scenarios, including fuels only, coproducts only, more than one coproduct, etc. For 2,3-BDO upgrading, we envision a flexible process where 2,3-BDO could be converted to either fuels and/or value-added chemicals (e.g., 1-butanol, isobutanol).
- The TEA was conducted within the first six months of effort for some upgrading pathways. Significant progress has been made by each catalytic-upgrading route within the last 18 months and the TEA will be updated in Q4 FY 2019 and will further inform opportunities for cost reduction.
- We thank the reviewers for their positive comments. We appreciate concerns regarding the cost dependency on the production of lignin-derived coproducts and will show the cost of producing the sugar-derived products with and without lignin valorization.

## **ONE-STEP, HIGH-YIELD PRODUCTION OF FUNGIBLE GASOLINE,** DIESEL, AND JET FUEL BLENDSTOCKS FROM ETHANOL WITHOUT ADDED HYDROGEN

#### Vertimass LLC

#### **PROJECT DESCRIPTION**

Most fuel ethanol is currently produced from starch in the United States and cane sugar in Brazil, and new technologies are emerging for production of ethanol from cellulosic biomass such as wood, grasses, and agricultural and forestry residues. However, U.S. ethanol is used primarily as 10% blends with gasoline, and current U.S. ethanol production has virtually saturated that market. The resulting "blend wall" and limited infrastructure to supply

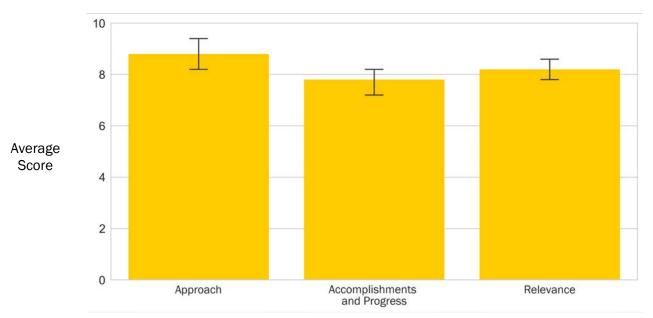
| WBS:                      | 2.3.1.201           |
|---------------------------|---------------------|
| CID:                      | EE0006875           |
| Principal Investigator:   | Dr. John Hannon     |
| Period of<br>Performance: | 7/15/2015-5/31/2019 |
| Total DOE Funding:        | \$1,650,000         |
| Project Status:           | Sunsetting          |
|                           |                     |

or use higher ethanol levels inhibit expansion of bioethanol production.

Vertimass LLC-through an exclusive license from Oak Ridge National Laboratory (ORNL)-seeks to commercialize novel catalyst technology to convert ethanol into gasoline blendstocks compatible with the current transportation fuel infrastructure and higher-value chemical coproducts, such as benzene, toluene, ethylbenzene, and xylene (BTEX), that provide valuable offsets, especially in low-oil environments. The gasoline blendstocks produced are anticipated to still fall under the Renewable Fuel Standard at the same level as feedstock ethanol. This catalytic process benefits from (1) production of minimal amounts of light components, (2) relatively mild temperatures and pressures, (3) ability to process 5% to 100% inlet ethanol



Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

concentrations, (4) product flexibility to respond to changing market demands, and (5) no need to add hydrogen.

In this project, Vertimass has taken major steps in advancing this technology to date to include (1) scaling up the process 300 times; (2) maintaining 100% conversion yields of ethanol; (3) increasing liquid yield product distribution from 36% to 82%; (4) moving from powder to pelletized and now commercial catalyst formulations; (5) running ethanol feedstocks with no dilution; and (6) decreasing metal loadings while maintaining performance, resulting in less-expensive catalysts. These technology advances through this project have enabled the economic feasibility of a Vertimass bolt-on for industrial application.

Commercialization of this novel technology would overcome fungibility issues that limit ethanol use in gasoline for light-duty vehicles and partially contribute to mitigating climate change in offering more than 90% GHG reductions. Vertimass plans to partner with ethanol producers (with particular emphasis on emerging cellulosic ethanol plants) as rapidly as possible to overcome the blend wall and also allow the airlines to achieve Federal Aviation Administration targets of one billion gallons of renewable aviation fuel by 2018. This technology would expand opportunities to use more sustainable fuels in the United States. BETO funding will accelerate the scale-up of this technology to realize important goals of reduced GHGs, enhanced energy security, and domestic jobs.

#### OVERALL IMPRESSIONS

- This project has set up an effective commercialization pathway model for BETO to accelerate towards its targets while carrying out all the great, exciting fundamental research and elegant science and engineering activities required to discover the new pathways. In this parallel multiscale development model, pilot-scale campaigns may be led by an engineering, procurement, and construction (EPC) contractor and a catalyst original equipment manufacturer (OEM) using existing developmental catalyst materials with both surrogate and real feedstocks in ample supply while lab-scale catalyst development takes place. The catalyst OEM must be able to quickly modify and provide small batch extrudates based on informs from ChemCatBio and incorporate in the next pilot plant run campaigns. This model establishes the technology developmental pipeline from the atomic-scale modeling level with CCPC through the ACSC lab-scale synthesis and characterization activities to the commercial-scale process simulation level with the TEA team as oversight to the EPC operating the pilot plant and making iterations to the feedstock work. These types of accelerated commercialization projects should follow the general partnership model demonstrated in part here by Vertimass from inception and should include: catalyst optimization with ChemCatBio (e.g., ACSC, TEA, Co-Optimization of Fuels & Engines [Co-Optimal initiative), a proven EPC with close enough design experience and pilot-to-commercialization experience, a catalyst OEM, an inspection company, an additive company with access to engine dynamometers, and taxi fleets.
- At a high level, this project is impactful because it provides a value add for ethanol producers. Specifically, it can allow ethanol to be converted to higher hydrocarbons and BTEX, which could increase bio-carbon injection into the transportation sector and improve the overall economics of a cellulosic ethanol facility. In terms of a project report, details were sparse, and the presentation is relatively nonspecific, so it is difficult to assess technical merit. Many of the milestones seem arbitrary and it was not clear how this project is leveraging capabilities at the national laboratories.
- This is a targeted sunsetting project with relevance to BETO objectives. The scale-up continues to seem promising from a technical perspective, though the direction of the system is somewhat unclear (e.g., is increased BTEX fractions a key to make the process economically competitive?). The target of ethanol to hydrocarbons, aside from closing a potential loop of bioconversion to fuels, needed stronger argumentation for a cost-competitive implementation.

- This is a nice project on scaling up an active catalyst for ethanol conversion and appears successful so far in terms of product yield at larger scale. The only thing missing is the TEA needed to allay doubts that starting with a relatively expensive feedstock like ethanol can still meet the <\$3/GGE target of DOE.
- Vertimass production of BTEX from ethanol is an example of a successful DOE-sponsored project. A viable commercial process resulted from initial work at a government lab that was licensed to a startup. The startup leveraged their work with a partnership with a catalyst manufacturer and engineering construction firm. They are working to provide an additional outlet for renewable ethanol production that is a value-added product that has no blending limit.
- The goal is to produce liquid hydrocarbons from ethanol using the catalyst licensed from ORNL. Their interest was to increase yield and scale up the process. The scale-up continues to seem promising from a technical perspective, though the impact of the coproduct on viability is somewhat unclear (i.e., is increased BTEX fractions key to making the process economically competitive or could this be an issue given the scale of a fuel-producing process?). Utilizing a technology developed at a national laboratory is of particular value. The advantages of the technology were mild conditions and one-step conversion. Management is clear and involves another two companies besides ORNL. The technology is relevant to the BETO mission. It is not clear how the knowledge acquired during this project could be transferred back to the lab and researchers involved within the consortium.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for this positive feedback. Vertimass chose to work with those with solid capabilities in the fields relevant to the project to avoid delays for purchasing and setting up equipment and analytical support, training of personnel, and startup of systems. Vertimass also greatly benefited from the expertise of these partners in terms of solving problems (e.g., substantially increasing yields from those realized at ORNL), transitioning to commercially relevant conditions (e.g., use of catalyst extrudates instead of powder), and providing a platform for rapid commercialization (e.g., ability to scale up to commercial operations from laboratory pilot/demo operations).
- Vertimass is working with the national laboratories for smaller-scale isotherm reactions that assist in directing pilot runs at pilot scale at TechnipFMC. Vertimass is also leveraging the catalyst characterization tools at national laboratories to examine the catalyst in its various states (e.g., fresh, run and regenerated, run and not regenerated, spent catalyst). Some details of the process and progress could not be presented at this time to protect potential patent applications.
- Utilizing the Vertimass bolt-on to make hydrocarbons from ethanol depends on the ethanol, gasoline, BTEX, and renewable identification number pricing. These prices are in constant motion though windows of opportunity, open where the ethanol produced can realize significant margin increases by using the Vertimass technology. In general, BTEX commands a premium as a chemical over fuels, so it is generally economically advantageous.
- Our TEA was presented and we displayed the detailed conversion cost transition from the start of the project (\$1.10/gal ethanol), intermediate validation (\$0.28/gal ethanol), current technology (\$0.14/gal ethanol), and our target of \$0.10/gal ethanol.
- Thank you for this positive feedback. We feel we are well positioned working with an engineering construction firm and a commercial catalyst manufacturer.
- Historically, BTEX has commanded a 40%–60% premium over fuel products, so it is generally economically advantageous.

## CATALYTIC PROCESSES FOR PRODUCTION OF ALPHA-OMEGA-DIOLS FROM LIGNOCELLULOSIC BIOMASS

#### **University of Wisconsin**

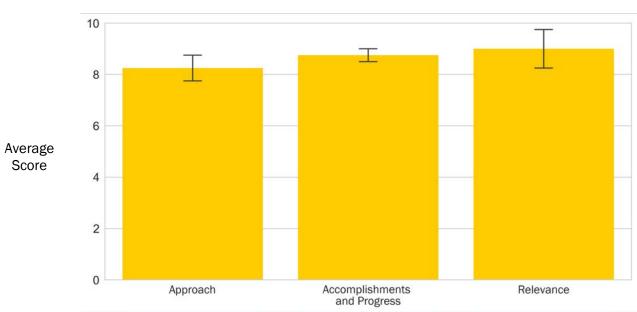
#### **PROJECT DESCRIPTION**

In this project, we have demonstrated and developed a multistep catalytic process for production of 1,5pentanediol (PDO) and 1,6-hexanediol starting from white birch. First, lignocellulosic biomass was converted into cellulose, furfural, and solid lignin via the TriVersa Process<sup>™</sup> developed by Glucan Biorenewables, LLC (GlucanBio). GlucanBio fractionated biomass into a solid high-purity stream of cellulose (90% purity and 90%)

| WBS:                      | 2.3.1.204         |
|---------------------------|-------------------|
| CID:                      | EE0006878         |
| Principal Investigator:   | Dr. George Huber  |
| Period of<br>Performance: | 2/1/2015-6/1/2018 |
| Total DOE Funding:        | \$3,004,132       |
| Project Status:           | Sunsetting        |
|                           |                   |

recovery) and a concentrated liquid phase of solubilized hemicellulose (90% of hemicellulose solubilized). The hemicellulose was then converted into furfural (85% yield) without any purification step. Furfural was converted into 1,5-PDO by four catalytic steps: (1) furfural was hydrogenated into tetrahydrofurfuryl alcohol (THFA), (2) THFA was dehydrated to dihydropyran (DHP), (3) DHP was hydrated to 2-

hydroxytetrahydropyran (2-HY-THP) and 2-HY-THP dimers, and (4) 5-hydoxyvaleraldehyde (5-HY-Val) was hydrogenated into 1,5-PDO. This pathway will be referred to in this report as the dehydration, hydration, and hydrogenation (DHH) route. A total yield of more than 80% 1,5-PDO was achieved via this new DHH pathway, which surpasses the 50% 1,5-PDO yields over traditional noble catalysts.



#### Weighted Project Score: 8.7

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%

 $oldsymbol{\mathbb{I}}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- The goal of this project was to develop a catalytic process for converting woody biomass into 1,5-PDO and 1,6-hexanediol that makes economic sense. The diol market offers a multibillion-dollar product capture opportunity. The process design involves a number of units and synthesis steps, and the project team provided excellent thorough TEA analysis with transparent, believable capital expenditure hurdles on the order of several hundreds of millions of dollars for grassroots conceptual design estimates. The synthesis chemistry was elegant and provided numerous precursor opportunities for alternative routes and pathways. The project team was able to prove the synthesis route at the lab scale in flow reactors. The project team was able to spin off a company, Pyran LLC, to commercialize 1,5-PDO products produced from woody biomass. Mechanistic elucidation for interaction of diols within zeolitic frameworks and pore cavities was accomplished and coupled with computational and experimental agreement. Overall, this was an impressive project with sizeable market potential and its success reaching all of the key milestones.
- Production of α,ω-diols from lignocellulosic biomass project is a great example of what is required to
  prepare an early-stage commercialization proposal, including a thorough TEA. This TEA was done
  independently from the DOE and would need to be validated; however, it does indicate that the overall
  process is feasible. The estimated cost of the plant is \$770,000,000. This is a very large investment for a
  grassroots startup even if the return on investment is achieved. It will be difficult to raise this capital
  without a major development project and demonstration of the key steps at scale. It is difficult to believe
  that a process with a catalyst with 10% platinum loading would be viable. However, the PI realized this
  issue and made sure to focus on critical steps that could be independently developed to use high-value
  chemicals and an intermediate (dihydropyran) which could be used as a platform for preparing
  bioadvantaged chemicals. This point was made in the prior peer review and was recognized by the PI.
- The conversion of lignocellulosic intermediate chemicals into diols presents a nice connection of development of a new technology, intimate study of the reaction mechanisms and catalyst operation, and attempts to transition the processes to a higher TRL. The TEAs are encouraging for incorporation of the one-diol conversion into cellulosic ethanol production. While the background materials and approach were sparse, the milestones and other achievements, including both technology transfer and several publications, were well detailed and indicate a strongly operated project that has successfully met its objectives. The relatively large body of publications, plus patents and spinoffs, are evidence of new knowledge being generated and the relevancy of the work to the BETO mission.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

## LIQUID FUELS VIA UPGRADING OF INDIRECT LIQUEFACTION INTERMEDIATES

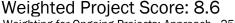
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

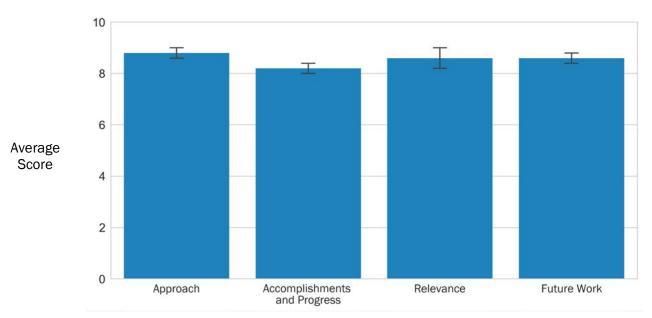
This project seeks to develop a responsive, integrated biorefinery concept based on IDL technologies that produces a suite of fuels and coproducts and provides control over the product distribution such that process operation can be adjusted to meet the shifting gasolinedistillate fuel market demand. Advanced upgrading technologies from syngas are critically needed for the successful commercial implementation of fuel production at a scale relevant for biomass. Research tasks within this project leverage light oxygenate intermediates from syngas and focus on the development of new catalytic pathways with lower-severity conditions to achieve high-carbon yields of gasoline, diesel, and jet fuel with integrated routes to coproducts that can improve overall economics.

| WBS:                      | 2.3.1.305           |
|---------------------------|---------------------|
| CID:                      | NL0013383           |
| Principal Investigator:   | Dr. Dan Ruddy       |
| Period of<br>Performance: | 10/1/2016-10/1/2019 |
| Total DOE Funding:        | \$11,550,000        |
| DOE Funding FY16:         | \$3,950,000         |
| DOE Funding FY17:         | \$3,200,000         |
| DOE Funding FY18:         | \$2,200,000         |
| DOE Funding FY19:         | \$2,200,000         |
| Project Status:           | Ongoing             |
|                           |                     |

Each pathway under investigation offers promise to generate high-quality fuels (e.g., high-octane gasoline with low aromatics, and desirable jet- and diesel-range hydrocarbons) and to achieve favorable cost targets by 2022. Finally, research progress is compared against the Mobil Olefin to Gasoline and Distillate (MOGD) process, which also offers control over the gasoline and distillate products, as an industrial benchmark. The new pathways seek to exceed the fuel product yields and reduce the cost of production versus the MOGD process. Recent catalyst and process development accomplishments are highlighted by improvements in carbon



Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${f I}$  One standard deviation of reviewers' scores

selectivity to fuels and catalyst productivity for all three of the pathways under investigation, resulting in reductions to the modeled MFSPs of 10%–33%.

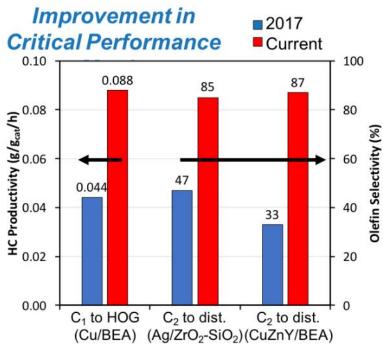


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- In general, the project has very focused tasks to develop a wide range of potential full candidates from low molecular weight oxygenates. The team successfully leverages interactions with many groups within ChemCatBio to enhance the project. The majority of the project has seen activity and selectivity metrics met, though room to improve catalyst reusability remains. In general, future studies appear to build on prior successes and will leverage capabilities in ChemCatBio to attempt to further catalyst performance. The project is productive in both connecting with fundamental science, publications in field-leading journals, technology, and several patents and a successful technology transfer with one of the processes.
- Overall, this seems like a comprehensive effort geared toward making IDL-based technologies commercially viable. It was not clear that the TEA estimates on biomass to liquids through the Fischer-Tropsch process and otherwise are presently realistic, and some comparison to commercial gas-to-liquids/coal-to-liquids would be useful, but that does not diminish from the work being done throughout this project.
- This project is making great progress already by delivering a promising pathway with several others to follow. This is the type of technology platform pipelining that BETO needs to continue funding in order to remain an innovative leader in bioenergy technology for the future. These types of processes that are rooted in alcohol conversion over modified zeolite chemistry will accelerate the progress toward the 2022 target. The information received from TEA and the CCPC make this project approach very robust. The team should stay vigilant and not trivialize the oligomerization chemistry and related unit operations required to drive the carbon-carbon bond formation to distillate-range material.
- Conversion of light oxygenates to drop-in hydrocarbon fuels is a flexible platform applicable to both biomass, CO<sub>2</sub> utilization, and natural gas, and as such is critical technology. There have been significant commercial efforts in this area; however, there are only a few operating plants even given the economies of scale. Improved catalysts could definitely facilitate the adoption of this approach, and the upstream

process, when integrated sustainably, would significantly impact GHGs. In the near term, it is unlikely that this approach will proceed without strong government support and mandates. However, in the long term this route is a likely component of future fuel supplies. The butadiene product produced and other intermediate olefins are more valuable than fuel and should be considered as the main product. The approach taken by the project team is extremely sound, allowing the comparison of multiple catalysts and routes in terms of both carbon efficiency and costs. Significant progress has made in the past two years and is likely to continue to be made going forward. The project with Enerkem would provide a potential near-term route to validate the new catalyst at a commercial scale.

- This is a heavyweight project at the heart of BETO's portfolio of catalytic technologies. It has made significant contributions to the field since its inception and will continue to do so as it sunsets.
- In general, the project has very focused tasks to develop a wide range of potential fuel candidates from low molecular weight oxygenates. The team successfully leverages interactions with many groups within ChemCatBio to enhance the project. The majority of the project has seen activity and selectivity metrics met, though room to improve catalyst reusability remains. In general, future studies appear to build on prior successes and will leverage capabilities in ChemCatBio to attempt to further catalyst performance. The project is productive in both connecting with fundamental science, publications in field-leading journals, technology, and several patents and a successful technology transfer with one of the processes. It involves NREL, PNNL, and a small portion (and more recent) to ORNL. Scaling is an important consideration on this project. It would be beneficial to evaluate modular processes as well and evaluate how synthetic catalysts work on large-scale processes.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that catalyst reusability remains an important part of our research. This is the focus of our endof-year goal, where we will explore deactivation and regeneration in all three of our oxygenate conversion pathways.
- Comparative TEA is an important part of our approach, and we will revisit our analyses of benchmark processes (Fischer-Tropsch, MOGD, and other gas-to-liquids/coal-to-liquids) to ensure we have realistic estimates.
- Although our focus is on the catalyst development for oxygenate conversion to versatile hydrocarbon intermediates, the reviewer is correct that the oligomerization cannot be trivialized. Due to time limitations, these results were not presented. However, this is an active area of research in the project, and based on these comments, it will remain as such.
- The reviewer provides an excellent overview of the versatility of our research approach, the challenges, and the opportunities for successful implementation. We have previously considered butadiene and mixed olefins as value-added coproducts. At our last peer review, we were cautioned against considering them as the final products, in light of the strict purity requirements required in the chemical industry that may not be trivial to meet. In the near term, our goal is to develop a market-refinery biorefinery concept around these pathways, which would enable the production of fuels and chemicals. Thus, we seek to maximize the carbon efficiency to these valuable intermediates, and to further explore and develop chemistry to convert them to fuel products.
- In addition to our ongoing efforts around catalyst reusability, the reviewer presents a useful suggestion to consider varying scales and modular processes. Our initial assessment of smaller scales suggested less favorable process economics, as typically associated with small-scale gasification technologies. However, we acknowledge that the opportunity to utilize renewable carbon sources may someday favor modular systems, and we will consider how our technology scales.

## CATALYTIC UPGRADING OF PYROLYSIS PRODUCTS

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

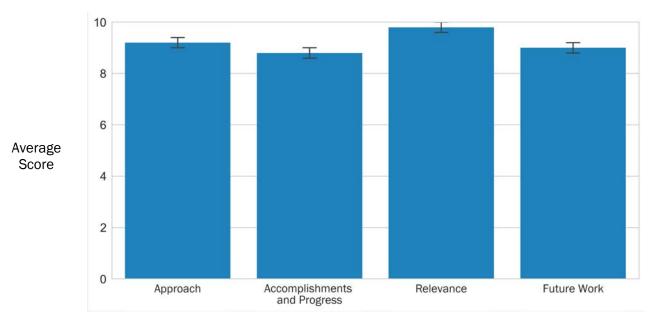
Fast pyrolysis of biomass is a promising route for converting lignocellulosic feedstocks into fungible biofuels; however, the resulting bio-oil must be upgraded prior to utilization as a fuel or blendstock. The focus of this project is to improve the fuel quality and stability of bio-oil through CFP, in which catalytic upgrading is performed in the vapor phase prior to condensation in either an *in situ* or *ex situ* configuration. The major challenge for CFP is to achieve high-carbon yields to the desired fuel-range molecules while operating under relatively harsh conditions that are conducive to catalyst deactivation via carbon deposition. To address this challenge, this project leverages a vertically integrated and collaborative

| WBS:                      | 2.3.1.314           |
|---------------------------|---------------------|
| CID:                      | NL0025579           |
| Principal Investigator:   | Dr. Josh Schaidle   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$16,388,556        |
| DOE Funding FY16:         | \$4,797,424         |
| DOE Funding FY17:         | \$4,897,723         |
| DOE Funding FY18:         | \$3,450,809         |
| DOE Funding FY19:         | \$3,242,600         |
| Project Status:           | Ongoing             |
|                           |                     |

approach, spanning from catalyst design to integrated bench-scale CFP. The overarching goal of this project is to reduce biomass conversion costs by developing catalysts and integrated processes for CFP that improve yield and enhance the fuel quality and stability of the resulting bio-oil by reducing the oxygen content (i.e., oxygen-carbon ratio), increasing the hydrogen content (i.e., hydrogen-carbon ratio), and increasing the carbon number into a range suitable for gasoline, diesel, or jet fuel. Ultimately, we seek to develop a CFP technology platform for an integrated biorefinery concept that is capable of producing both cost-competitive biofuels at greater than 75-GGE dry tons of biomass and high-value coproducts and can be market responsive by controlling the product distribution to meet market demand.



Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

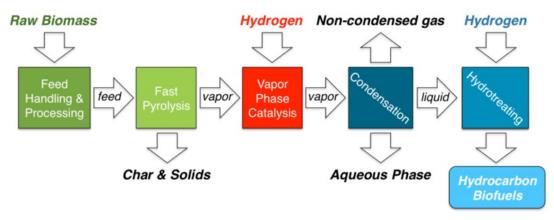


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- Overall, this is a very nice project that is targeting the cost drivers in CFP.
- The project interactions approach to this work is commendable, involving the lab community, consortiums (ChemCatBio, Bioprocessing Separations), cooperative research and development agreements (CRADAs) with energy (Exxon Mobil Corporation), material and catalyst companies (Johnson Matthey), scale-up (Advanced Development and Optimization), and engine application (Co-Optima) functions. This has been a successful effort thus far with strong partners and steering efforts.
- This catalytic upgrading of pyrolysis products project has made significant advances since the last review. The CFP continues to be extremely attractive with an identified path to low-cost fuel when supplemented by separation of a value-added product. It is a role model for other projects in terms of progress and organization. The team has incorporated the feedback from past reviews into their plan and have made great progress. Significant additional development work is needed to commercialize the process. Improvements in yields and product quality are still likely, if work continues. The cost of the value-added products needs to be compared to that of the current products. The fixed-bed flow scheme with new catalysts has a good probability of successfully reaching the commercial targets.
- This is a difficult project. The devil is in the details and the details are being addressed. TEA shows the promise of \$3.50/GGE. The work is at the heart of ChemCatBio and must be considered a crown jewel not only of ChemCatBio but of the entire BETO program.
- This is a successful, large-scale project with a rich history in BETO. Given the somewhat welldeveloped systems, the metrics are well defined and targeted to improve carbon efficiency, product distribution, and overall process costs. The recent progress is promising, and the future areas of focus expand on the recent successes to continue to improve catalyst performance and leverage coproducts effectively. Progress is heavily based on foundational science and the program is encouraged to leverage some of the work by coordination with other academic/national laboratory basic science programs. TEA and industrial relationships are important and working well. Feedstocks are key in their economic analysis and it is beneficial to encourage strong ties with bioenergy feedstock research partners.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their constructive feedback. We agree that CFP is a complex process and have sought to address this complexity through a collaborative approach leveraging both foundational science and applied engineering. Moving forward, we will continue to target improvements in carbon yield, catalyst performance, and product quality while identifying and developing routes to value-added chemical coproducts.

# CONDENSED PHASE CATALYSIS TECHNOLOGY FOR FUELS AND CARBON PRODUCTS

#### **University of Tennessee**

#### PROJECT DESCRIPTION

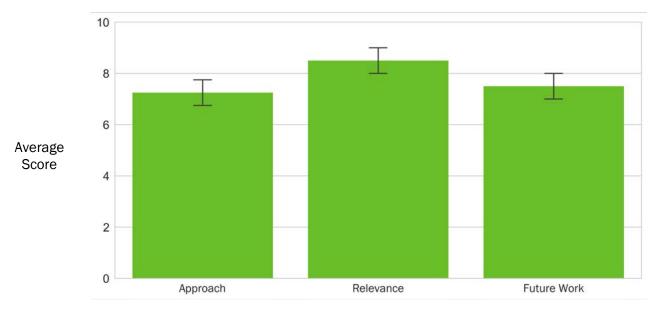
We propose a condensed phase catalysis technology with the biomass-derived solvent gamma-valerolactone (GVL) to deconstruct, fractionate, and upgrade lignocellulosic biomass to aviation liquid fuels (alkanes) and high-purity lignin. The lignin will be converted into functional carbon materials, such as activated carbon foams. Intermediate chemicals preceding the alkanes include furfural, highpurity cellulose, HMF, levulinic acid, and GVL. GVL is an effective solvent for biomass conversion because

| WBS:                      | 2.3.1.413          |
|---------------------------|--------------------|
| CID:                      | EE0008353          |
| Principal Investigator:   | Dr. David Harper   |
| Period of<br>Performance: | 8/1/2018-7/31/2020 |
| Total DOE Funding:        | \$1,400,000        |
| Project Status:           | New                |
|                           |                    |

hydrolysis and dehydration reaction rates increase 100 time and 30 times, respectively, relative to water. Fast kinetics enable mild biomass deconstruction severity (time, temperature, acid concentration, and pressure) and lead to clean fractionation into concentrated liquid hemicellulose, solid cellulose, and lignin. The biomass fractionation produces high yield and purity for the C5, C6, and lignin streams at high biomass loadings, enabling downstream processing and product recovery with less energy. The fractionated biomass components are independently and simultaneously converted to products in GVL, leading to process intensification by reducing the number of separation steps. These capabilities are critical to achieve below a \$3/GGE fuel cost target. The GVL-derived lignin readily converts into high-quality carbons. The GVL-enabled mild biomass digestion conditions produce lignin that has high purity, molecular weight, and glass transition temperature, yet also fusible. These characteristics are desirable for carbon materials with commercial applications. Our preliminary data suggest that we can use this lignin stream to create a range of carbon materials. Its high purity and low ash content make it ideally suited to produce high-temperature foam insulation, activated carbon, and

#### Weighted Project Score: 7.7

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



L One standard deviation of reviewers' scores

electrodes. Each of these products has high market value and will displace materials derived from fossil sources. Since roughly 25%–30% of lignocellulosic biomass is lignin, making biofuel production viable requires lignin valorization beyond its fuel price. Our goal is a continuous process integrated biorefinery that uses condensed-phase catalysis technology and the environmentally friendly biomass-derived solvent GVL to convert biomass into aviation fuel and functional carbon materials. By fully using and upgrading all major biomass components, the project will demonstrate the technical and economic feasibility of producing aviation fuel below \$3/GGE.

#### OVERALL IMPRESSIONS

- Generally, the project seems well structured. The management appears adequate. Preliminary results are promising and suggest potential interesting science and a useful technology can result from the work. The relevance to DOE and BETO is clear. For a project ramping up, additional details about thoughts on overcoming potential challenges, non-catalysis aspects of the work (solvent recycling), and better-defined timelines of future work would have been beneficial.
- This project is definitely in the early proof-of-concept stage involving simple characterization of a few biomass feedstock options followed by a few solvency runs monitoring pH and temperature. The focus should be on the future work of screening more BETO-relevant feedstocks and accelerating the solvency testing to probe more fundamental characteristics and thermodynamics first principles. PIs should engage the BETO computational group on areas to focus the basic research part of this program. A related benchmark study from open literature would be helpful to improve the efficacy of the GVL solvent. There may be more opportunity in the economic analysis task to include a cellulosic ethanol partner and provide additional processing details.
- The condensed phase catalyst project is a high-risk and high-reward project. Achieving the target would provide a new commercial route to biofuels. However, the scope of the project is very broad, and it is likely under-resourced. The economic evaluation is critical and still remains to be done. Pieces of this approach have been evaluated by these and other researchers in the past, which reduces the technical risks. Cost reduction and simplification are the critical parameters, along with product quality and suitability for high-value applications. Two of the most important aspects are demonstrating the feedstock flexibility and developing higher-value products from lignin and should continue to be the focus. Feedstock flexibility is critical to the future of biofuels because lowering the costs will involve using lower-cost feedstocks.
- The approach to biomass utilization by breaking it down into C5 and C6 sugars and lignin is simple and tractable. Yield goals are high. The gathered team has world-leading expertise to successfully perform the work.
- The goal is to separate biomass into high-purity streams of its three main components—cellulose, hemicellulose, and lignin—in an integrated process to enable efficient and cost-effective downstream conversion processes. Eventually, the team should convert hemicellulose and cellulose to an aviation fuel (alkanes) through intermediate chemicals derived from biomass polysaccharides (i.e., furfural, levulinic acid). The goals are clearly relevant to BETO's mission. Partners are University of Wisconsin and GlucanBio. Tasks are clear and logically divided, including TEA, and management is adequate. It would be beneficial to have an analysis of how this process compares with the state of the art. For a project ramping up, additional details about thoughts on overcoming potential challenges, non-catalysis aspects of the work (solvent recycling), and better-defined timelines of future work would have been beneficial.

#### **RECIPIENT RESPONSE TO REVIEWER COMMENTS**

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# CHEMCATBIO DFAS: LOW-PRESSURE HYDROGENOLYSIS CATALYSTS FOR BIOPRODUCT UPGRADING WITH VISOLIS

#### Pacific Northwest National Laboratory

#### **PROJECT DESCRIPTION**

In late 2017, the ChemCatBio consortium 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 biothermochemical process to produce high-value monomers at near-theoretic yields.

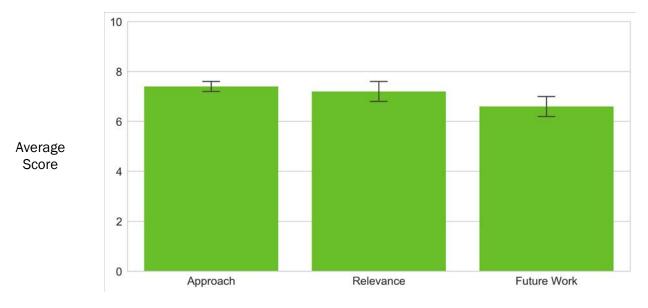
Visolis has previously demonstrated demo-scale (6,000 L) fermentation to produce an intermediate with low projected costs at commercial scale. Development of hydrogenolysis to convert the bio-derived intermediate to the desired monomer was proposed to ChemCatBio. A

| WBS:                      | 2.3.1.700            |
|---------------------------|----------------------|
| CID:                      | NL0033617            |
| Principal Investigator:   | Dr. Karthi Ramasamy  |
| Period of<br>Performance: | 1/20/2018-12/31/2019 |
| Total DOE Funding:        | \$525,000            |
| DOE Funding FY16:         | \$0                  |
| DOE Funding FY17:         | \$0                  |
| DOE Funding FY18:         | \$525,000            |
| DOE Funding FY19:         | \$0                  |
| Project Status:           | New                  |
|                           |                      |

major production cost in hydrogenolysis is the requirement for very high pressures—typical pressures for hydrogenolysis exceed 25 megapascals (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.

#### Weighted Project Score: 7.2

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

Objectives of the current effort are to develop and demonstrate a stable and robust hydrogenolysis catalyst by the end of FY 2019 for the conversion of the fermentation-derived intermediate to high-value monomer at  $\geq$ 80% selectivity under 4-MPa pressure. The solution entails a bimetallic catalyst system, a challenge requiring the screening of hundreds of potential catalysts and to fine tune the catalyst to achieve the desired product yield and stability. The team will also provide TEA for pilot-plant design using ASPEN Plus process models and discounted cash flow analysis.

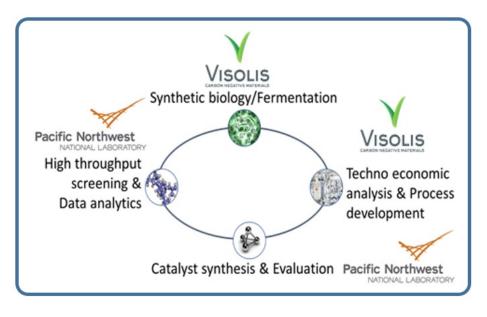


Photo courtesy of Pacific Northwest National Laboratory

#### **OVERALL IMPRESSIONS**

- This is a very targeted project with existing ties to PNNL catalyst development. Appears to be on track for meeting goals. More details could be provided regarding future work and justifying the fit with PNNL beyond the preexisting relationship.
- Overall, this is a good project in that it leverages high throughput synthesis and characterization abilities at PNNL to solve a relatively challenging selectivity issue (favoring reduction vs. carbon-carbon scission). Acknowledging this is a DFA, I understand that the level of detail has to be somewhat limited, but this also makes it very difficult for reviewers to comment on the relevance and quality of the work.
- The project team has done a wonderful job of showing how combinatorial catalytic research in bioenergy systems should be done. The high throughput screening apparatus should be used throughout ChemCatBio in every catalysis design project as a guide tool working parallel with rational *ab initio* design approaches simply for vector and ranking validation. The approach is sound by including commercial catalysts in the screening, working at real hydrotreating pressures near 1,800 psi. The presentation showed 100 catalytic materials, but it assumed that thousands have been screened. The project goal is highly relevant to BETO's objective of upgrading intermediate feedstocks from biocatalytic processing steps. In this case, C5 oxygenates produced by Visolis' demonstration-scale fermentation process are hydrotreated catalytically by PNNL to various alkanes of unknown speciation at 50% selectivity with a target of 80%.
- The PNNL/Visolis development of low-pressure hydrogenolysis catalysts for bioproduct found several new candidate formulations for improving the process. It would be easier to evaluate this project if more specific information was provided about the target products or catalysts. Presumably, intellectual

property protection is being prepared that will include this information. Hydrogenolysis catalysts that are active at low pressure and are water tolerant are highly attractive and could greatly facilitate the adoption of biomass conversion technology. The expertise gained can be applied to other BETO projects that require catalysts with similar functionality.

- This is a very sparse presentation, conveying some success at high throughput catalyst screening but offering no rationale for why these catalytic processes will give high yield as the pressure is lowered.
- Develop a low-pressure and water-tolerant hydrogenolysis catalyst to convert the fermentation-derived C5 oxygenate to a high-value monomer. A very targeted project with existing ties to PNNL catalyst development. The project appears to be on track for meeting its goals. More details could be provided regarding future work and justifying the fit with PNNL beyond the preexisting relationship. In addition, it is not clear what the lab and the consortium are learning from this project. One of the advantages could be data made available through the data hub.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The insightful comments provided by the reviewers are greatly appreciated. As pointed out by the review team, this project leverages the high throughput synthesis, screening, and characterization abilities at the ChemCatBio consortium to solve a relatively challenging issue in upgrading intermediate feedstocks from biocatalytic processing steps.
- We apologize for not being able to provide detailed technical information during the peer review presentation. This is due to the constraints of confidentiality with a commercial partner. Once the novelty is protected by patent, our goal is to make the information available to public and document all the information in the data management hub operated by ChemCatBio consortium.
- The commercial catalyst tested is designed to promote hydrogenolysis chemistry but is not specifically tuned to accommodate the bio-derived intermediate and feed composition. Thus, the commercial catalyst is not active to produce the high-value monomer of interest. The lessons learned from the commercial catalyst, through knowledge on the feedstock property and prior expertise in the hydrogenolysis chemistry, guided our team to develop an active catalyst that can operate at low pressure.
- Synthetic biology and fermentation are Visolis' core competencies, and this hybrid process requires heterogeneous catalyst discovery and development. PNNL's prior-demonstrated technical expertise in the hydrogenolysis catalyst development space and the equipment capability for heterogeneous catalyst development under the ChemCatBio consortium made PNNL the logical partner in accelerating this process.
- Even though the goal of this project is to develop a low-pressure and water-tolerant hydrogenolysis catalyst to produce a specific high-value monomer from a bio-derived intermediate, we strongly believe the successful outcome of this catalyst development with fundamental understanding will facilitate the adoption of other biomass conversion technologies that are under the BETO portfolio.

# CHEMCATBIO DFAS: TEREPHTHALIC ACID SYNTHESIS FROM ETHANOL VIA *P*-METHYL BENZALDEHYDE WITH LANZATECH

#### **Pacific Northwest National Laboratory**

#### **PROJECT DESCRIPTION**

To date, the only readily available renewable component of polyethylene terephthalate (PET) is ethylene glycol. Renewable terephthalic acid (TA) is a ready complement for renewable plastics (e.g., bottles and packaging films). In 2012, the global demand for TA was 47 million tons. The TA market is expected to grow continuously, reaching nearly 80 million tons in 2020. Ethanol could be a promising feedstock for renewable TA.

The development of ethanol-derived *p*-methyl benzaldehyde offers the possibility of producing 100% renewable PET from ethanol, adding flexibility and opportunities for a healthy industry that continues to grow.

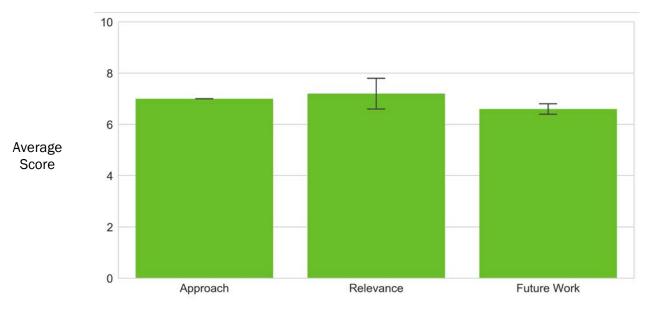
| WBS:                      | 2.3.1.701           |
|---------------------------|---------------------|
| CID:                      | NL0033621           |
| Principal Investigator:   | Dr. Karthi Ramasamy |
| Period of<br>Performance: | 4/3/2018-3/31/2020  |
| Total DOE Funding:        | \$200,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$200,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | New                 |

In addition, dehydrogenation of ethanol and the subsequent dehydrocyclization step in the *p*-methyl benzaldehyde synthesis generates hydrogen, which improves economics and life cycle impacts by reducing the need for external hydrogen for biorefineries having both a PET product line and a hydrocarbon fuels line.

The conversion of acetaldehyde occurs via a complex sequence of reaction mechanisms over a mixed-oxide catalyst. The complexity of the multistep cascade chemistry requires multifunctional catalysts with the acid base surface chemistry necessary for aldol condensation, paired with an active site that can promote the

#### Weighted Project Score: 7.0

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

dehydrocyclization step to achieve high conversion and selectivity. In addition to the multifunctionality, shape selectivity is required to maintain the high selectivity to the *p*-methyl benzaldehyde over the ortho isomer.

Objectives of the current effort are to develop and demonstrate the catalytic conversion of acetaldehyde (derived from renewable ethanol) to a methyl benzaldehyde(s) intermediate to establish the path to a marketable process for the economical and renewable production of TA and phthalates.

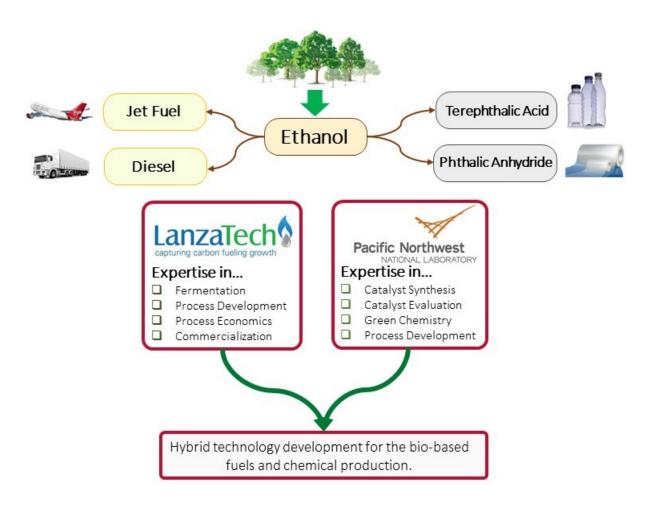


Photo courtesy of Pacific Northwest National Laboratory

#### **OVERALL IMPRESSIONS**

- A narrow focus effort with some level of productive results. Very little detail was provided on any aspect of the system, making this difficult to evaluate. Parts of the review criteria were omitted completely (i.e., a statement from the industrial partner).
- Producing aromatic aldehydes is an attractive addition to the ethanol upgrading portfolio. Consistent with other DFAs, it is difficult to assess the technical merit and progress due to a relatively high-level presentation, but overall, this seems like a technology that has some potential.
- Although this project is in the early stages, it feeds into BETO's long-term strategy for the flexible integrated biorefineries chemical pathway options. The project lead should continue to engage

ChemCatBio's resources and seek support for the next generation of catalytic materials in the future work.

- The PNNL/LanzaTech project to produce renewable precursors to terephthalic acid from ethanol is a route to a higher-value product that can lower the cost of coproduced fuels. Terephthalic acid is an important target because of the desire to create beverage and other containers with biomass-derived plastics. This project builds on the platform of finding higher-value use for biomass-derived ethanol. This project contributes to this effort; however, there are other approaches to preparing PET and other renewable substitutes that may be more attractive.
- Seed one-year project to verify if the chemical pathway proposed is viable for utilization of ethanol being produced by LanzaTech. The group seems to have a large degree of freedom in terms of selection of catalyst and process. New expertise and new processes for aldol condensation can be of advantage to the consortium despite the narrow focus that brings justification for BETO's investment. Parts of the review criteria were omitted completely (i.e., statement from the industrial partner).
- Initial results from the two-bed reactor system have demonstrated a very significant improvement in yield—from 10% or 20% to about 50%. The description of how additional improvement to the level of 70% yield was achieved was not provided.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The thoughtful comments provided by the reviewers are greatly appreciated. As mentioned by the reviewers, producing aromatic aldehydes is an attractive addition to the ethanol upgrading portfolio and the successful outcome of this project will feed into BETO's long-term strategy for the flexible integrated biorefinery chemical pathway options.
- We regret not including the statement from LanzaTech. As mentioned during the presentation, LanzaTech highly appreciates the PNNL collaboration and their statement is as follows, "This research has the potential to provide a high-yield pathway from ethanol directly to C8 aromatics without the yield loss to paraffins and higher aromatics. This pathway would provide an opportunity to leverage LanzaTech's sustainable ethanol into the PET supply chain. This project is in the catalyst discovery phase, TRL 2–3. This type of work requires expertise, resources, equipment, and a skilled staff in the catalyst discovery space, to which LanzaTech does not have access."
- We recognize the other renewable approaches to prepare PET. Compared to other routes, this process has advantage to produce C8 aromatics at high yield due to the nature of chemistry and mild operating temperature. In addition, the cogeneration of hydrogen from this chemistry enables the balanced biorefinery to produce fuels and chemicals in tandem. Current selectivity to the C8 aromatic aldehyde is ~60% and this is due to the generation of hydrogenated products from the feed and intermediates. Incorporation of gallium in the catalyst will reduce the hydrogenation and improve the product selectivity. A series of modified zeolites are being investigated to increase the *p*-methyl benzaldehyde to approximately a 20% level through isomerization.
- This project is in the early phase, so the work was not protected by patents at this time, and this made it difficult to present the technical details in the public forum. Our goal is to document all the information in the data management operated by the ChemCatBio consortium at the end of this project.

## CHEMCATBIO DFAS: TACTICAL AVIATION FUELS WITH GEVO

#### Los Alamos National Laboratory

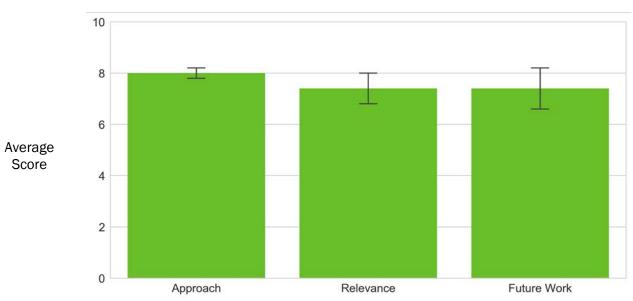
#### **PROJECT DESCRIPTION**

Increasing the energy density of an aviation fuel is nontrivial. Current branched-chain saturated hydrocarbons suitable for unleaded kerosene (Jet A-1) or Jet Propellant 8 (JP-8) applications produced by Gevo have a density of 0.76 g/mL and have an energy density of 33.44 MJ/L. While this exceeds the specification for ASTM D1655 7566 for aviation turbine fuel, performance advantaged fuels with higher energy densities are desirable. Increasing the density and energy density can be achieved through dimerization and cyclization reactions, and in particular through the formation of strained ring systems. For example, cyclobutanes can add approximately 100 kJ/mol of energy through ring strain alone and dimerization

| WBS:                      | 2.3.1.702          |
|---------------------------|--------------------|
| CID:                      | NL0033622          |
| Principal Investigator:   | Dr. Andrew Sutton  |
| Period of<br>Performance: | 4/1/2018-3/31/2020 |
| Total DOE Funding:        | \$667,000          |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$O                |
| DOE Funding FY18:         | \$667,000          |
| DOE Funding FY19:         | \$0                |
| Project Status:           | New                |
|                           |                    |

further increases the energy density. However, typical dimerization of olefins is performed industrially using strong acid catalysts such as sulfuric acid or hydrofluoric acid, which presents handling and environmental concerns and generates large quantities of corrosive waste to either dispose of or recycle.

We aim to use Gevo intermediates to produce higher energy density fuels in order to provide a performance advantage over current aviation fuels.



#### Weighted Project Score: 7.7

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 ${f I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- Overall, the project has some innovative ideas applied to upgrading of unfunctionalized alkenes to jet fuels. The link between the Los Alamos National Laboratory (LANL) performers and the company is clear. The multifaceted approach allowed some progress on this exploratory project. The path forward in both success areas and tasks needing improvement (copper sensitizers) is clear. Additional details about milestones, catalyst systems, and rationale for a photochemical over a thermal approach would have been valuable.
- This project aims to upgrade olefins from the Gevo process into targeted cyclobutene-type molecules to dramatically improve the energy density of jet fuels. This is based on some type of [2+2] addition reaction that is photoinitiated. It may be helpful to consider the scale of cyclopentenone availability (suggested to come from CFP) in comparison to Gevo alkenes and aviation fuel markets, which might provide a better assessment of whether the work will ultimately be practical at scale.
- The chemistry is interesting from a science-elegance standpoint, working through the enone-ene intermediate and then doing the coupling. The research appears to offer opportunities in solid alkylation conversions as well following a reducing step. Enone-ene production rates from Gevo should be disclosed and the other constituents present in an actual feedstream. More mechanistic details should be offered regarding the partial hydrogenation of the carbonyl group to produce the final cyclic alkane at the end via a phenol intermediate. If so, this is not a trivial step and the reactor exotherms may become dangerous at scale and difficult to control along with the catalyst. More information regarding the poisoning of this catalyst should also be gathered, especially those with the potential for trace metals like silicon or copper and some other things at parts-per-billion levels. The issue of ring strain in the presence of mostly straight molecules in kerosene hydrocarbon should be examined by fuel oxidation stability testing. Naphthenes may not be present at high amounts in some Jet A compositions and the influence of visible light on fungible mixtures should be determined.
- Production of high-performance tactical aviation fuels is an important target for both military and commercial projects. This is a very early-stage proof-of-principle project with a long road to commercialization. Photoreactors are not common in the chemical processing industry and are generally costly. However, gaining experience with photoreactors would significantly add to the repertoire of the laboratory. Production of less-costly alternatives to JP-10 is an important target for the national defense community and a side benefit of the program. The product would provide a source of income to Gevo while it is going through its development phase.
- This is something of a high-risk, high-reward project. If the [2+2] cross coupling can only be achieved with an external reagent, the impact will be severely lowered. It will be exciting to see if a photocatalyst (ultraviolet or visible) can be found to impact the homocoupling of the Gevo substrate.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their thoughtful and helpful responses to our project. We fully agree with them that this is a high-risk, high-reward project and we have tried to develop a stepwise approach towards increasing complexity as we progress to a set of building blocks that can be fully sourced from Gevo product streams. Our initial work was to demonstrate the [2+2] cycloaddition using bioderived molecules, such as cyclopentenone. While cyclopentenone can be produced in small quantities in CFP, it is a known product from furfural through a set of high-yielding and selective transformations. The efficiency of cyclopentenone cycloadditions led us to incorporate Gevo isopentenes in this reaction approach to produce strained ring molecules. The promising initial physical properties of the resulting cycloaddition products suggest they do have potential for application as high energy density fuels, assuming the long-term stability of these cyclobutanes can be demonstrated. Further expansion to use Gevo isopentenes as the sole carbon building blocks is ongoing and following analysis of these potential fuel molecules we will attempt to develop a feasible and economic strategy to produce these molecules at scale.

# CHEMCATBIO DFAS: IMPROVED VALUE OF THE GASOLINE AND FUEL OIL COPRODUCT FRACTIONS WITH LANZATECH

#### Pacific Northwest National Laboratory

#### **PROJECT DESCRIPTION**

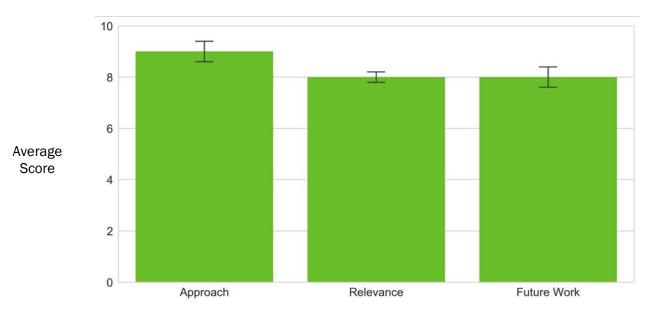
The ChemCatBio consortium invited industry to partner with national laboratories and leverage ChemCatBio capabilities in late 2017. LanzaTech, a small biotech company, led the charge to answer a challenge that all integrated biorefineries must face—finding a market or use for all carbon entering the plant, a necessity for economic and environmental sustainability. PNNL's alcohol-to-jet (ATJ) process primarily yields synthetic isoparaffinic kerosene in the jet range. This project is increasing the value of the gasoline (light) and fuel oil coproduct (heavy) fractions. The technical goals of this project are to (1) increase the research octane number (RON) of the lighterthan-jet gasoline fraction above 98 and (2) create a synthetic lubricant base oil from the heavier-than-jet fraction.

| WBS:                      | 2.3.1.703          |
|---------------------------|--------------------|
| CID:                      | NL0033624          |
| Principal Investigator:   | Dr. Rob Dagle      |
| Period of<br>Performance: | 4/3/2018-3/30/2020 |
| Total DOE Funding:        | \$600,000          |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$0                |
| DOE Funding FY18:         | \$600,000          |
| DOE Funding FY19:         | \$0                |
| Project Status:           | New                |
|                           |                    |

To produce a high-octane RON gasoline blendstock, we are utilizing an intermediate stream from the current ATJ process that is rich in linear butenes. Low-temperature oligomerization of this intermediate has resulted in a lower-than-desired octane rating, restricted by limited branching. Thus, we are investigating high-temperature skeletal isomerization prior to oligomerization, which will result in more branched iso-olefins, thus increasing the RON of the mixture. For example, 2,2,4-trimethyl-1-pentene has an RON of 103, making it

#### Weighted Project Score: 8.5

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oxed{I}$  One standard deviation of reviewers' scores

a valuable gasoline blendstock component. We are targeting a 98+ RON blendstock that has a cost premium of 25% above gasoline. Shape-selective and non-shape-selective catalysts have been investigated for skeletal isomerization. After isomerization, controlled oligomerization using commercially available strong acid resin catalysts (e.g., Amberlyst-36) has been performed. Thus far, the RON of the gasoline fraction has been increased from 86 to 94. However, in order to reach the target RON of 98, further octane enhancement is required, and this will be accomplished through process improvements and/or by eliminating heavier constituents from the feedstock (e.g., C6+ olefins).

To produce lubricant, we have started to evaluate the isoparaffins that are produced by the heavier-than-jet-fuel oil fraction as a Group III base oil. Group III base oils with four centistokes viscosity have been valued from \$3.80–\$4.60 per gallon in 2017, a significant value improvement versus diesel spot prices of \$1.40–\$1.70 per gallon over the same period. Base oils are the name given to the hydrocarbon portion of fully formulated lubricants such as passenger car motor oils. Base oils typically consist of compounds with 18–40 carbons and boil between 288°C and 566°C. ASTM D6074 is the standard for characterizing hydrocarbon lubricant base oils. Group III base oil must contain more than 90% saturates, possess less than 0.03 wt % sulfur, and have a viscosity index (VI) above 120. Isoparaffinic content is a primary contributor to a significantly high base oil VI value. Hydrocarbons produced by the PNNL ATJ process are virtually all isoparaffinic and contain no sulfur. Thus, with minimal catalytic processing, we expect the material will classify as high-value Group III base oil. We are currently investigating hydroisomerization of the greater-than-jet-fraction in order to improve the viscosity index from 100 to greater than 120 and meet the specification as a Group III base oil.

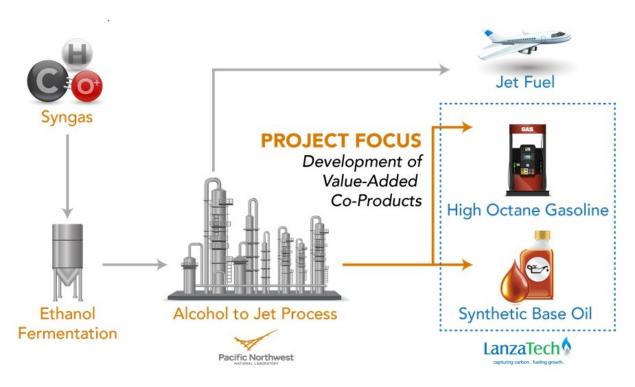


Photo courtesy of Pacific Northwest National Laboratory

#### **OVERALL IMPRESSIONS**

• The project continues a unique collaboration between LanzaTech and PNNL. The results look promising to complete the project milestones. There is clear perceived value of having PNNL participate in the studies. While some additional details of the system would contribute to a more thorough evaluation, this is still perceived as a well-organized and potentially successful project.

- I like the effort to make targeted oligomerization products that offer high RON and/or perform well as lubricants. I have some concerns that oligomerization-based chemistries can be very selective, particularly at high temperatures. I think carbenium-type oligomerization will, at these temperatures, probably lean toward a thermodynamically controlled distribution of oligomers, aromatics, cracking products, etc., and it wasn't clear that one could selectively target a specific class at 400°C. I think it might be possible to make isobutene at lower temperatures, provided one can find a way to turn on skeletal isomerization without encouraging too much oligomerization.
- In general, this work is headed in the right direction and is well done so far. The next phase is to work with real feeds that could exacerbate the coking and deactivation events. It is time to discuss the process options with LanzaTech from an engineering design perspective.
- The cooperative project between PNNL and LanzaTech to improve the quality of the gasoline and fuels made from ethanol has good commercial potential. It supports the technology that converts alcohol to hydrocarbons, which is a major potential route for producing biofuels from excess ethanol. Technically, the project should work, and a process can be developed; the questions are the cost versus the benefits. The production of renewable lube stocks is particularly attractive. The project furthers PNNL with LanzaTech, which is already licensing ethanol-to-hydrocarbon technology from PNNL.
- This project makes the most out of ethanol, addressing the previously unattended light and heavy hydrocarbon fractions from the LanzaTech jet fuel process. Strong teams give the sense that success is highly likely. The impact that improving the light and heavy fractions has on the TEA of the overall process would be interesting to see but has not been proposed.
- Develop new reaction routes and process to produce high-quality fuel/lubricants from fermentationderived feedstocks from LanzaTech. Again, there is a clear advantage to both sides justifying BETO's investment: LanzaTech finds a new market to their product and the consortium creates new knowledgebased processes. Progress is appropriately demonstrated, and future work is commensurate to their goals. There is already a good relationship and technologies licensed from PNNL from work with LanzaTech. The partnership seems solid. While some additional details of the system would contribute to a more thorough evaluation, this is still seen as a well-organized and potentially successful project.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer's positive comments and agree that this project continues a strong collaboration between LanzaTech and PNNL. This project builds upon the codeveloped alcohol-to-jet process being commercialized by LanzaTech. We appreciate the reviewer's positive comment about our approach for making a targeted, oligomerized, high-RON coproduct and lubricant.
- We agree with the reviewer that at high temperatures the product distribution is more varied. Selectively producing isobutene at lower temperatures would be preferred; however, controlling selectivity against oligomerization is difficult indeed. Our approach has been to investigate both processing options, each with their own set of challenges. Results thus far indicate that at lower temperatures some degree of branching occurs but not enough to achieve our high-RON target. Operating at a higher temperature produces isobutene, but byproducts are formed, including aromatics—in fact a high-RON constituent—and undesirable cracking products and coke. Ultimately, both approaches will be evaluated with TEA. Here the tradeoff between a high-RON process—requiring more frequent catalyst regeneration and two-step processing—will be investigated versus a lower-RON process with a more simplified process scheme. TEA will also be performed for the lubricant processing and will be included in the final report.
- We agree that working with real feedstocks provided by LanzaTech will be important. We will verify RON and lubricant properties using ASTM methods. Additionally, we will evaluate catalyst stability when using real feedstocks, and study catalyst regeneration.

• We appreciate the reviewers' positive comments about this project having good commercial potential. This project aims to find coproduct opportunities and find value for all of the carbon in the plant. We agree with the reviewer that the production of renewable lubricant is particularly attractive. We note that at the time of the review we had just initiated the lubricant study, as the project began with development of the high-RON coproducts. We have since initiated hydroisomerization studies of the lubricant fraction using metal-promoted zeolite catalysts. We are evaluating the effects of the zeolite structure and acidity on resulting lubricant properties, particularly viscosity.

# CHEMCATBIO DFAS: CATALYTIC PROCESS INTENSIFICATION OF BIO-RENEWABLE SURFACTANTS PLATFORM WITH SIRONIX RENEWABLES

#### Los Alamos National Laboratory

#### PROJECT DESCRIPTION

Surfactants are the key active ingredient in cleaning products, with long lists of additional builder ingredients added to boost function while maintaining product safety and shelf life. These builder chemicals increase product cost and volume and biodegrade poorly. Sironix Renewables has invented a new class of surfactants, called Oleo-Furan Surfactants (OFS), which eliminate the need for these additional chemicals, reducing volume and resulting in a product that biodegrades readily. Our OFS link the function of bio-based furan building blocks with natural oils to produce multifunctional and eco-friendly cleaning products. Our technology gives improved performance, and by eliminating builder chemicals, we

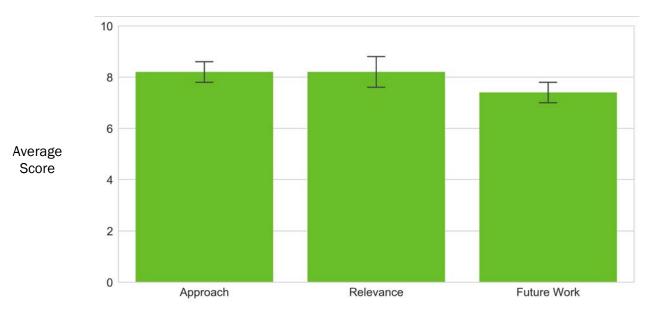
| WBS:  | 2.3.1.704               |
|---|-------------------------|
| CID:  | NL0033626               |
| Principal Investigator:                                     | Dr. Andrew Sutton       |
| Period of<br>Performance:                                   | 7/1/2018-6/30/2020      |
| Total DOE Funding:  | \$667,000               |
| DOE Funding FY16:   | \$0                     |
| DOE Funding FY17:   | \$0                     |
| DOE Funding FY18:   | \$667,000               |
| DOE Funding FY19:   | \$0                     |
| Project Status:   | New                     |
| DOE Funding FY17:<br>DOE Funding FY18:<br>DOE Funding FY19: | \$0<br>\$667,000<br>\$0 |

reduce the volume (and therefore packaging) by 30%. This reduces overall energy consumption while producing a more environmentally friendly product.

The proposed joint research project with Sironix Renewables is designed to leverage the catalytic reaction engineering, catalyst development, and furan chemistry resources of the ChemCatBio consortium with the

#### Weighted Project Score: 8.0

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $\square$  One standard deviation of reviewers' scores

surfactants platform of Sironix Renewables to accelerate the DOE-invented and DOE Small Business Innovation Research-funded technology toward market commercialization. Technical goals include process improvements to achieve efficient scale-up of existing surfactants and the development of a new class of furanbased structures to address an emerging market need for nonionic surfactants.

#### **OVERALL IMPRESSIONS**

- The project seems like a strong and successful collaboration. The link to the LANL performers is clear and perceived as a benefit to the industrial partner. Significant progress has been made on the project. Future work on the project is well delineated in time and metric milestones. Additional details on scarcely mentioned aspects of future work would have strengthened the case for expansion of the project into new areas involving computational and catalyst characterization.
- The furan coupling approach/play into the surfactant market seems like a viable pathway with high margins. Work is being done on optimizing an industrial problem that impacts commercial margins directly when progress is made on the project. Current lab setup looks reasonable with the batch reactor configuration. There is a good approach to demonstrate yield improvements over the current state-of-the-art copper-chromium mixed oxide-based catalyst under same conditions and even optimized conditions. The chemistry is sound and reliable to reproduce under the observed operating conditions. It appears that there are even more opportunities to reduce space time even more and go out further with time on stream (TOS) with an hydrodeoxygenation (HDO) catalyst operating at 99% conversion. Partial HDO seems like it will be tricky to scale even though lower pressures of 150 psi are used. Process safety hazard analysis should start early. Feed composition currently has 3 wt % of reactant in the feed, so increasing the concentration in future work to keep equipment sizing modest could be a near-term goal. The project team should continue to benchmark with commercial catalyst materials in parallel and develop a technology milestone chart to visually see progress. There has been good progress achieved in this work thus far.
- This is a really interesting technology that may have a fairly short-term path to market, in that it specifically targets performance-advantaged bioproducts. This is perhaps due to the nature of the DFA program, but it is challenging for an external reviewer to comment on progress as technical details are relatively sparse. I had some concerns about the ways that stability and selectivity are being assessed. They may not be appropriately benchmarked, and it may give a false impression as to the origin of enhanced selectivity and/or stability.
- The initial catalyst development for both the carbon-carbon coupling and HDO of the intermediate appear to be quite successful. Additional process intensification would be achieved if both reactions could be conducted simultaneously (though no explanation was given for why this might work), and if the process could be demonstrated to work in continuous mode.
- The collaboration with Sironix Renewables has a clear short-term commercial target. The production of nonionic surfactants is a good approach to adding value to biomass-derived furans. The product is an example of a bioadvantaged chemical. A new surfactant was discovered by the LANL group. There has been good progress in a short period and has already transferred materials to Sironix Renewables, LANL's industrial partner. The project is very likely to produce a commercial product.
- This is a new technology to accelerate and develop an emergent market of new surfactants.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for the opportunity to present our current results on this successful CRADA with Sironix Renewables. Our collaboration to this point has been extremely productive and we acknowledge the reviewer's comments regarding the need to fully investigate our catalysts in terms of recyclability, stability, and effective lifetimes. Our initial efforts for the nine months of the project presented at peer

review were focused on developing alternative catalysts to those currently employed to increase overall yield and selectivity to the desired product, a task which was achieved and successfully transitioned from batch to continuous flow reactors. As we refine and optimize the reaction conditions, we are excited to probe the extent and limits of our catalyst performance in order to fully support the commercialization efforts of Sironix Renewables, which will include a TEA of a fully refined process.

# DIRECT CATALYTIC CONVERSION OF CELLULOSICS

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

The Direct Catalytic Conversion of Cellulosics (DC3) project is set out to (1) develop a semicontinuous solvolysis and chemo-catalytic process to upgrade cellulosics residuals from woody biomass and (2) evaluate the resulting mixed oxygenate products for fuel applications. The abundancy of delignified cellulosics from the pulp and paper industry, as well as a byproduct from a lignin-first biorefining process, offers the opportunity to valorize an inexpensive feedstock to performance-advantaged fuels. While enzymatic hydrolysis is a leading and highly selective approach for cellulosics depolymerization, it can be economically challenged by recalcitrant feedstocks that require high enzyme loadings. As such, direct solvolysis with chemo-

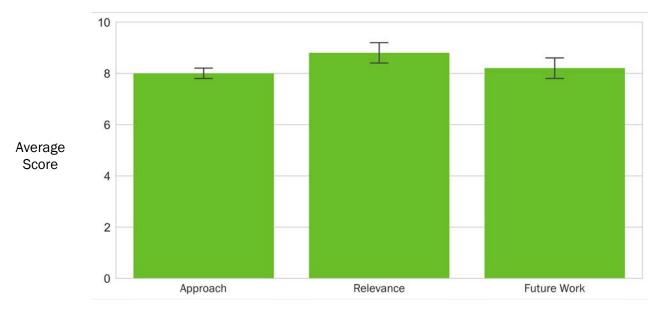
| WBS:                      | 2.3.4.503           |
|---------------------------|---------------------|
| CID:                      | NL0034402           |
| Principal Investigator:   | Dr. Derek Vardon    |
| Period of<br>Performance: | 10/1/2018-10/1/2020 |
| Total DOE Funding:        | \$200,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | New                 |
|                           |                     |

catalytic conversion is a promising alternative for delignified woody feedstocks.

DC3 aims to develop a dual-bed semicontinuous design with the capability to separate biomass feed and catalyst to overcome the inherent challenges associated with the current state-of-the art batch processes. These challenges include: (1) problematic separation of feed and catalyst, (2) challenging scale-up considerations, and (3) convoluted reaction network for solvolysis and monomer conversion. In addition, DC3 has the advantage of being able to utilize the same initial biomass, reactor system, and solvent system employed for biomass delignification during lignin first. Following lignin removal, DC3 can convert the cellulosic residuals from lignin first to C2–C6 aliphatic alcohols for fuel applications.



Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

DC3 is a new start seed project within ChemCatBio that will leverage the consortia's catalytic process development capabilities. Collaborators from the enabling capabilities include the ACSC task, as well as the Catalyst Cost Model Development task. In addition, DC3 will interface closely with lignin first to coordinate on feedstock and solvent selection, as well as the Co-Optima consortia to leverage the latest fuel property prediction and characterization tools.

DC3 will achieve its first phase objectives by (1) synthesizing, characterizing, and testing various multifunctional mixed metal-oxide catalyst designs and correlating their properties to product distribution; (2) outfitting a high-temperature, high-pressure dual-bed semicontinuous reactor for testing downselected catalysts; and (3) evaluating the fuel properties of oxygenated products and tuning catalyst and process variables to improve target product yields.

Preliminary data obtained in the first 25% of the project will lay the foundation for future work. In FY 2019 and FY 2020, research efforts will focus on (1) preparing delignified biomass as the feedstock for DC3; (2) establishing analytical methods for the complex solid, liquid, and gas product mixtures; (3) benchmarking inhouse catalyst design against commercial formulations and evaluating the effects of catalyst properties on product distribution; (4) commissioning a high-temperature, high-pressure dual-bed semicontinuous reactor to test reactivity and stability of downselected catalysts; (5) assessing the mixed oxygenate product fuel properties; and (6) integrating the process with preliminary TEA in conjunction with lignin first. Milestones are crafted to measure progress towards success outcomes with risk analysis and go-no-go decisions to refine options.

In summary, DC3 employs a science- and engineering-driven approach with a collaborative team to enable a pathway to advantaged oxygenated fuels from residual cellulosic biomass.

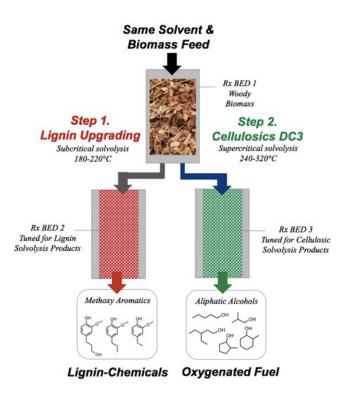


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- Overall, a very thoughtful project which clearly defined goals, approaches, and future directions of the seed effort. Makes a clear connection to the characterization efforts of ChemCatBio but could provide stronger connections to other ChemCatBio capabilities. The integration with the solvolysis portion of the processing could have been further delineated, as only catalyst development may not lead to an effective semicontinuous process.
- This project is in the early stages, but it has a very straightforward, clear pathway to success with the proper support team, tools, and knowledge-leveraging resources throughout ChemCatBio.
- TEA has made it clear that biomass upgrading is unlikely to be economical without lignin valorization, and lignin-first approaches have emerged in response. They seem more amenable to lignin upgrading than conventional lignin removal by, for example, Kraft pulping, and so should have an impact on valorization and possibly be more economical. This project is aimed at devising technologies to upgrade the residual carbohydrate fraction, in particular, converting them into monooxygenates by solvolysis and (probably) hydrotreating. Academic partners already working in this area appropriately inform this project. I like the interface with the Co-Optima project to determine what type of upgrading will provide the best biofuel/engine design.
- Direct catalytic conversion of cellulose couples a lignin-first separation with continuous direct cellulose conversion. It provides another potential route to renewable fuels and chemicals. This is an early-stage low-TRL project that evaluates an emerging approach that is receiving increasing attention in the literature. There are several groups that have evaluated organosolv and subcritical water separations coupled with fermentation of the obtained cellulose. Any direct catalyst conversion process could replace fermentation in these processes. The mixed aliphatic alcohol products are not a drop-in fuel and will require a follow up to ensure their utility. This would likely fall under the Co-Optima program, as discussed in the presentation.
- Seed project from the Catalytic Upgrading of Biochemical Intermediates effort and coordinated with lignin first.
- The conversion of dissolved cellulosics left over from lignin-first processing is a superb example of utilizing all the carbon in biomass feed. The research plan is thought out in detail and is very involved—so much so that the adequacy of the budget is in question.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We appreciate that the reviewers of the DC3 project found value in our approach to convert a residual waste stream from lignin-first processing. Per the reviewers' suggestions, DC3 will continue to focus on transitioning to semicontinuous processing in close coordination with lignin valorization efforts to ensure feedstock and process consistency with harmonized economic analysis. In addition, future efforts will focus on the biomass solvolysis step, as we agree this is as important as the catalytic upgrading step. Interactions with the Co-Optima team will help de-risk the novel oxygenates as a fuel. The DC3 team thanks the reviewers for their support of this effort and constructive feedback for project next steps.

## CONSORTIUM FOR COMPUTATIONAL PHYSICS AND CHEMISTRY

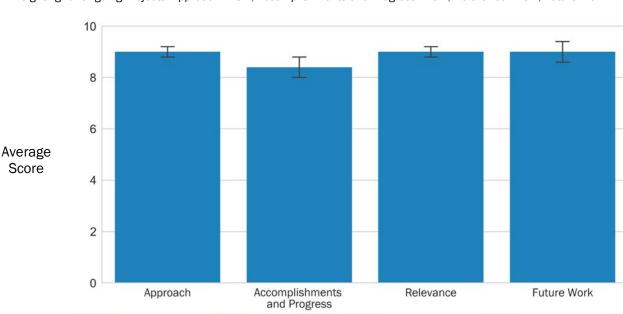
#### **Oak Ridge National Laboratory**

#### PROJECT DESCRIPTION

The ChemCatBio-enabling project Consortium for Computational Physics and Chemistry (CCPC-CCB) accelerates progress in catalytic conversion R&D through theoretical simulation of surface chemistry reactions to enable ChemCatBio experimental teams to achieve the BETO targets for each conversion technology (e.g., goal of \$2/GGE fuel for CFP). Furthermore, the CCPC-CCB enables verification of core BETO pathways via modeling of conversion reactions and critical transport phenomena at meso and process scales. Overall, the CCPC-CCB verifies scalability and translation of biocomplex surface science technologies to biomass-to-fuel product conversion processes at scales relevant to the bioenergy industry. Our

| WBS:                      | 2.5.1.301             |
|---------------------------|-----------------------|
| CID:                      | NL0025890             |
| Principal Investigator:   | Dr. James E. Parks II |
| Period of<br>Performance: | 10/1/2015-9/30/2021   |
| Total DOE Funding:        | \$12,854,800          |
| DOE Funding FY16:         | \$3,144,000           |
| DOE Funding FY17:         | \$3,150,000           |
| DOE Funding FY18:         | \$3,280,400           |
| DOE Funding FY19:         | \$3,280,400           |
| Project Status:           | Ongoing               |
|                           |                       |

mission is to utilize core computational capabilities across the DOE national laboratory system to enable and accelerate the development of new materials and optimize process scale-up to advance the bioenergy economy. The CCPC-CCB is a well-developed and actively functioning consortium that combines synergistic technical capabilities across five core national labs (ORNL, ANL, NREL, PNNL, and the National Energy Technology Lab) and critical collaborating partners to advance bioenergy research rapidly and cost effectively. The consortium began in FY 2013 by request of BETO Director Jonathan Male to develop a cohesive plan and structure for modeling activities in the conversion program. The specific technical focus and scope change as needed based on needs identified by collaborating BETO experimental projects and feedback provided by



#### Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

industry through an advisory panel and periodic program peer reviews. As such, the CCPC-CCB represents a flexible and rapid response team of computational expertise to enable success toward critical BETO objectives. The enabling aspect is a core tenet of the project, and close collaboration with partner experimental projects is essential to success. The CCPC-CCB provides a culture to promote the necessary technical exchange and collaboration, which is key to achieving the project objectives.

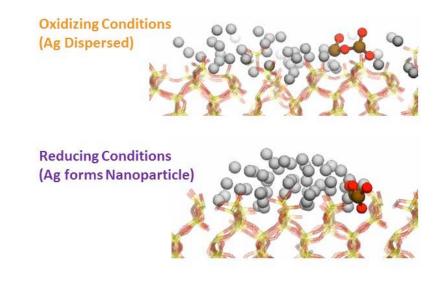


Image of a Ag catalyst supported on a metal-oxide support under oxidizing vs. reducing conditions. Image from PNNL (Wilkelman, Akhade, Kovarik, Glezakou, Rousseau, Dagle, Dagle).

Photo courtesy of Oak Ridge National Laboratory

#### OVERALL IMPRESSIONS

- A well organized, expansive center-level effort, which did an excellent job of demonstrating its pervasive value throughout ChemCatBio. Tends to lean a little more toward the basic science side than most ChemCatBio projects, but this has advantages. The center strives to continue to increase level of systems complexity in new proposed projects, which can still lead to significant technology impact while also contributing to basic science.
- CCPC is a strong organization with a good foundational direction. Experimental validation will always continue to be the key to computational programs, building both the researchers and process design engineer's confidence as a reasonable agreement is reached at all scales. This consortium is equipped with all the right resources.
- CCPC was the first consortium-type project and is still a role model for demonstrating the potential impact of the approach on many different projects centered at multiple labs. The organization and management of the project are major factors in its success. It shares its findings and methods both within and outside BETO projects. The approaches taken by the CCPC team are the scientifically sound applications of mathematical models to problems that arise from biomass conversion technologies. They have established two goals for the project involving catalyst selection and scaling function for one technology. Establishing these types of general goals as a metric for the consortium project enables a more objective evaluation. However, the work of the consortium is much more expansive and impacts many different projects.

- This is a very impressive effort that covers many scales of catalyst/reactor performance. It will be interesting to see continued outputs from this work going into the evolving data hub. I think machine-learning algorithms might be a great fit for these multiscale reactor models as they can lump much of the model complexity and avoid much of the effort in parameterization and model solution, but still allow meaningful predictions about reactor performance.
- The operation of the CCPC is what all the enabling capability projects might aspire to. What a solid, helpful, impactful consortium.
- The goal of providing a computational toolset developed by CCPC and facilitating the modeling of biomass industrial technologies from atomic to process scales, thereby reducing the cost, time, and risk in commercializing bioenergy technologies, is certainly an important cross-cutting capability. It's a very large effort with a large outreach that is also involved with other BETO consortia (especially the relevant Bioprocessing Separations Consortium). It involves many national labs and has evolved throughout the years. It tends to lean a little more toward the basic science side than most ChemCatBio projects, but this has advantages. In addition, the group is encouraged to pursue partnerships with the existing basic science programs. The approach is comprehensive and involves many scales, and the group is commended for investing in the kinetic work, which is absolutely necessary for this effort. CCPC strives to continue to increase level of systems complexity in new proposed projects which can still lead to significant technology impact while also contributing to basic science.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Regarding feedback in specific areas, we agree that the data hub and associated machine-learning tools offer interesting opportunities for modeling. We intend to further support the data hub and will seek opportunities for machine-learning applications. However, we intend to be cautious with machine learning to ensure that our modeling outcomes have a tangible science-based underpinning, which is critical to the accuracy of our results.
- We agree completely that experimental validation is a critical aspect of our efforts. We have benefited greatly from validation data supplied by our experimental colleagues, and we intend to grow the interactions with experimentalists as we move forward. Specifically, we seek to jointly define critical experiments that will yield specific model parameter data critical to accurate model predictions.
- Thank you for the reinforcing guidance to (1) leverage the basic science programs and (2) continue to define and apply kinetics. Our liaison approach of defining a specific person to track key partnerships, such as with the basic science catalysis program, is relatively new but has provided benefits to date, and we will continue that approach to strengthen our awareness and connections to the basic energy science programs. Our kinetics efforts are relatively new as well but are critical to bridging ChemCatBio catalysis successes to larger scales. We will continue kinetics development in close collaboration with our experimental colleagues.
- The CCPC appreciates the numerous positive feedback comments on our project's approach, organization, accomplishments, relevance, and future work. We appreciate the compliment on the wide range of scales we are addressing, and we consider our multiscale approach to be critical to success. We also thank the reviewers for the compliments on the impacts demonstrated across many projects in the BETO program.

# CATALYST COST MODEL DEVELOPMENT

#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

The goal of the joint NREL-PNNL Catalyst Cost Model (CCM) project was to develop a free and publicly available catalyst cost estimation tool that enables rapid and informed cost-based decisions in early-stage research and commercialization of catalysts. This goal was successfully realized in October 2018 with the release of the complete web- and spreadsheet-based CatCost<sup>TM</sup> tool, online at catcost.chemcatbio.org. CatCost is a first-of-its-kind, publicly available tool for determining the costs of precommercial catalysts that employs state-of-the-art estimation methods coupled with an intuitive user-interface and comprehensive visualizations. CatCost dramatically simplifies the process of assembling cost estimates for

| WBS:                      | 2.5.4.301           |
|---------------------------|---------------------|
| CID:                      | NL0030154           |
| Principal Investigator:   | Dr. Fred Baddour    |
| Period of<br>Performance: | 10/1/2015-9/30/2018 |
| Total DOE Funding:        | \$900,000           |
| DOE Funding FY16:         | \$300,000           |
| DOE Funding FY17:         | \$300,000           |
| DOE Funding FY18:         | \$300,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

precommercial catalysts, enabling synthetic chemists and process design engineers alike to prepare rigorous early-stage economic assessments for the production of catalytic materials. This information enables researchers to (1) focus R&D efforts on areas of greatest cost, (2) make informed decisions based on combined performance and cost data, and (3) guide catalyst synthesis early in development. CatCost was industrially reviewed throughout its three-year development to ensure the accuracy and relevance of the integrated estimation methods and tailor the user interface based on expert feedback. This presentation will highlight the cost estimation methods developed and integrated in FY 2017 and FY 2018, the methodologies for considering spent catalyst value, and demonstrate use cases in which CatCost has been successfully deployed to give insight to the value proposition of catalysts being developed within BETO's catalysis portfolio.

# Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25% Average Score Approach Accomplishments and Progress Relevance Relevance

Weighted Project Score: 8.9

 ${\mathbb I}$  One standard deviation of reviewers' scores

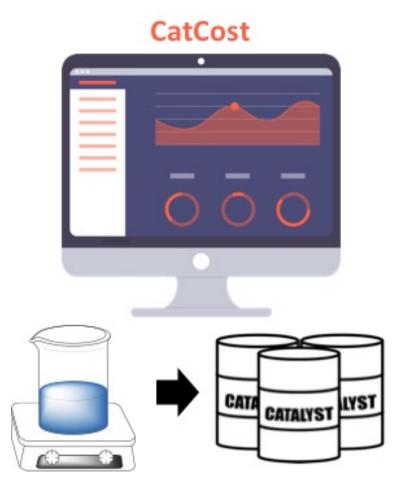


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- The concept of a catalyst cost estimation tool for R&D professionals designing and characterizing new catalytic materials that show technical promise is invaluable. Often, the engineering design basis has to make many assumptions by using the most similar commercial catalyst in order to provide a reasonable estimate for the novel catalyst. With catalyst costs making up close to 4%–20% of the MFSP for some bioenergy pathways, an estimation tool to help design engineers avoid a "show-stopping" commercial factor when moving the project along to greater scales and higher risk is essential. Now with this tool, researchers can make resource priorities at the R&D and front-end loading (FEL)-0 conceptual design phases for projects.
- The catalyst cost-estimating tool is an extremely useful tool for biomass conversion and all chemical processes. The project team has done a remarkable job of collecting the data and rolling it into a usable model. They have produced a usable user interface that is freely accessible to the public. They have included appropriate safeguards to protect internal and external user data because the spreadsheet input and outputs are only stored on the user's computer. Reclamation costs for the catalysts are included. However, the recycling costs do not reflect the consequences of U.S. Environmental Protection Agency regulations, which limit the storage, recycling, and disposal of smaller quantities of catalyst. Also, the market dynamics of metal prices are not adjusted for the new demand added by the catalyst manufacture.

- This is a very nice complementary effort to general catalysis research in the field. It allows those working in a range of fields from material design to scale-up to account, at least partially, for catalyst cost. It's a huge outcome to provide a user-friendly tool to the community, and this group has been very active in improving awareness and educating potential users. Overall, to be commended. There may be slight concerns over deployment and whether a nonexpert can use the tool to generate a meaningful cost, particularly for a more complex catalyst, but the project leads have taken some measures to ensure the robustness of the tool.
- Public availability of a catalyst cost-estimation tool is a service to the field and helps provide more accurate TEA of a particular process. The impact of the work is diminished to the extent that catalyst cost is usually a small percentage of capital and operating costs. What works: Appears to be an accurate method to evaluate costs for precommercial and novel catalysts. What doesn't work: Can't necessarily address nonstandard methods of synthesis.
- The project has successfully developed an excellent tool for both ChemCatBio and the greater catalysis community. It has already shown direct impact on the consortium and will be a valuable tool for researchers and educational efforts moving forward. Some level of continued oversight should ensure the tool evolves to meet the needs of ChemCatBio and other users. It is only focused on catalyst cost, which averages about 10% of total process cost, including process costs to produce the catalyst, which somehow limits the impact. It would be interesting to see mechanisms of incorporating new synthetic methods in the tool. BETO should be encouraged to keep some funding for the maintenance and improvement of the tool. It is especially important to get input from the advanced synthesis effort.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer's feedback and hope that the tool will prove to be valuable in helping researchers prioritize resources at early R&D stages.
- We appreciate the feedback about the utility of the tool and agree that there are some limitations regarding waste handling and market dynamics. We agree that there are a number of external influences that may affect catalyst price and have sought to include these types of boundary conditions into the documentation to make users aware of the potential impact of market and policy factors on catalyst manufacture.
- We thank the reviewer for their insight and agree that there is always a tradeoff between accuracy and complexity. The CatCost tool has been released in two versions with this in mind, with a more visually oriented online interface and a companion spreadsheet that is more flexible and customizable.
- We agree with the reviewer that there are some limitations to the tool regarding nonstandard synthesis methods, but we have included some process templates for synthetic methods that may fall into this category (e.g., millifluidic nanoparticle synthesis). We concur that increasing the types of synthetic methods and templates that are included in the tool will increase the value and reach of the tool.
- We appreciate the reviewer's feedback and hope that we can continue to expand the tool to include additional synthesis methods and manufacturing techniques to be better aligned with the advanced synthesis efforts that are ongoing within the ChemCatBio consortium.

# ADVANCED CATALYST SYNTHESIS AND CHARACTERIZATION

#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

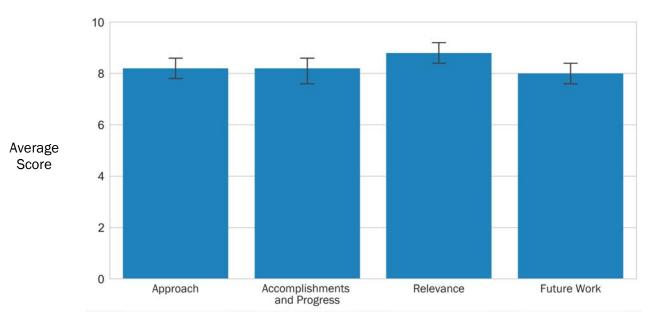
The ACSC project provides fundamental insight into critical research challenges leading to actionable recommendations for ChemCatBio catalysis projects by leveraging world-class synthesis and characterization capabilities across multiple DOE national laboratories. The ACSC was based on a collaboration between ANL and NREL, in which X-ray absorption spectroscopy (XAS) studies performed by ANL at the Advanced Photon Source (APS) user facility coupled with experimental work at NREL identified the active sites responsible for the enhanced performance of a copper-modified zeolite catalyst for the conversion of dimethyl ether to hydrocarbons. This highly successful collaboration

| WBS:                      | 2.5.4.304           |
|---------------------------|---------------------|
| CID:                      | NL0032282           |
| Principal Investigator:   | Dr. Susan Habas     |
| Period of<br>Performance: | 10/1/2017-9/30/2019 |
| Total DOE Funding:        | \$4,427,500         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$1,492,500         |
| DOE Funding FY18:         | \$1,342,500         |
| DOE Funding FY19:         | \$1,592,500         |
| Project Status:           | Ongoing             |
|                           |                     |

identified a need for access to advanced characterization for all ChemCatBio catalysis projects. As the ACSC, this collaborative effort was expanded to encompass (1) *in situ* and operando spectroscopic techniques for bulk and surface structural and chemical characterization, including XAS at ANL, Raman spectroscopy at NREL, and neutron scattering at the Spallation Neutron Source at ORNL; (2) *in situ* and operando spatially resolved imaging and characterization, including sub-ångström resolution electron microscopy and spectroscopy at the Center for Nanophase Materials Sciences at ORNL; and (3) a dedicated synthetic effort focused on developing next-generation catalysts through innovative synthetic routes, including solution synthesis methods for highly controlled nanostructures at NREL and metal organic frameworks at Sandia National Laboratories (SNL). As a

#### Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

ChemCatBio-enabling technology, the ACSC works closely with the CCPC and the Catalyst Deactivation Mitigation for Biomass Conversion project, with cost insight from the CatCost tool, to (1) identify active site structures in working catalysts, (2) inform computational models to predict structures with enhanced performance, and (3) deliver cost-effective next-generation catalysts that exceed performance targets. The ACSC portfolio of capabilities is reevaluated annually to ensure that we are meeting the evolving needs of the ChemCatBio catalysis projects as well as tackling overarching research challenges to enable rapid response to new conversion technologies. Since the start of the project, the ACSC has collaborated with all of the ChemCatBio catalysis projects to provide fundamental insight leading to actionable recommendations for critical research challenges, supported the 2022 engineering-scale CFP verification by enabling improvements to catalyst performance that minimize the loss of carbon, and directly interacted with industry through the nearly 50% of ChemCatBio DFA projects that are leveraging ACSC capabilities and expertise. The ACSC has also facilitated the complete catalyst and process development cycle for the dimethyl ether to hydrocarbons pathway, leading to next-generation catalysts with increased dehydrogenation activity. The end of the threeyear goal is to rationally design bimetallic zeolite catalyst formulations with tailored dehydrogenationhydrogenation activity to enable products with targeted fuel properties. The capabilities and expertise developed for this effort will be leveraged to develop next-generation metal-modified zeolite catalysts with increased C3-C6 olefin selectivity during the conversion of ethanol to distillates, and to assess the accelerated catalyst and process development cycle with the goal of enabling demonstrated performance enhancements in half the time.

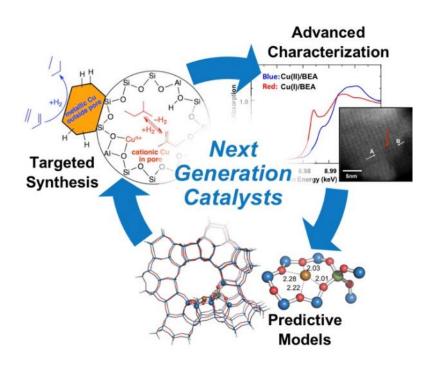


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• Overall, a well-integrated activity that strengthens the entire ChemCatBio project portfolio. The expertise of the group complements the needs of the ChemCatBio projects. The value has been demonstrated in past and existing projects. The future projects ask clear questions, which the current characterization efforts assist in answering. The attempt to remain responsive to the needs of the

ChemCatBio portfolio by introducing new techniques is very important but should continue to be evaluated so the right tools are used in the appropriate settings.

- The ACSC is another solid, good technical story coming out of ChemCatBio with money well invested and the scientific discovery return on investment very important. The ACSC is a well-managed project knowing where their targets, challenges, and milestones lie. They should be applauded by ChemCatBio for their ability to work together across labs as a unified organization that will most likely change the trajectory of the biofuels industry. Their work is impressive, and they understand that they must create actionable recommendations that also allow for practical implementation.
- The ACSC project can impact most of the process development work supported by BETO. The characterization portion of the project has clearly impacted a number of BETO projects and has helped several bioeconomy startups. The synthesis portion is less evolved and has not yet had a major impact. However, it is difficult to show the clear benefits of fundamental research in this area in the short term. It is a high-risk, high-reward project. Most new catalysts are not successful. The work done by the ACSC team is similar to that conducted as part of R&D at leading commercial and government catalyst and development labs throughout the world. There is wide agreement that this work is worthwhile. What makes the ACSC team unique is the focus of the BETO mission and integration into the BETO project teams. One area in which the project is lacking is in the ability to prepare industrial-style formed catalysts. The BETO team relies on outside industry groups to provide this expertise and to prepare the volumes of these types of materials required for testing.
- This is a nice foundational effort that really goes toward enabling all other upgrading research within the various DOE-supported consortia. Susan Habas gave an excellent presentation. It is really difficult to make sense of catalyst performance without an accompanying effort in controlled synthesis and characterization. I like the nice effort toward characterizing materials under reaction conditions and/or complex media (to the extent that the capabilities will allow). Our conventional approach has been to study the reactor performance of a material under steady-state conditions, where the structure of the material is almost certainly different from the synthesized material. This effort goes toward addressing that discrepancy.
- The ACSC project is vital to the entirety of ChemCatBio and meshes nicely with CatCost and CCPC. One area which might be added to the portfolio is a controlled deposition of metal precursors onto catalyst supports (as opposed to solution synthesis of nanoparticles [NPs] followed by deposition). This suite of methods did not appear in the presentation.
- The goal of providing fundamental insight leading to actionable recommendations for critical research challenges by leveraging world-class synthesis and characterization capabilities across multiple DOE national laboratories is certainly a core need for all the projects within the consortium. Integration with the ChemCatBio Data Hub seems to be working really well and the researchers are encouraged to continue this effort. The attempt to remain responsive to the needs of the ChemCatBio portfolio by introducing new techniques is very important but should continue to be evaluated so the right tools are used in the appropriate settings. For instance, neutron efforts should be evaluated to make sure it is suitable for the work being emphasized in this project, as well as have a good justification for inclusion of MOF synthesis work. Also, the synthesis portion of the project was downplayed relative to characterization efforts and should be better highlighted in the future.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for the positive feedback regarding the value of the ACSC project to the ChemCatBio catalysis projects and fully agree that it is important to remain responsive to the needs of these projects and to continue to create actionable recommendations to support the catalysis portfolio.

- We agree that the characterization component of the ACSC has been impactful and was well highlighted during the review, and we will make similar efforts to highlight the synthesis capabilities similarly in the future. The synthesis platform has been critical to advancing the state of technology for a number of catalysis projects. For example, within the IDL project, the synthesis of model catalysts with defined active sites was essential to enabling the identification of the active site for dehydrogenation by operando characterization. Realization of the next-generation catalysts, identified by the CCPC, relied on targeted synthesis methods to controllably incorporate dehydrogenation and hydrogenation active sites. We are addressing the absence of technical catalyst synthesis capabilities by engaging with the Engineering of Catalyst Scale-Up project that started in FY 2019.
- As part of the review, we sought to highlight what we believe are the unique capabilities of the ACSC, including advanced synthesis methodologies. However, the controlled deposition of metal precursors and impregnation-based methods are core components of our catalyst synthesis capabilities and have been instrumental in the development of model catalysts and next-generation materials for the IDL and CFP projects.
- We are encouraged by the reviewer's thoughts on introducing new capabilities into the ACSC project and we will continue to evaluate the suitability of the techniques for the catalysis projects. The neutron scattering characterization and MOF synthesis efforts will be subject to a go-no-go decision point to assess their ability to meet the needs of the consortium, as will all future efforts.

## CATALYST DEACTIVATION MITIGATION FOR BIOMASS CONVERSION

#### **Pacific Northwest National Laboratory**

#### PROJECT DESCRIPTION

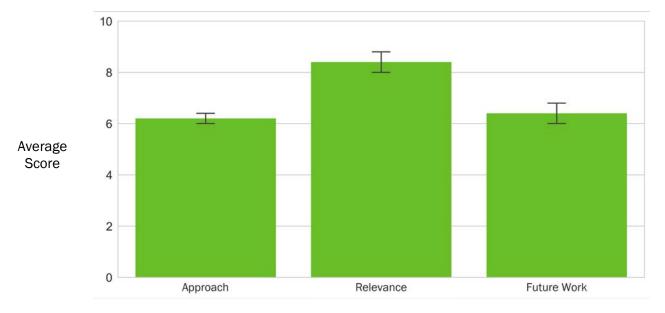
This project is a new "enabling" capability of ChemCatBio for addressing catalyst deactivation issues associated with catalytic conversion of biomass materials. Industrial catalyst lifetimes are on the order of years, while catalysts being developed under ChemCatBio may not see times on stream beyond 500 hours while in early-stage R&D. As an enabling capability, this project serves as an R&D team specialized in correlating catalyst deactivation with characteristics of biomass-derived process streams, identifying catalyst deactivation mechanism, and developing solutions for improved catalyst lifetime, stability, and regeneration.

| WBS:                      | 2.5.4.501           |
|---------------------------|---------------------|
| CID:                      | NL0034446           |
| Principal Investigator:   | Dr. Huamin Wang     |
| Period of<br>Performance: | 10/1/2018-10/1/2021 |
| Total DOE Funding:        | \$300,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | New                 |
|                           |                     |

The concept for this project is based on a systemic need within ChemCatBio to address catalyst deactivation issues. Some unique qualities of biomass materials (e.g., high oxygen content, high moisture content, highly reactive functional groups) bring significant issues to catalyst longevity, which is an overarching challenge for ChemCatBio technologies. Previous successes addressing this challenges include (1) improvement of sulfided catalyst lifetimes for fast pyrolysis bio-oil hydrotreating (extended operation time from approximately 90 hours to 1,400 hours); (2) improvement of reduced metal catalyst for bio-oil hydrogenation (extended lifetime from approximately 150 to 800 hours); and (3) improvement of zeolite catalyst for aqueous phase dehydration of alcohols (over five times improvement of lifetime).

#### Weighted Project Score: 6.8

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

This project will achieve greater success by (1) coordinated and formal collaboration with ChemCatBio catalysis projects; (2) systematic approaches to accelerated deactivation evaluation, deactivation mechanism identification, and development of catalyst regeneration protocols; and (3) documenting, publishing, and communicating summaries of the connections established between characteristics of biomass-derived feedstocks and catalyst deactivation for guiding more rational catalyst and process designs. This project will provide needed information on catalyst deactivation and mitigation to catalysis R&D communities. The Catalyst Deactivation Mitigation project directly addresses the catalysis barrier of improving catalyst lifetime and ChemCatBio's goal of accelerating catalyst development and technology readiness for industrial application.

# Addressing catalyst deactivation challenges associated with unique properties of biomass feedstocks

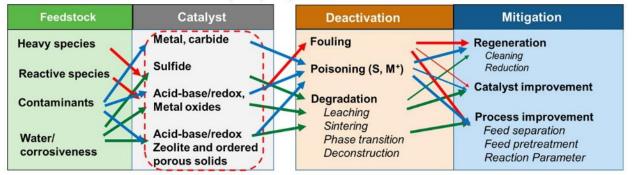


Photo courtesy of Pacific Northwest National Laboratory

#### OVERALL IMPRESSIONS

- This overarching project, along with the theory program, can be a broad but impactful component of ChemCatBio. The initial systems of investigation are "low-hanging fruit" that have been studied in related systems. However, impact can certainly still result in these studies across all the ChemCatBio portfolio. Management of this component seems in order and will be critical moving forward, as the diverse catalysis-related portfolio may be a challenge to home in on specific challenges for maximum impact rather than spread the project too thin.
- This project has the potential of becoming an entire center of excellence focused on deactivation of catalysts in bioenergy applications. This will require many researchers and possibly much more when the time is right. More industrial partners, especially catalyst OEMs, should be involved in this work. The approach of elucidating the various modes of deactivation, controlling rates, and then establishing accelerated deactivation methods is quite plausible. This project has a huge task and requires many more resources and partners.
- Overall, this is an important project that aims to address catalyst stability in a variety of biomassupgrading technologies. It would be helpful to see more specifics about the important modes of deactivation in a specific technology, how they will be investigated, how they will be mitigated, etc. The slide deck would benefit from decreasing redundancy; several figures appear repeatedly and did not seem to add substantially to the discussion.
- Catalyst deactivation is a critical reason for the poor economics of a variety of different proposed biomass conversion processes. Highlighting this problem both in terms of finding ways to assess the long-term deactivation rate and design catalysts with longer useful lives may help develop robust cost-effective processes. The project needs to focus on identifying clear targets and approaches. It would have

benefited from a better discussion of the hypothesis involving catalyst deactivation being studied and the approaches. The impact of the project on BETO projects needs to be more clearly demonstrated.

- The goal of the project—to improve catalyst stability (lifetime) for ChemCatBio catalysis projects through understanding catalyst deactivation and developing mitigation approaches—is surely relevant for the core work of the consortium. This reviewer had more concerns about the presentation being too general rather than the overall idea of the project being faulty. It would be interesting to see more solid and articulated ideas on how to provide stability on the more complicated systems being studied in this consortium, such as the multifunctional systems.
- The correlations, mitigation strategies, and documentation to be produced are potentially valuable. It seemed like more homework could have been done by the authors of the proposed work to identify the needs of the consortium, instead of making one of the tasks to find out what the needs are.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their support of the relevance and potential impact of this new enabling project to the overall program and the fundamental importance of understanding and mitigating catalyst deactivation to the ChemCatBio and scientific community.
- We agree that addressing deactivation is a broad and impactful component of ChemCatBio. As an enabling project, one important objective is to support ChemCatBio core catalysis projects, and this project should target the most impactful process and not "reinvent the wheel." We will work with two multifunction catalysts, Pt/TiO<sub>2</sub> catalyst for CFP and Ag/ZrO<sub>2</sub>-SiO<sub>2</sub> for ethanol conversion. Both processes are unique and recently developed within ChemCatBio for their specific application, and their deactivation and mitigation still require extensive research to extend/verify their lifetime. The study of the two different multifunctional catalysts for different reactions, including simple alcohol or complicate pyrolysis vapor, will not only improve the individual catalyst deactivation issues for similar processes.
- We agree with the importance of having catalyst developers being involved. Modification of catalysts is one approach to address deactivation, and this project will provide an understanding to guide catalyst modification. We will specifically focus on catalyst regeneration to enhance lifetime. We will get input from the industry by subcontracting with an industrial consultant and meeting with an industrial advisory board. We will further identify industrial collaborators and access their inputs.
- We developed the specifics about the hypothesis for modes of deactivation, the approach to investigate and mitigate, and the targets with the core team for the two specific catalytic processes. Based on their current experimental results and understanding of activity-function relationship, we hypothesized a possible deactivation mechanism and mitigation approach. The goal is to conduct an analysis of the working catalysts and specify a hypothesis on the deactivation mechanism and verify through controlled experiments or accelerated aging. Based on the determined deactivation mechanism, the mitigation approach will be developed.
- We discussed extensively with the ChemCatBio catalysis teams to identify the need. We will continue to communicate with them to ensure the most impactful needs to be included. The ChemCatBio catalysis teams include various labs and research areas, and will also have an adjustment of scopes and focus areas, especially in FY 2020, for starting a new three-year project period. We will include the task to ensure a good connection and relevance with the core catalysis projects.

# CHEMCATBIO DFAS: COMPREHENSIVE CHARACTERIZATION OF MIXED-METAL OXIDE CATALYSTS WITH GEVO

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

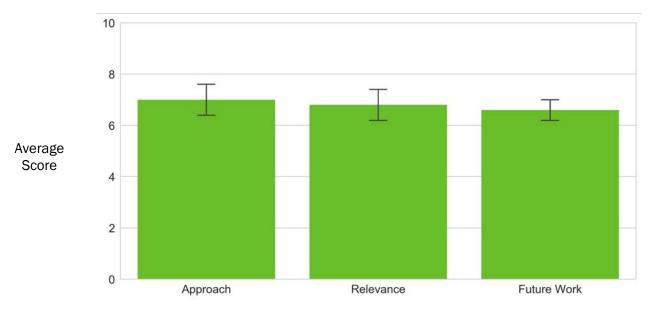
Gevo has developed mixed-metal oxide MMO catalysts to selectively convert biomass-derived C2–C6 oxygenates to olefins and then hydrocarbon fuels to meet DOE 2022 fuel targets. Selective conversion of ethanol to isobutylene with mixed-metal oxide catalysts requires low ethanol feeds to maintain performance. Increasing the feed results in rapid catalyst deactivation. Gevo has increased catalyst stability by adding additional metal oxides. However, variations in performance based on the level and type of additive and catalytic conditions have been observed. This project will use advanced catalyst characterization capabilities and expertise available through the ChemCatBio ACSC project to gain insight into key catalyst features and deactivation

| WBS:                      | 2.5.4.700           |
|---------------------------|---------------------|
| CID:                      | NL0033614           |
| Principal Investigator:   | Dr. Susan Habas     |
| Period of<br>Performance: | 4/1/2018-12/31/2019 |
| Total DOE Funding:        | \$125,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$125,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | New                 |
|                           |                     |

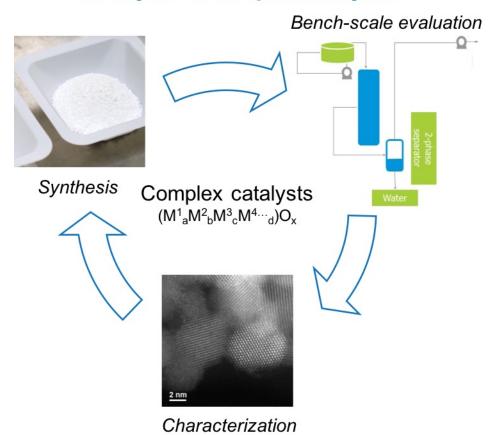
modes with the goal of tailoring catalyst composition to improve performance.



Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores



# **Catalyst Development Cycle**

Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- This is an early-stage project that fits into BETO's strategy model for working with industrial partners on novel catalytic materials that can be launched in a few years. These types of projects are good to keep in the technology pipeline.
- The direct-funded NREL/Gevo characterization of mixed-metal oxide catalysts provided useful data that would aid Gevo's commercial development. This type of limited, highly focused progress is a good example of how the national labs can help improve the economics of biofuel production. While the impact of this program will be somewhat limited due to its failure to enable a major new product route, it will have an incremental benefit on the cost of ethanol. The mixed-metal catalysts identified could be licensed to other ethanol producers. The technology could also be extended to other light oxygenate streams. The benefits to BETO include developing expertise at analyzing commercial catalysts, proving the consortium can impact industry, building relationships with key players in the bioeconomy, and developing joint intellectual property.
- This is a project that allows Gevo to leverage the expertise of the ACSC. Overall, this seems like a good way to answer questions that Gevo would be otherwise unable to address. Comments raised the issue that characterization revealed deactivation modes, but it did not necessarily provide guidance on how to address them with new synthesis and application strategies.

- The collective team appears to lack the expertise with which to infer from the characterization—which revealed that deactivation was correlated to phase segregation of the mixed-metal oxide—what steps could be taken to stabilize the mixed-metal oxide. One wonders if the CCPC could help out here.
- This mid-cycle DFA effectively outlines how the capabilities of ChemCatBio are leveraged to assist in mixed-metal oxide catalyst development in collaboration with Gevo. The intellectual contribution of the ChemCatBio performers is vital to the project and the clear benefit to ChemCatBio is evident, given expanded expertise gained in synthesis and characterization of the complex catalysts. This new knowledge may well assist efforts in complex catalyst development described in other projects within ChemCatBio. Characterization work demonstrating a structure-performance relationship is clear, but catalyst design goals and stability are yet to be demonstrated.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer's positive feedback on the role of novel catalyst development work in collaboration with industrial partners.
- We agree with the reviewer that the highly focused scope of the Gevo project can help to aid Gevo's commercial development. Towards this goal, the project has focused on enhancing the commercial viability of catalysts for both the ethanol-to-olefins process and a new process around fusel oil conversion.
- We agree that it has been helpful for Gevo to be able to leverage the capabilities and expertise of the ChemCatBio consortium, and as such, we have been able to provide them with insight into catalyst deactivation modes. Catalyst development at Gevo based on the insight provided by advanced characterization and corresponding guidance is ongoing.
- With the goal of providing guidance to Gevo around catalyst development based on insights gained from advanced characterization, we have made sure that the team includes catalyst synthesis and characterization experts as well as catalysis researchers from relevant ChemCatBio catalysis projects. We regret our inability to communicate fully the planned catalyst modifications due to intellectual property concerns. However, we agree that collaboration with the CCPC could be useful and opportunities to collaborate will be evaluated.
- We thank the reviewer for highlighting the synergy between industry and ChemCatBio within this project. We agree that the catalyst design and stability goals have yet to be demonstrated, as these are the focus of upcoming efforts in this project.

# CHEMCATBIO DFAS: ADVANCED CHARACTERIZATIONS TO ACCELERATE COMMERCIAL CATALYST DEVELOPMENT WITH VERTIMASS

#### **Oak Ridge National Laboratory**

#### PROJECT DESCRIPTION

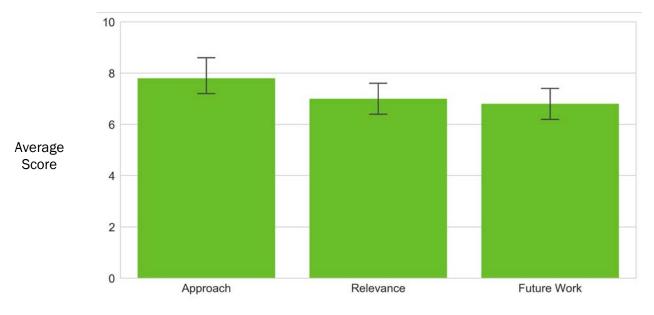
The goal of this project is to provide advanced catalyst characterizations to accelerate Vertimass LLC ethanol upgrading commercial catalyst development. Vertimass has a worldwide exclusive license for catalytic technology originally developed by ORNL in 2014 that converts ethanol into hydrocarbons over metal-modified zeolite catalysts. Vertimass is now taking the next critical step in scaling up to commercialize this technology by moving from pilot-scale catalysts to commercial catalysts. There is a critical need in the extensive catalyst characterizations to correlate the structure to catalyst performance, and to further provide critical information during successful catalyst commercialization and reformulation. In this project, we will utilize ORNL, ANL, and NREL's unique

| WBS:                      | 2.5.4.703          |
|---------------------------|--------------------|
| CID:                      | NL0033618          |
| Principal Investigator:   | Dr. Zhenglong Li   |
| Period of<br>Performance: | 4/9/2018-9/30/2020 |
| Total DOE Funding:        | \$325,000          |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$0                |
| DOE Funding FY18:         | \$325,000          |
| DOE Funding FY19:         | \$0                |
| Project Status:           | New                |
|                           |                    |

catalyst characterization capabilities and experienced staffs to bridge both catalyst synthesis production and catalyst testing at pilot scale (two types of industry partners: a catalyst producer and process engineering company), which will provide valuable catalyst characterization information to accelerate the commercial catalyst development. The characterization information will provide key data to mitigate risk on moving to commercial catalysts, save time and money for both catalyst and process development, and to optimize

#### Weighted Project Score: 7.3

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



L One standard deviation of reviewers' scores

formulation to improve catalyst performance. More importantly, the lessons learned in this proposed work will have a broader impact on the biofuels and bioproducts industry by providing suggestions to avoid unnecessary catalyst development failures and accelerate their commercialization. More specifically, both fresh and used catalysts will be analyzed to examine the structural and compositional changes after ethanol-upgrading reactions. ORNL, ANL, and NREL will provide the following characterizations to understand these catalysts: (1) ORNL will apply scanning transmission electron microscopy (STEM), X-ray 3D tomography, acid sites measurements, thermogravimetric analysis, physisorption, X-ray diffraction, and elemental composition analysis to analyze the metal distributions, coking, and catalyst structural and compositional changes after the reaction; (2) ANL will utilize *in situ* operando X-ray absorption spectroscopy to understand the metal distributions and oxidation states for both fresh and used catalysts; (3) NREL will use solid-state <sup>27</sup>Al nuclear magnetic resonance spectroscopy to examine the changes of aluminum. In the beginning three quarters, this project has provided valuable catalyst structural information to correlate with catalyst performance in the pilot-scale operation. We also developed a correlation between catalyst changes and the water vapor concentration. We will continue to characterize both the fresh and used commercial catalysts to understand the difference between pilot and commercial catalysts.

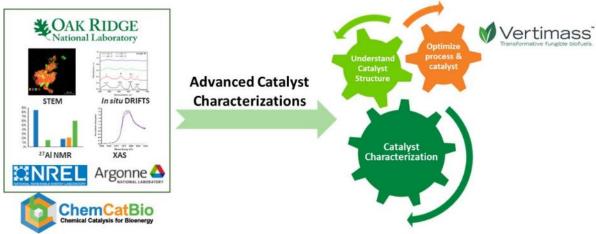


Photo courtesy of Oak Ridge National Laboratory

#### OVERALL IMPRESSIONS

- This project allows Vertimass to leverage national lab tools and expertise to identify modes of deactivation in their catalysts. It was not completely clear that the project is effectively leveraging prior knowledge from partner Clariant. The presentation did not establish a clear path forward for addressing challenges in future work.
- This project has straightforward goals. Smaller industrial organizations often don't have the characterization tools to do this work, so the efforts of ChemCatBio are commendable to help this effort. The communication plan is appreciated showing how frequently and openly the project members will meet. This is important strategy and should be continued. This type of work takes quite a bit of coordination. There was a lot of effort put into the characterization effort in this work using really advanced methods like extended X-ray absorption fine structure, STEM-energy-dispersive spectroscopy and Al-nuclear magnetic resonance (solid state). These are not inexpensive analytical methods and take significant professional resources to maintain, so a careful project plan must be executed to conserve resources. Other members in the CRADA should get involved in this early work. For instance, it would be useful for Clariant to assist from an industrial perspective on the catalyst characterization activities with one of their quality-control labs. All catalyst manufacturers have quality-control labs offering minimal characterization techniques. It may also be useful to see some overlap in the characterization activities between ChemCatBio and Clariant on some parameters to make sure the reproducibility is reasonable. In general, project stewardship using an official, professional project manager taking on major roles to keep tasks moving and hold targets accountable, also serving as conduit with other third-

party vendors, may be a good strategy for this work. The project team should provide quality assurance specifications on the final catalyst material on behalf of Vertimass to Clariant.

- The ORNL/Vertimass project to characterize their ethanol conversion process provided data that was used to develop improved formulations and operating conditions. The ORNL relationship with Vertimass is a great example of how a national lab can work with a startup to push forward new technology. The production of hydrocarbons from alcohols is one of the most promising routes to biomass-derived fuels. The cost of production is the main limiting factor but leveraging development by using the national labs provides support for this development process. However, this type of catalyst development could have been accomplished by Vertimass' commercial partner Clariant without the help of the lab.
- The project seeks to leverage catalyst development for ethanol upgrading, leveraging the expertise of ChemCatBio performers for catalyst characterization. In general, the partnership shows clear value for the company but not so much for the lab/consortium. It is vital these projects are not ultimately merely service relationships. ChemCatBio is uniquely positioned to participate in the project. A higher level of detail regarding the scientific questions studied and approaches was needed to evaluate the project more effectively.
- This is a relatively simple project on catalyst characterization in which a nicely complementary suite of techniques has been assembled. The interpretation of the characterization data is not well presented and calls into question the ability to further refine the catalyst.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that it's useful to leverage the knowledge from Clariant regarding catalyst scale-up. Due to limited presentation time, we didn't cover the role of Clariant clearly. Vertimass has a separate service contract with Clariant to obtain commercial samples. Clariant is not directly involved in this DFA's R&D work. We do have a clear path forward to address challenges in the future work, including characterization of both fresh and spent commercial samples to understand catalyst changes (if any) during ethanol upgrading.
- We agree that some level of interactions with Clariant will benefit the whole project. The ChemCatBio team is planning to discuss this topic with Vertimass and will try to make a reasonable plan within the scope of the project and in light of intellectual property protection.
- We agree that it's helpful to involve Clariant in some typical scale-up characterizations from an industrial perspective. Meanwhile it's critical for ChemCatBio to be heavily involved. ORNL originally developed the new catalyst and has a broad depth of knowledge about the catalyst structures and performance. It's very important to leverage that knowledge to accelerate the understanding of pilot-scale catalysts and commercial catalysts. ChemCatBio provides unique characterizations (e.g., extended X-ray absorption fine structure, advanced STEM) to help Vertimass understand the catalysts. It's critical to keep the involvement of ChemCatBio to accelerate the catalyst development for Vertimass. This is consistent with the reviewer's comment that ChemCatBio is uniquely positioned to participate in the project.
- Ethanol upgrading represents a revolutionary bioenergy technology to produce fungible hydrocarbon fuels and bioproducts from ethanol, one of the largest biofuels produced in the United States. Leveraging ChemCatBio capabilities to accelerate this type of technology development will help to achieve BETO's mission. It also helps to meet the BETO's goal to enable sustainable, nationwide production of biofuels that are compatible with today's transportation infrastructure.
- Not all the interpretations were presented in this short presentation. The characterization information already provides useful insights to Vertimass to help understand catalyst changes under different conditions. We feel confident that we will be able to further help Vertimass with the next level of catalyst development.

# CHEMCATBIO DFAS: ENHANCED CATALYST DURABILITY AND SULFUR TOLERANCE BY ATOMIC LAYER DEPOSITION WITH ALD NANOSOLUTIONS AND JOHNSON MATTHEY

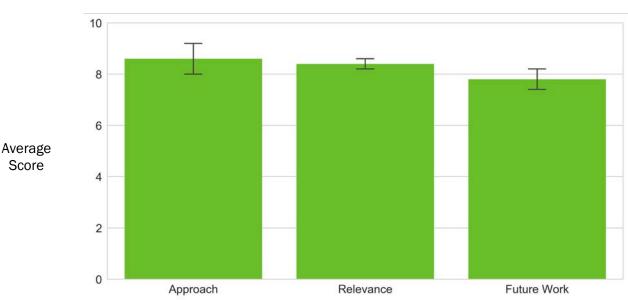
#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

One of the multiyear program goals of ChemCatBio is to accelerate the development of catalysts and related technologies for the commercialization of biomass-derived fuels and chemicals. Biomass processing often requires challenging environments that conventional catalyst materials cannot withstand, leading to catalyst deactivation by leaching, organic fouling, and poisoning. These modes of deactivation result in reduced catalyst lifetime productivity due to the requirement for frequent catalyst regenerations, or, more severely, irreversible catalyst deactivation. The development of a new class of catalytic materials that can address these challenges is critical for the progression of the bioeconomy. Atomic layer

| 2.5.4.706          |
|--------------------|
| NL0033623          |
| Dr. Derek Vardon   |
| 4/1/2018-9/30/2020 |
| \$536,000          |
| \$0                |
| \$0                |
| \$536,000          |
| \$0                |
| New                |
|                    |

deposition (ALD) is a method for improving the durability of catalysts by depositing an atomically thin protective metal oxide coating that still retains access to catalyst active metal sites. This project seeks to develop and advance the industry relevance of ALD catalyst coatings to improve durability and enhance biogenic sulfur tolerance of supported metal catalysts.



#### Weighted Project Score: 8.3

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 ${f I}$  One standard deviation of reviewers' scores

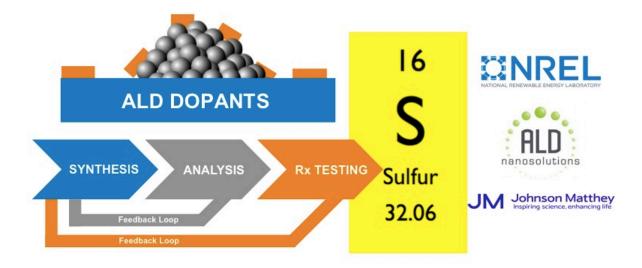
Internally, the NREL project team is composed of technical experts in bench-scale ALD coatings, experimental catalyst testing, characterization, computational modeling, and TEA. Our team includes industry partners ALD NanoSolutions and Johnson Matthey, who are world leaders in ALD manufacturing and large-scale catalytic materials production, respectively. Leveraging the unique capabilities of each partner, the objective of this project is to achieve the goal of improved understanding and accelerated commercialization of ALD for next-generation catalytic materials.

Our project team will achieve this goal by:

- Developing novel ALD-coated catalyst materials to increase durability during muconic acid hydrogenation and catalyst regeneration in the presence of sulfur impurities
- Incorporating computational modeling to address ALD impacts based on a first-principle basis
- Utilizing laboratory-scale findings to inform a final ALD coating formulation for scalable synthesis
- Updating existing ALD manufacturing and process TEA for refined sensitivity analysis at scale.

During the initial stages of this project, we have made progress towards enhanced catalyst stability using targeted ALD coating strategies. We have demonstrated catalyst stability improvements against leaching and sulfur poisoning during the hydrogenation of muconic acid—an emerging biochemical intermediate—to adipic acid. Furthermore, we have shown dramatically enhanced thermal stability of our materials as compared to a conventional, uncoated catalyst. Using data gathered through reaction testing and application of advanced characterization techniques, we have gained materials insights used to inform continued ALD coating refinement by our industrial partners.

Planned activities for the continuation of this project include (1) utilizing computational modeling to inform relationships between ALD coatings and sulfur tolerance, (2) scaled synthesis of ALD-coated materials for validation, and (3) further refining preliminary cost models for ALD manufacturing and bio-based adipic acid production at scale. Collectively, these efforts are progressing the development and commercialization of robust ALD coatings for lowering the cost of biomass conversion through enhanced catalyst lifetime productivity in harsh reaction environments.





#### OVERALL IMPRESSIONS

- In general, a well-integrated effort with clear connection of the resources of ChemCatBio enhancing the partnership in a unique way. Results indicate targets are achievable while also providing some general understanding of catalyst function that may be translatable to other systems and potential technologies. Organized management with clear and achievable milestones suggests continued success for the project in the future.
- Catalyst stability is always a challenge, and biomass-upgrading technologies face some unique challenges, particularly in liquid media and when upgrading crude feedstocks. ALD provides a nice way to stabilize metal nanoparticles against various deactivation modes, and so this project could have a significant benefit to process economics.
- This project had a well-organized presentation and story. This project has a good start at reaching the end-of-project objectives, especially in the area of critical partnerships.
- ALD has been shown to produce unique catalytic materials with superior performance; however, it has not been used commercially because of perceptions that it is difficult and expensive. Developing a cost-effective way to produce a catalyst with controlled structure by atomic deposition has long been the goal because it is believed that this approach can yield unique performance. This project is an industry and national lab collaboration aimed at determining how this can be done practically. It leverages the developments in the commercial application ALD to the production of sensors and electronic products. It couples the nanoparticle and atomic deposition skills, testing and computational skills of the national labs with industrial catalyst suppliers. NREL characterization capabilities provide critical information for adjusting the preparation procedures. The project would not be possible without the direct funded project team that brought together capabilities from a government lab, ALD NanoSolutions, ForgeNano, and Johnson Matthey.
- Initial work on a small-scale batch of sample shows promising results for NP stability and reactivity durability, though sulfur resistance is yet to be tested. No details are provided on the means for scale-up; this will be critical for the method to be translated to industry.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We appreciate that the reviewers of the DFA ALD found value in our approach to address catalyst deactivation through improved material design. Per the reviewers' suggestions, the DFA ALD project team will continue to leverage the private-public partnership to address major cost and scaling barriers for catalyst stabilization by ALD. In addition, future efforts will specifically address scale-up concerns as downselected materials are identified in the project. Ongoing sulfur tolerance testing will inform which ALD coatings are of most interest based on process cost considerations. The DFA ALD team thanks the reviewers for their support of this effort and constructive feedback for project next steps.

# CHEMCATBIO DFAS: CATALYST DEVELOPMENT FOR SELECTIVE ELECTROCHEMICAL REDUCTION OF CO<sub>2</sub> TO HIGH-VALUE CHEMICAL PRECURSORS WITH OPUS 12

#### National Renewable Energy Laboratory

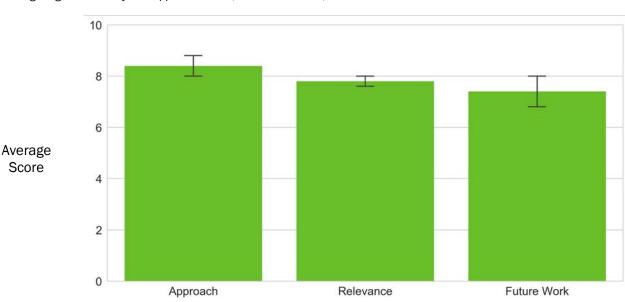
#### PROJECT DESCRIPTION

Cost-effective electrochemical reduction of  $CO_2$  (ECO2R) is considered one of the holy grails of green chemistry. ECO2R combines just three inputs:  $CO_2$ , water, and electricity, and converts them into cost-competitive fuels and chemicals. However, widespread commercial fuel and chemical production via ECO2R 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, over 4.5 million metric tons per year of  $CO_2$  are generated from existing domestic biorefineries. Utilization of this domestically produced

| WBS:                      | 2.5.4.707           |
|---------------------------|---------------------|
| CID:                      | NL0033625           |
| Principal Investigator:   | Dr. Fred Baddour    |
| Period of<br>Performance: | 1/1/2018-12/31/2019 |
| Total DOE Funding:        | \$250,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$250,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | New                 |

CO<sub>2</sub> to make fuels and chemical products has the potential to create a multibillion-dollar market.

The core innovation developed by Opus 12 is a reactor design that enables ECO2R in a polymer electrolyte membrane (PEM) electrolyzer. A novel polymer blend and CO<sub>2</sub>-reducing transition metal NP catalysts on carbon in the cathode layer transform a PEM water electrolyzer into a PEM CO<sub>2</sub> electrolyzer. The goal of this



#### Weighted Project Score: 8.0

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 ${f I}$  One standard deviation of reviewers' scores

project is to gain a fundamental understanding of the impact of metal NPs and carbon support physical properties on electrochemical CO<sub>2</sub> reduction performance. Leveraging the synthesis and characterization expertise developed within the ChemCatBio consortium through the ACSC project and the advanced PEM diagnostics developed by the Hydrogen and Fuel Cells group at NREL, this project seeks to generate insight that enables the development of customizable reactors that can convert CO<sub>2</sub> with high selectivity to CO, CH<sub>4</sub>, or C2+ products for the specific needs of customer segments within the biofuels and bioproducts industry.



Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- This targeted project seems to have a logical partnership between the performers. Results appear promising, both in catalyst development and performance. While scant on some details that could be valuable in assessing fully the current and future trajectory of the project, the NREL portion provides a unique expertise in catalyst synthesis and characterization that is clearly valued by the industrial partner.
- This program has a great long-term future with a potential for many breakthrough design optimizations that can reach commercial application swiftly. The overall spend of the project is quite reasonable for the commercialization story being told from the partnership. Funding should continue for this work, especially with the TEA/LCA efforts. The opportunity to develop large-scale electrochemical units for the future integrated biorefinery is critical and needed for the bioenergy industry. The project team should continue to be more transparent about technical barriers to solicit support across BETO with the cross-cutting efforts and CCPC.

- This is an interesting and important effort geared toward electrochemical upgrading of CO<sub>2</sub>; however, the level of detail was somewhat light. This may be due to nondisclosure agreement requirements from the commercial partner, but it is a difficult to assess the project without full technical details.
- It is not clear how the second-generation catalyst will be improved over the first-generation catalyst. The products of the reaction are not specified, nor is there a TEA to justify the expense of running the cell.
- The ability to convert CO<sub>2</sub> to fuel and chemicals would be a major boon to the fight against global warming. Electrochemical catalysis is one of the more promising approaches because it would allow the conversion of renewable electricity available from a variety of sources into an easy-to-store high energy density liquid fuel. Demonstrating improved performance and determining the potential costs are critical for the continued development of the technology.
- The topic is the investigation of catalysts for electrocatalytic CO<sub>2</sub> reduction. This targeted project seems to have a logical partnership between the performers. Results appear promising, both in catalyst development and performance. While scant on some details which could be valuable in fully assessing the current and future trajectory of the project, the NREL portion provides a unique expertise in catalyst synthesis and characterization that is clearly valued by the industrial partner. Opus 12 in return provides the lab feedback of the performance of the materials. There is a clear advantage of obtaining some expertise on electrocatalytic CO<sub>2</sub> reduction for the consortium.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewer for their positive feedback and regret our inability to communicate fully the results due to intellectual property concerns.
- We appreciate the reviewer's feedback that this type of collaborative effort is necessary to address many of the economic and technical barriers of highest priority to BETO. We agree that increasing the transparency around this type of effort may assist in achieving these targets and expanding opportunities to collaborate across ChemCatBio.
- We have targeted established methods to modify the first-generation materials related to increasing current density and catalyst lifetime for Opus 12's targeted products. The current scope of the collaborative project has focused on catalyst development and characterization at NREL and evaluation at Opus 12 with the economics surrounding the process are ongoing at Opus 12.
- We agree with the reviewer on the promise of electrochemical catalysis and the value in demonstrating performance and understanding the economics of deployment of this technology.
- We appreciate the reviewer's insight and agree that there is an advantage to expanding the expertise in electrocatalytic CO<sub>2</sub> reduction for the ChemCatBio consortium as a whole.

## CHEMCATBIO DATA HUB

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

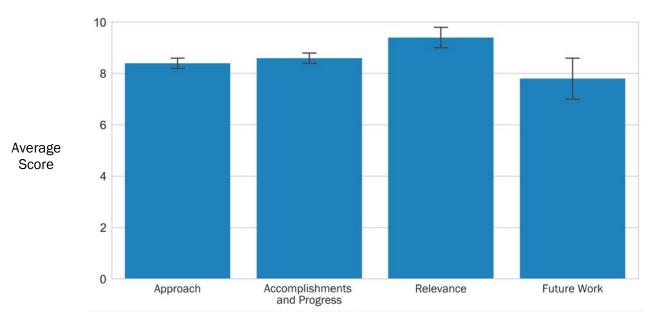
The goal of this project is to accelerate the catalyst and process development cycle by establishing the ChemCatBio Data Hub for (1) centralized and secure data storage, sharing, and analysis and (2) development and application of publicly available advanced analytics tools to provide predictive capabilities for catalyst research and development. Toward the first goal, a secure data repository for storage and sharing of data amongst project team members has been constructed, and a data release process for knowledge dissemination through sharing of data with the public has been established. Alongside the repository, this project develops and releases plug-ins for ease of data upload, search, filter, and visualization while allowing data to be easily and quickly mined and

| WBS:                      | 2.6.2.500           |
|---------------------------|---------------------|
| CID:                      | NL0033706           |
| Principal Investigator:   | Dr. Carrie Farberow |
| Period of<br>Performance: | 11/1/2017-9/30/2020 |
| Total DOE Funding:        | \$400,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$200,000           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

processed into formats that provide key actionable information to researchers. The design and development of data tools in this project are achieved through (1) continuous input from ChemCatBio researchers ensuring that deliverables are responsive to researcher needs and (2) close collaboration with the other DOE Energy Material Network consortia to avoid redundancy and address common and complementary data analysis needs efficiently. With the data repository in place, based on researcher feedback obtained through the FY 2018 go-no-go, the focus of this project has now shifted heavily toward the development of transformational tools to enable predictive capabilities in catalyst research and development. Specifically, the ChemCatBio Data Hub project aims to develop a pathway-independent catalyst design engine, which will be a publicly available tool



Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

for application by both ChemCatBio researchers and the bioenergy industry. The catalyst design engine tool would consider the critical tradeoff between predicted performance and material costs to accelerate the design of optimized catalyst formulations for the production of a diversity of end products from biomass and waste resources.

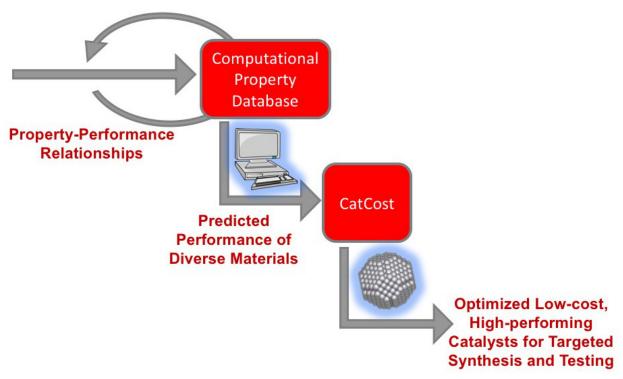


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- The ChemCatBio Data Hub is an important component of ChemCatBio. No real issues with the presented objectives, structure, and future goals. The researcher-centric approach is great to ensure maximum use and potential impact. Performers should continue to strive to implement new concepts to better manage and use data in innovative ways.
- This is an exciting project for ChemCatBio, and resources should be dedicated to make sure it continues to upgrade in functionality year after year. The catalyst design engine will be a major innovation. ORNL has a long and documented history of successful software application launches, and they should be engaged at some point in the future before the next few version releases. There is a story in cost savings and efficiency that must be told at some point. This metric should be established as a measure of success, as well as usage and any other business-process streamlining benefits like the sample management tool.
- This is a very timely effort that seeks to centralize data and make it accessible to project partners to streamline collaboration. I think we see considerable duplication of efforts in catalysis research, and I like the effort that has gone into providing unique sample identifiers that code data about specific materials, etc. I would love to be able to log into this type of a repository and view, for example, binding energies, vibrational spectra, reaction mechanisms, etc., so I think this can provide a very powerful impact for the greater catalysis community. The PIs may need to take additional precautions in providing extremely user-friendly tools to a public audience. The tools will ultimately be crafted to be easy to use; however, the methods they depend on are actually sophisticated and require detailed knowledge. There is some concern that an uninformed user might generate bogus outputs and give them undue weight

because they are generated by a tool that has been vetted by experts. I used the example of Gaussian software in our discussions about this project; it is extremely easy to use and so it often gets misused.

- The ChemCatBio Data Hub is an enabler of the consortium project and provides public access to BETO project information that can be used to advance biofuel development. This is increasingly important as BETO and the national labs move to a more collaborative and consortium-oriented approach to research. A single gateway to the publicly shared computational tools is particularly useful. The approach taken by the project of integrating user feedback throughout the process is appropriate. In the past, the need for multistage review has delayed the release of reports and information to the research community. This needs to be balanced with the need for accuracy and control of proprietary information. The ChemCatBio Data Hub project should be expanded to allow the inclusion of more tools and perhaps data from outside sources; this would require some additional curating. It would be good to continue to support this project in the future to maintain and expand the database.
- The group should strive to implement a clear mechanism to require/maintain data storage. Data storage and data tools are very distinct efforts, and both are important.
- The group is also encouraged to have a mechanism to receive feedback from users to measure their success. Also, performers should continue to strive to implement new concepts to better manage and use data in innovative ways (machine learning/advanced data mining). Another missing objective is use of the data for benchmarking purposes.
- The ChemCatBio Data Hub is the easy-access bank vault and safety net of the ChemCatBio consortium. Data storage, manipulation, and retrieval is a very necessary, if not glamorous, role to have. It will be interesting to see how the catalyst development engine pans out.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The ChemCatBio Data Hub project thanks the reviewers for support for the project goals and insightful feedback. The team will work throughout the coming year to implement the recommendations. The reviewers identified the need to establish a metric for measuring project success in terms of cost savings or process efficiency. This project's FY 2019 annual milestone requires comparison of a conventional data analysis workflow with a workflow enabled by tools developed to demonstrate a 50% reduction in time used to share, store, or analyze data. Thus, we agree that demonstrating achievement through similar quantitative metrics should remain a criterion for project success. As noted by the reviewers, misuse of tools developed is a concern that warrants careful consideration. Public release of any tool will be accompanied by a publication and documentation to advertise tool features, define assumptions, and provide clear guidance on application. While we acknowledge we cannot eradicate misuse or misinterpretation, we firmly believe the value of the transformational tools envisioned necessitates continued development and deployment despite this concern. Ultimately, it is the responsibility of the user to follow best practices in research toward tool application. We agree with the reviewers' point that extensive and diverse data are needed for predictive tools. Current efforts toward developing a computational catalyst property database are not limited to data generated within ChemCatBio; greater than 95% of the data in the database to date are published data generated by external organizations. In the future, should the project scope enable development of similar public databases of experimental data, processes to incorporate data from external organizations will be included. Similarly, we agree that it is desirable to utilize the databases developed for benchmarking, and while it was not discussed in detail, this is within the scope of current goals. The reviewers recommended engaging experts to plan a software release. We agree and have initiated discussions with the NREL technology transfer team and will proceed with leveraging software development expertise at the other national labs. Lastly, the reviewers' suggestion to establish a clear mechanism for user feedback is well taken and will be integrated in FY 2020 milestones.

# LIGNIN UTILIZATION

TECHNOLOGY AREA

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## INTRODUCTION

The Lignin Utilization Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place on March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 11 projects were reviewed in the Lignin Utilization session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$20,312,772, which represents approximately 2.4% of the BETO portfolio reviewed during the 2019 Peer Review. During the Project Peer Review, the principal investigator (PI) 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 approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the Lignin Utilization Technology Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. Jay Fitzgerald as the Lignin Utilization Technology Area Review Lead, with contractor support from Ms. Jessica Phillips (Allegheny Science & Technology). In this capacity, Dr. Fitzgerald was responsible for all aspects of review planning and implementation.

## LIGNIN UTILIZATION OVERVIEW

Lignin constitutes 15%–40% of biomass carbon, but it is currently considered a waste stream in biorefineries, generally burned for heat and power. Techno-economic modeling suggests that for current biochemical routes to hydrocarbon fuels to be economically viable, lignin must be transformed into a higher-value coproduct stream that is able to reduce effective fuel cost by >\$2 per gasoline gallon equivalent (GGE). Given BETO's focus on large commodity markets for coproducts, analysis suggests that >40% of the carbon in a lignin-rich stream will need to be converted into value-added products in a biochemical conversion process to achieve this reduction in fuel cost.<sup>1</sup>

The Lignin Utilization Technology Area focuses on research and development (R&D) of biological, thermochemical, and hybrid approaches to lignin valorization in support of cost reduction for biochemical conversion pathways. Approaches to valorize lignin fall into two main categories:

- 1. Breaking lignin down into small molecules and upgrading those into value-added products
- 2. Utilizing the native structure of polymeric lignin for materials applications.

Projects in the Lignin Utilization Technology Area work closely with projects in the Biochemical Conversion Technology Area and the Bioprocessing Separations Consortium to utilize real lignin streams and produce purified products.

<sup>&</sup>lt;sup>1</sup> Davis, Ryan, Nicholas Grundl, Ling Tao, Mary J. Biddy, Eric C. D. Tan, Gregg T. Beckham, David Humbird, David N. Thompson, and Mohammad S. Roni. 2018. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-71949. https://www.nrel.gov/docs/fy19osti/71949.pdf.

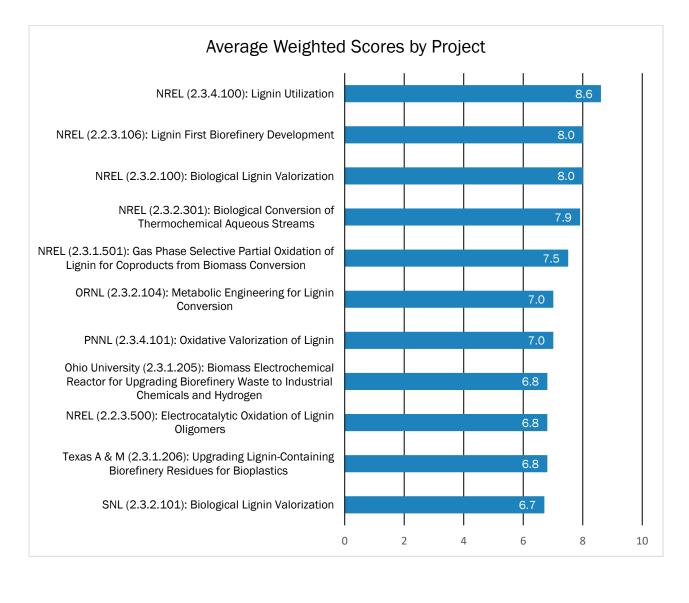
## LIGNIN UTILIZATION REVIEW PANEL

The following external experts served as reviewers for the Lignin Utilization Technology Area during the 2019 Project Peer Review.

| Name               | Affiliation                   |
|--------------------|-------------------------------|
| Emma Master*       | University of Toronto         |
| Joseph Bozell      | University of Tennessee       |
| Matthew Tobin      | Matthew B. Tobin Consulting   |
| Jeff Scheibel      | J. J. Scheibel Consulting LLC |
| W. Michael Sanford | Prisma Renewable Composites   |

\*Lead Reviewer

## TECHNOLOGY AREA SCORE RESULTS





## LIGNIN UTILIZATION REVIEW PANEL SUMMARY REPORT

#### Prepared by the Lignin Utilization Review Panel

A broad range of conversion strategies and product targets are represented by BETO's Lignin Utilization Technology Area projects. Both physicochemical and biological pathways are represented, including electrochemical and solvolysis approaches, improved and low-cost oxidation catalysts, and engineered microorganisms with ability to funnel useable lignin monomers to specific chemicals. Moreover, multiple projects directly integrate upstream lignin processing technologies with downstream bioconversions to specific products. A good example of this is the Coprocessing of Lignin and Residual Sugar (CLARS) process, which demonstrates improved overall product formation through low-severity pretreatment of the starting biomass. Likewise, the Lignin First Biorefinery Development project improves upon thermochemical approaches with its reductive catalytic fractionation (RCF) method to stabilize reaction products from lignin, ultimately producing aromatic monomers and oligomers of value or that can be funneled to specific end products through microbial processes.

Lignin breakdown strategies mainly concentrate on carbon-carbon (C-C) bond cleavage, but also include carbon-hydroxyl group (C-OH) conversion to the more reactive carbonyl group (C=O) functionality. Synthesis of lignin model compounds, application of robotic systems for sample handling, and robust application of statistical methods have together advanced the development of technologies that convert industrially relevant lignin streams into targeted end products.

The main products targeted to date include diacids (e.g., muconic acid, adipic acid, terephthalic acid, and itaconic acid), medium-chain alcohols, polyhydroxyalkanoates (PHAs), aromatics, hydrogen, and low molecular weight lignins for resin applications. The multiple end products considered reflect the complexity of the starting material and its potential value in many applications.

Each project demonstrated good relevance to BETO's overall effort to reduce biofuel costs through coproducts from underused biomass fractions. As next steps, it will be important to consider challenges relating to technoeconomic analysis (TEA), technology scale-up, and product recovery.

Project presentations included reasonable descriptions of the project management process and approach, including resources, skills, critical success factors, goals and objectives, and meetings/interactions. However, some reviewers noted that risk analysis (identification, weighting, and mitigation) was underrepresented in most projects. More rigor here would be a welcome upgrade and would help to prioritize project tasks and derisk project activities.

#### IMPACT

Lignin represents a significant challenge to the biorefinery, as its heterogeneous structure (as either native or technical lignin) has historically seemed to defy efforts to accomplish its selective conversion to high-value products. The projects chosen by BETO hold the potential for overcoming this challenge.

Biochemical work being supported by BETO targets a 40% yield of usable monomers from isolated, technical lignin, which is an ambitious goal in itself. The program further aims to use genetically modified *Pseudomonas putida* to convert those monomers to key industrial chemicals, including various diacids, medium-chain alcohols, and PHA. Despite a potentially growing market, the choice of PHAs as a target product may be a difficult one, as there is a history of commercialization difficulties. Licensing activity around some of the developed PHA technology signals industrial interest; however, the focus on PHA would be strengthened by performing a TEA to consolidate assumptions, and clarification of whether this effort generates PHAs that are significantly different than those generated through previous work.

*P. putida* strains were developed that transform syringol and compounds from syringyl lignin. In most cases, however, engineered *P. putida* strains were tested for ability to convert ferulate or *p*-coumarate to targeted diacids and medium-chain alcohols, with typically 30% conversion efficiency. DOE's Agile BioFoundry Consortium, along with DOE's large-scale sequencing and synthetic biology platforms, are expertly leveraged by the lignin bioconversion projects. By consequence, these projects have already demonstrated the potential to biologically funnel defined lignin-derived compounds to specific chemicals, while uncovering fundamental insights into regulation circuits and tolerance mechanisms that influence lignin bioconversion efficiency. The eventual impact of this program will depend on ongoing efforts to directly funnel complex and changing aqueous streams resulting from lignin pyrolysis or other pretreatments. Moreover, as there are few industrially useful (and manipulatable) organisms available, a licensing or other customer-friendly approach to getting new *P. putida* strains into industry hands could further advance BETO objectives.

Parallel to bioconversion pathways, BETO complements their long-term thermochemical efforts to convert lignin via pyrolysis with electrochemical options for controlled depolymerization to aromatics and hydrogen gas, as well as improved oxidation catalysts for C-C bond breakage. Bond cleavage between lignin monomers and oligomers has been highlighted previously as a critical node in achieving favorable economics via lignin valorization. To convincingly demonstrate the impact of corresponding advances, however, it will be critical to prove economic conversion of complex mixtures to specific final products. The program would further benefit from a clear description of how the newly developed catalysts and approaches offer advantages over similar, earlier efforts that evaluated a wide range of conditions and catalysts.

As a whole, the impact of the lignin effort benefits greatly from the National Renewable Energy Laboratory's (NREL's) analytical capacity for lignin analysis. Two of the current lignin projects expand upon this core capacity by synthesizing new lignin compounds that support the analytical characterization of processed lignin samples or are used in microbial and enzyme screens. Compounds that support biological screens provide a differentiating resource, because we can only find what can be screened for, and many compounds relevant to lignin conversion cannot be bought commercially. So far, compounds developed for screening reflect native lignin structures. This is valuable for some projects—for example, the Lignin First Biorefinery Development project. As a next step, however, compound synthesis for biological screens ought to leverage the information now available through other projects, which clarify main lignin structures present in pretreated lignin streams that remain difficult to biologically convert to target chemicals.

Relating to this aspect, the impact of both bioconversion and physicochemical conversion efforts suffer slightly by the use of lignin model compounds or representative native lignins, which likely have little connection to the actual structure of the technical lignins available for conversion to high-value products. To this end, each project would be strengthened by defining exactly the sources of lignin intended for use.

#### INNOVATION

Scientifically, the panel was presented with a solid and innovative program. The scientific strength of the program was illustrated by the effort to frequently publish research results, and in top journals. Moreover, the program contains efforts to understand the molecular-level processes that control lignin conversion. For example, the Pacific Northwest National Laboratory (PNNL) and NREL efforts to understand mechanisms in lignin pyrolysis may lead to greater process control and address the very long-standing issue of product complexity in lignin thermochemical conversion. More broadly, incorporation of these types of fundamental efforts need to remain at the core of biomass research efforts, as it couples basic scientific knowledge to successful biorefinery development and bridges fundamentals with applications. The willingness of BETO to include such efforts—in contrast to efforts supported by earlier incarnations of BETO—is a real strength of the program.

The program has identified adipic acid as a key industrial target from their lignin conversion work, and a successful development of an industrially viable production of bio-based adipic acid from lignin would be truly innovative. Nonetheless, the program's focus on ferulate and coumarate as adipic precursors would be

strengthened with a clearer justification of why (yield, conversion, availability) these are good models of what the biorefinery will actually have to work with. The same question would apply to the choice of base-catalyzed depolymerization (BCD) lignin as an initial feedstock. If (1) BCD lignin fails to be recognized as a viable industrial starting material and (2) the amount of ferulate/coumarate is insufficient to make an economic case, do these processes have a chance to be adopted at a commercial scale? The program needs to be clear that it is not backing into a pretreatment simply because it gives the largest amount of the substrates (ferulate/coumarate) needed for bioconversion. If industry determines that other pretreatments are better, this work will remain scientifically interesting, but will fail to meet larger BETO goals.

#### SYNERGIES

Presentations in the lignin session did a good job in describing existing and possible synergies. A particular strength was seen in the NREL effort where multiple presentations by different PIs referred to one another and how their work was informing a colleague's effort. The NREL electrochemistry project is attempting to increase the utility of lignin oligomers generated during BCD deconstruction. NREL's biochemical work is trying to convert the small amount of lignin generated during thermochemical treatments. Electrochemical transformation of lignin incorporates work from the electrochemical CO<sub>2</sub> reduction project. The panel saw again and again that problems arising in one project were addressed in parallel projects. The program's multipronged approach to lignin conversion and utilization frequently described applicability to parallel efforts in pyrolysis, biological funneling, and oxidative or reductive conversion.

Whereas projects led by national labs appear to be tightly integrated, the competitive projects appeared less well connected. For example, both Oak Ridge National Laboratory (ORNL) and Texas A&M University described work on PHAs in their projects. A clearer description of the level of integration and coordination between the labs continuing to examine PHAs would be helpful. Notably, the presentation from Texas A&M University was rather long, and yet it was difficult to discern specific advances since the last review and rationale for changes in direction (e.g., apparent discontinuation of laccases). Emphasizing connections between PHA projects across BETO is strongly recommended.

Similar aims and approaches were also noted between the Ohio University and NREL electrocatalysis projects. Despite this, the only point of connection appeared to be the provision of lignin by NREL to Ohio University. Clarification on how these efforts differ from one another (other than specific product targets) is important.

Mutual benefits are expected through closer collaboration of national lab and competitive projects, given the availability of complementary analytical tools, data analysis methods, and TEA expertise.

#### FOCUS

First and foremost, BETO's willingness to support multiple projects and approaches to lignin conversion is a real strength and must remain a driver in future work—the technology for lignin conversion still requires a broad-based and flexible effort to define the best approaches, even if it takes longer to reach an answer.

The project reviews, however, would have benefitted from a more detailed description of the base case biorefinery. The background information presented by BETO (e.g., block diagrams in the *Multi-Year Program Plan*) are clear at a high level, but the specifics of the feedstock, separation processes, and targets being used as benchmarks for GGE analysis would provide a better understanding of the value and feasibility of each project. For example, additional context would clarify if the base case is using a pretreatment that is scalable and likely to be adopted by industry. This is particularly relevant for electrochemical approaches, where important advantages (e.g., selective lignolysis, hydrogen cogeneration) must be shown in light of an overall process to justify the apparent complexity of this option. Additional context would also clarify the merit of generating monomers from lignin that are also generated from carbohydrates (e.g., adipate, muconate). Similarly, deeper context would help to underscore key differences between the hydrogenolysis work through the Lignin First Biorefinery Development project and the similar work being actively pursued through the BioEnergy Engineering for Products Synthesis program at Spero Energy.

Bioconversion research teams have made an impressive and focused effort to develop *P. putida* as a platform host for lignin conversion to valuable chemicals. Many fundamental insights have emerged from that work, which also have applied relevance. Moreover, molecular tools and methods established along the way provide an important resource for the broader research community. Whereas the concerted effort to engineer *P. putida* for lignin conversion presents a strong point of focus that links several research teams, it will be important to further justify this strategy in light of the potential advantages afforded by microbial communities, especially when attempting to transform particular toxic process streams.

Several projects presented a well-organized TEA template developed at NREL. However, this methodology was not employed uniformly. There is an opportunity to use the TEA more effectively as a research tool, to focus efforts, and illustrate the most feasible technology development pipelines. For example, a TEA for technologies at initial, mid, and final stages of the project could help teams (1) report progress in terms of the percentage of the way to reaching an economically feasible solution and (2) point to specific constraints to economic feasibility, uncovered by the TEA, which then informed their research direction.

At the same time, there is an opportunity to develop a "TEA-light" evaluation so that a promising program would not be missed because sufficient data were not yet available to confirm feasibility. This type of evaluation would be a "best-case" scenario to prioritize low-TRL projects where the cost of an effort could be evaluated assuming each step reached the maximum possible yield (i.e., a simple demonstration of broad economic possibility), but, more importantly, an initial demonstration of where the greatest impact of research would be on the cost of a process.

#### TECHNOLOGY DEVELOPMENT PIPELINE

Each lignin project demonstrated high scientific quality; however, in several cases, the path to commercialization was less clear. This may not be a weakness at this stage—the concept of selective lignin conversion is still poorly understood, and the efforts to carry out more fundamental efforts is worthwhile. It should be given sufficient time to reach fruition without being fully driven by efforts to reach commercialization.

However, even at a preliminary stage, a project's discussion of potential industrial utility needs to make sure that their rationale is well laid out. As an example, the NREL project in gas phase lignin oxidation of lignin to phenols describes a coproduct value of about \$0.90/lb. If this is the value used in the TEA, it appears at odds with the price of pure phenol that only commands a value of \$0.40–\$0.50/lb. As another example, in a conservative industry such as wood products, it is difficult to envision ready acceptance of electrochemical processes, despite the large amount of interesting transformations that it can enable. In this case, rather than production of phenolic resins where many options already exist, it will be important to demonstrate a pipeline to products that leverage unique transformations from electrochemical processes.

For several projects, the corresponding TEA shows that research has led to a projected reduction in cost. However, it was not clear that they could achieve the numbers necessary to make the best use of lignin in the portfolio. It would be helpful to clarify/justify the metrics used when reporting product targets. For example, reporting gram of product/gram of lignin would help compare technologies and their progress. Relating to this, corresponding metrics should be in terms of the initial lignin source, rather than only isolated individual phenolic streams.

Lastly, scale-up required to achieve commercial relevance and plans for product recovery will be important to carefully consider as a next step. In most cases, such challenges were not addressed in the project presentations. A hard look at scalability risks and product recovery options is needed to demonstrate a convincing technology development pipeline.

#### RECOMMENDATIONS

The review panel sees the following as key recommendations for the program going forward:

- Continue the multifaceted approach by supporting multiple lignin conversion efforts. This strategy will be critical to understanding the technology space needed for selective and high-value use of lignin. At the same time, strengthen each project by supporting efforts to carefully consider anticipated challenges relating to scale-up and product recovery.
- The integration of science and molecular-level understanding with industrial applications should continue, as this will form the best foundation for process development and control. As part of that effort, support research activities that utilize industrially relevant lignin sources, and synthesize the most challenging lignin-derived compounds for bioconversion processes.
- There are opportunities to improve the focus of the program, but it must not be done at the expense of promising but unproven approaches to lignin conversion. TEA approaches can be used as a tool to help uncover the most important research questions. For example, the technology development pipeline for each project could be extracted from a TEA performed at initial, mid, and final stages of the project. As part of that effort, teams could highlight examples where a TEA informed the research direction, and clarify metrics as well as key assumptions (e.g., product yield based on relevant lignin source, anticipated market size for targeted products, anticipated environmental benefits).
- Where numerous lignin monomers are obtained, teams should look for ways to group together these monomers or dimers, maximizing total yield for alternative high-value uses. For instance, one suggestion is to sulfonate the mixture to provide water-soluble chelant mixtures, which may be applicable for industrial use.

## LIGNIN UTILIZATION PROGRAMMATIC RESPONSE

#### OVERVIEW

The program would like to thank the reviewers for their time and thoughtful comments throughout the review process. The program responses to reviewer recommendations are found in the following section.

#### Recommendation 1: Portfolio diversity.

The panel recommended continuing to support multiple approaches to lignin valorization to ensure industrial relevance while strengthening approaches to scale-up. The program will continue to invest in a variety of lignin valorization technologies while ensuring that at least one technology will be able to be benchmarked for a state of technology. We are also actively pursuing scale-up challenges through multiple competitive awards involving industry as well as the BETO Bioprocessing Separations Consortium.

#### **Recommendation 2: Fundamental understanding and lignin sources.**

The panel recommended continuing the integration of molecular understanding with industrial applications as well as utilization of industrially relevant lignin sources and synthesis of model compounds. We will continue to pursue molecular understanding of lignin along with industrial applications as suggested by the panel. Diversified sources of lignin will be used in the portfolio, including deacetylation and mechanical refining-enzymatic hydrolysis (DMR-EH) lignin from a variety of sources, acid/base pretreated corn stover, as well as poplar and miscanthus. The Lignin Utilization Technology Area has synthesized >20 model compounds, many of them containing recalcitrant carbon-carbon linkages, and will be testing and sharing those compounds in Fiscal Year (FY) 2020.

#### Recommendation 3: TEA.

The panel noted that highlighting examples of where TEA has been used in the past to guide research as well as key assumptions during the peer review would be useful. We agree and will implement steps to make sure that these are included more thoroughly in the template for national laboratory projects. For competitive projects, the program utilizes independent experts who conduct a verification process, including vetting TEA assumptions as each project is negotiated. This verification process will be highlighted in the next peer review in order for the panel to have a better sense for the process.

#### **Recommendation 4: Grouping of streams.**

The panel recommended that searching for practical ways to group deconstructed lignin streams to maximize yield would be very useful. We agree and are currently investigating two main strategies to group monomer/dimer streams. First, we are investigating ways to funnel monomers/dimers into single products either through metabolism or through gas phase catalysis through projects at NREL, ORNL, and Sandia National Laboratories (SNL). Second, we are exploring ways to functionalize monomers to make use-based groupings in projects at NREL, Spero Energy, and Clemson University.

## LIGNIN-FIRST BIOREFINERY DEVELOPMENT

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

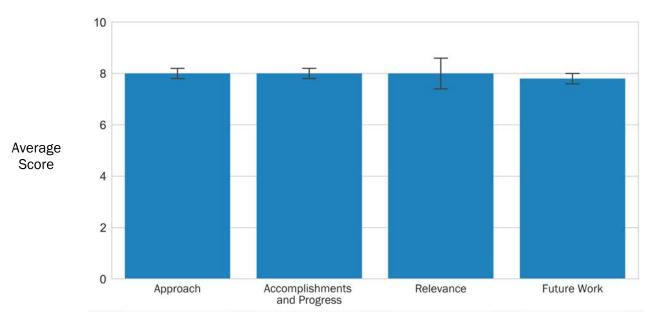
The Lignin-First Biorefinery Development (LFBD) project aims to develop an industrially relevant, lignin-first biorefining concept to fractionate lignin and polysaccharides through RCF. RCF is an active stabilization method wherein lignin is first solubilized from whole biomass through a polar protic solvent, such as methanol, and the lignin is contacted with a hydrogenation catalyst in a reducing environment to cleave aryl-ether bonds and stabilize the reaction products. RCF has been shown to be able to achieve high yields of a narrow slate of monomers—essentially acting as a catalytic funneling process—from hardwood feedstocks at high extents of delignification. The LFBD project is a close collaboration

| WBS:                      | 2.2.3.106            |
|---------------------------|----------------------|
| CID:                      | NL0033400            |
| Principal Investigator:   | Dr. Gregg Beckham    |
| Period of<br>Performance: | 10/20/2017-9/30/2020 |
| Total DOE Funding:        | \$1,400,000          |
| DOE Funding FY16:         | \$0                  |
| DOE Funding FY17:         | \$0                  |
| DOE Funding FY18:         | \$700,000            |
| DOE Funding FY19:         | \$700,000            |
| Project Status:           | Ongoing              |
|                           |                      |

with the Massachusetts Intitute of Technology and aims overall to replace standard pretreatment methods that are carbohydrate-centric (e.g., acid pretreatment) with a fractionation method that produces highly digestible polysaccharides and a lignin stream that can be separately valorized, thus equally weighting the lignin and polysaccharides in biomass. Moreover, most hardwood feedstocks are not compatible with the standard biochemical conversion paradigms of pretreatment and enzymatic hydrolysis, which the RCF process could potentially enable. The LFBD project is conducted in close collaboration with the Lignin Utilization project (for lignin analytics and model compound synthesis), the Bioprocessing Separations Consortium (for advanced separations technologies applied to the RCF process), the Performance Advantaged Bioproducts (PABP) via

#### Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

Selective Biological and Chemical Conversion project (for valorization of lignin products), and the Direct Catalytic Conversion of Cellulosics (DC3) and Enzyme Engineering Optimization (EEO) projects for carbohydrate valorization.

The LFBD project comprises two primary tasks: the first focuses on the RCF solvolysis and catalysis steps. The emphasis of this task is to develop an industrially relevant, semicontinuous, flow-through reactor system and associated robust catalyst that can efficiently solubilize lignin from whole biomass and cleave aryl-ether linkages to produce high yields of monomers, respectively. Accomplishments thus far include the construction and commissioning of a new flow system that is highly versatile and has been demonstrated to achieve greater than 35% monomer yield from hardwood feedstocks. This effort also includes lignin solvolysis modeling efforts, which leverage expertise developed in the Consortium for Computational Physics and Chemistry and will ultimately inform reactor optimization for solvolysis efforts.

The second task in the LFBD project encompasses the overall lignin-first biorefining process, with an emphasis on unit operations development outside the solvolysis and catalysis steps, namely separations of the lignin oil, recovery and characterization of water-soluble products, and solvent recovery and recycle. Accomplishments to date include the development of a rigorous techno-economic model in close collaboration with the Biochemical Platform Analysis task that highlights process challenges and opportunities for the RCF concept and preliminary evaluations of basic separations technologies for RCF oil (e.g., liquid-liquid extraction and distillation).

Ongoing work includes the examination of reduced solvent usage, improved catalyst stability, and reduced process severity, all of which can impact the techno-economics of the lignin-first process concept. Evaluations with the DC3 and EEO projects are ongoing for polysaccharide conversion. Additionally, future work includes collaboration with the PABP efforts to valorize the monomers and oligomers resulting from RCF processing towards the goal of 60% lignin conversion to value-added products by the end of the three-year project.

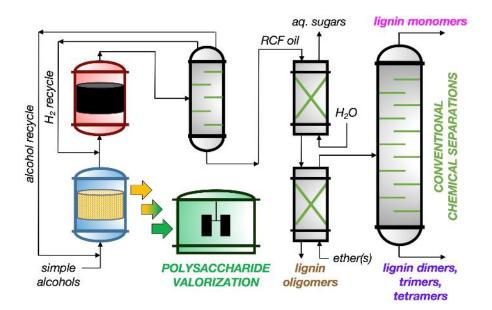


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

• This project is establishing a process to simultaneously fractionate and valorize lignin and polysaccharides. The process concentrates on producing stable lignin products that are usable by

microorganisms, while minimally impacting sugar recovery and use. The team designed and built a flexible reactor system for their process, which is operating very nicely; as a next step, the scalability of their design will be important to demonstrate.

- Revisiting existing biomass pretreatments that were developed for sugar usage in order to valorize more process streams is an appropriate, fundamental approach to improving economics of biorefineries. This project improves upon thermochemical approaches with its RCF method to stabilize reaction products from lignin, ultimately producing aromatic monomers and oligomers of value. Capital expenditures of the approach need to be considered due to methanol and hydrogen, as well as separation operations to recover multiple products.
- A lignin-first approach is a great idea. Great progress to date on results coming from thoughtful reactor design and processing approaches. Evaluation of commercial catalysts may advance the work faster, especially if they purchase a pelletized catalyst for flow through the reactor systems. Access to a variety of these were recommended to the team to access through a catalyst recycling company. The team modeled a recirculating reactor, but is this really a loop reactor-type design? Catalytic is the way forward for lower temperatures and pressures. There seems to be a resurgence in work on supercritical water approaches as of late, albeit extreme temperatures and pressures require unique, smaller, multiple reactor designs. Has the team considered that perhaps their lowest-cost solvent could be a mixture of their more volatile lignin products? This could perhaps lower the pressure requirements substantially and create a holistic approach versus using external purchased solvents. Perhaps only a portion of the stream could be used as a solvent while the rest goes to other products.
- Overall this is a well-conceived project, which has made some significant progress. Changing the biorefinery paradigm to lignin first versus sugar first could have significant value if this approach enables significantly higher lignin value capture with minimal impact on the fuels derived from the carbohydrates. The team is taking a holistic, integrated approach to the problem and should be commended for that. A quantitative analysis through TEA on how an RCF compares in economic performance versus alternative-process technologies would be a useful added study. This would help assess the value of continuing to follow this approach versus trying to improve and optimize the sugar-first biorefinery.
- The PIs present their take on catalytic biomass hydrogenolysis. This is an old process, but one that shows promise in that it can be used on whole biomass and affords an overall yield of 20%–30% propylphenols from lignin conversion. The potential for using this process to eliminate a biorefinery pretreatment step is important. The project would benefit by including more work on improving the hydrogenolysis itself, and by giving a better sense of its coordination with similar efforts in industry.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewer for the positive feedback. We completely agree that scalability will be critical to demonstrate, and we are working actively on new reaction engineering concepts that would enable fully continuous RCF chemistry to occur, which could significantly reduce solvent demand.
- We agree that the captial expenditures must be carefully considered. we have developed the first publicly available TEA for the RCF process, which will be published soon. This TEA work has helped identify key cost drivers and areas for research.
- The bench-scale work is not currently a closed-loop reactor design, but we are retrofitting existing equipment to be able to do this. Preliminary experiments have already shown that this process concept is feasible. We also completely agree and think that it is a great idea to use some of the lignin components as a solvent. We are planning to investigate this process concept in FY 2019 and FY 2020.

- We have conducted TEA. More details on this will be forthcoming.
- We agree that the hydrogenolysis step must be improved, and we are working towards that in collaboration with multiple academic groups. We are in close contact and directly collaborate with the only company to our knowledge scaling up RCF chemistry at the moment, thus we are keeping close contact with industrial efforts in this space as we can.

## **ELECTROCATALYTIC OXIDATION OF LIGNIN OLIGOMERS**

#### National Renewable Energy Laboratory

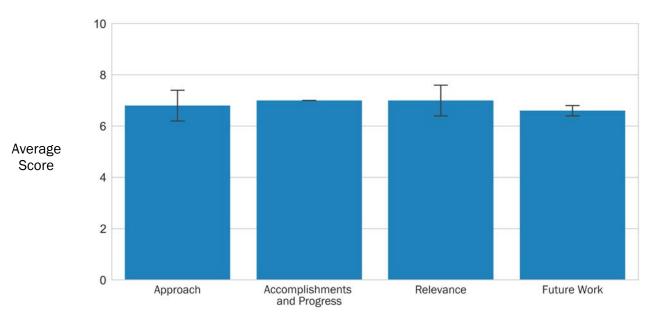
#### PROJECT DESCRIPTION

Deconstruction of lignin by "lignin-first" approaches like RCF produces functionalized monomers, but a significant portion of soluble lignin oligomers still remain. These oligomers are generally linked through recalcitrant C-C bonds. Thus, selective cleavage of C-C linkages in RCFderived oligomers into functionalized monomers is critical to the success of lignin valorization. To address this challenge, this project will (1) demonstrate proof of concept for electrocatalytic oxidative cleavage of the C-C linkages in RCF-derived soluble oligomeric lignin to selectively produce functionalized monomers for further upgrading and (2) advance the technology by targeting yield improvements.

| WBS:                      | 2.2.3.500          |
|---------------------------|--------------------|
| CID:                      | NL0033914          |
| Principal Investigator:   | Dr. Josh Schaidle  |
| Period of<br>Performance: | 4/1/2018-9/30/2020 |
| Total DOE Funding:        | \$450,000          |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$0                |
| DOE Funding FY18:         | \$300,000          |
| DOE Funding FY19:         | \$150,000          |
| Project Status:           | Ongoing            |
|                           |                    |

#### Weighted Project Score: 6.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${f I}$  One standard deviation of reviewers' scores



Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- The PIs present an interesting approach for further upgrading of recalcitrant lignin oligomers generated during lignin hydrogenolysis. The science behind the process is quite compelling, as is the project's link to solar photovoltaics. The project would be strengthened by a better understanding of the expected phenolic oxidation mechanism. It also remains to be seen whether electrocatalytic approaches can be demonstrated as useful in an industrial context or not.
- Valorization of soluble lignin oligomers resulting from RCF is targeted by development of electrocatalysts and electrolyte/solvent systems to cleave C-C bonds. Good progress has been made in the initial development. A large increase in usable monomers is possible assuming the project can achieve its yield and selectivity targets. More discussion on the scalability of the technology would be helpful to ascertain likelihood of commercial use and success.
- The very low concentration on model compounds is key concern for this approach. Also concerning is the high concentration of lithium perchlorate (LiClO<sub>4</sub>) and the acetonitrile solvent. Conversion of models to date also are fairly low, making this a very challenging program to meet the BETO goal for this project. The next steps on the RCF stream will define whether there is any right to succeed. Platinum electrodes used in the process raises a question: what is the cost of electrodes at a future potential commercial scale?
- This project has already led to three nanoparticle formulations for controlled potential electrolysis studies. Advantages of the electrocatalytic approach include low temperature, low pressure, and potential catalytic selectively. As for the next steps, the team is advised to address questions concerning scale-up and use TEAs as a research tool to evaluate the impact of electricity costs on the economic feasibility of the technology.
- This appears to be a relatively early-stage project with ambitious goals to try a new approach to improve lignin monomer yields. The team has made good initial progress with the proof of concept, although several challenges remain.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their constructive feedback and guidance, especially regarding our future directions. As noted, this project is an early-stage proof-of-concept effort in which we have leveraged a systematic approach to evalute the process and gain foundational insight into the reaction chemistry. We appreciate the reviewer's support of our initial progress and acknowledge that there are many challenges and key questions that need to be addressed for this process. These challenges and key questions relate to both the scale-up and commercial application of the technology as well as the fundamental reaction chemistry. During the remainder of this project, we will work to address these challenges and key questions, especially in regard to (1) assessing economic viability and identifying key cost drivers and (2) providing a deeper understanding of the fundamental chemistry and reaction mechanisms so that this technology can be advanced.

## BIOMASS ELECTROCHEMICAL REACTOR FOR UPGRADING BIOREFINERY WASTE TO INDUSTRIAL CHEMICALS AND HYDROGEN

#### **Ohio University**

#### **PROJECT DESCRIPTION**

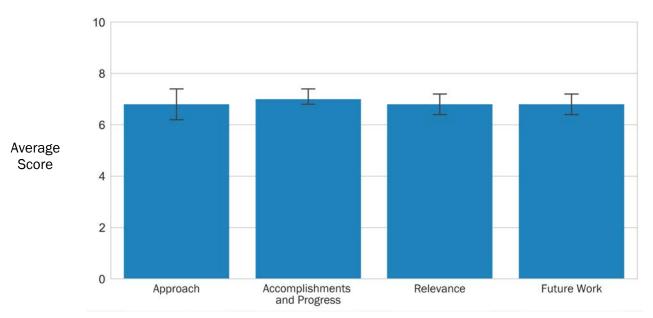
The goal of this project is to develop electrochemical processes to convert biorefinery waste lignin to industrial chemicals. The additional revenue stream resulting from these lignin-derived chemicals will enhance biorefinery economics and ultimately lead to a reduction in the cost of biofuels. Researchers at Ohio University have partnered with the Biorefining Research Institute at Lakehead University and an industrial partner to evaluate the

| WBS:                      | 2.3.1.205          |
|---------------------------|--------------------|
| CID:                      | EE0007105          |
| Principal Investigator:   | Dr. John Staser    |
| Period of<br>Performance: | 3/1/2016-4/30/2020 |
| Total DOE Funding:        | \$1,472,724        |
| Project Status:           | Ongoing            |
|                           |                    |

electrochemical conversion product streams in resin formulations and to determine the potential economic impact of this electrochemical process on the biorefinery. Key to this project is electrochemical conversion product analysis, which is used to determine metrics like the extent of lignin conversion and predominant product compound class (i.e., functionalized aromatic compounds resulting from electrochemical depolymerization of the lignin biopolymer). We are applying robust statistical analysis to understand with confidence how the electrochemical process modifies the biorefinery lignin. The electrochemical depolymerization of biorefinery lignin results in lower molecular weight products that are more reactive than the lignin biopolymer, both of which could render the product stream suitable for incorporation into resin formulations. This is being evaluated by our industrial partner. By the end of this project, we will have gone through two iterations of a continuous-flow electrochemical reactor, increasing the reactor size and the rate of lignin conversion over the project benchmark and the current state of the art. We will have evaluated

#### Weighted Project Score: 6.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

electrochemical reactor product streams in resin formulations, and will have optimized reactor operation to generate streams most suitable for incorporation into resin formulations. We will also have completed a TEA describing how the electrochemical reactor may affect biorefinery economics.

#### OVERALL IMPRESSIONS

- This is an innovative approach using electrochemistry for controlled depolymerization of lignin to produce high value aromatics. Excellent progress has been made on technical targets such as conversion, purity, and selectivity. Power consumption of the process and cost of electricity are key areas of concern, although the latter may be helped by hydrogen cogeneration during the process.
- This project is well thought out and has solid technical insights. The achievements to date on conversion are impressive, assuming sound analysis results. This project could have used more input from the BETO analysis team or Ohio University resources to confirm preliminary techno-economic input considering the amount of DOE money also involved in this program. This is a very high-potential project but very challenging to reach industrial-scale success because very few large-scale complex oxidative electrochemical processes exist today, if any, as complex as this one with such a variable feedstock. The early progress seems to indicate good potential to improve further towards viable commercial processes. One question: is there a reason why they have not already evaluated multiple sources of lignin that could have been supplied by BETO teams, or was this done in a previous year? Also, I am surprised there is no result on resin formulation work, even if preliminary, considering how long this project has been in progress. Is it not feasible to do a preliminary batch on a small scale to test the properties?
- This project harnesses the ability of electrochemical processes to achieve three significant outcomes: (1) tighter control over the lignin depolymerization process, (2) more reactive lignin species, and (3) a hydrogen coproduct. The emphasis on statistical consideration of large data sets is commendable. The team includes a close industrial partnership, which will help ensure the translation of the research in practice. To accelerate that process, the team can further integrate data from industry partners into the TEA of the product pathway.
- Conceptually, this appears to be a good project and the team has made good progress on the catalyst and process development. This program apparently started at a pretty low technology readiness level relative to other projects, but has come a long way. The inclusion of an industrial partner to assess the products of their process for use in producing a phenolic resin is commendable. In the event that the initial outcome of the phenolic resin evaluation is not positive, the team should consider what their options are, either to modify the process to achieve an acceptable result or to consider other potential outlets for the product mix. The TEA should be used as a tool to assess the degree of flexibility the team has to adjust the process and/or catalyst to make acceptable products. They have all the tools in place as part of the team to do this.
- The project will use electrochemical approaches for the conversion of lignin into smaller fragments targeted at the phenolic resin industry. The partnership offers an interface with a large and well-established industry. Further, the research team is well integrated across the various steps involved in moving from lignin to final products, and the PI brings important expertise in the design of larger-scale reactors that will eventually be needed. There are gaps in the process to date, especially with regard to understanding of the structures being generated during electrolysis and the mechanism of the electrochemical process. Inclusion of nuclear magnetic resonance as an analytical tool will address many of these issues. In addition, the project will be strengthened by a clear description of how this approach to phenolic resins offers improvements over the many other literature efforts to carry out similar activities.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# UPGRADING LIGNIN-CONTAINING BIOREFINERY RESIDUES FOR BIOPLASTICS

#### Texas A&M University

#### **PROJECT DESCRIPTION**

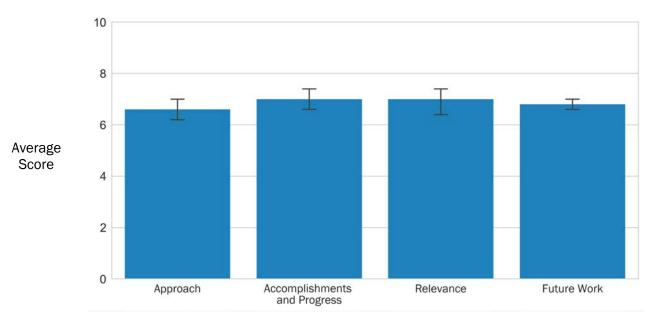
The proposed research will integrate the latest advances from a multidisciplinary academic-industrial coalition to address one of the most challenging issues in lignocellulosic biofuel production: the use of lignincontaining biorefinery residues for cost-effective bioproduct production. The success of a modern biorefinery heavily depends on the diverse product streams and the utilization of all fractions of input material. Even

| WBS:                      | 2.3.1.206            |
|---------------------------|----------------------|
| CID:                      | EE0007104            |
| Principal Investigator:   | Dr. Joshua Yuan      |
| Period of<br>Performance: | 4/15/2016-12/31/2019 |
| Total DOE Funding:        | \$2,499,993          |
| Project Status:           | Ongoing              |
|                           |                      |

though extensive progress has been made to process cellulose and hemicellulose into advanced biofuels, the utilization of lignin for fungible biofuels and bioproducts has not been achieved. Lignin is much more underresearched as compared to cellulose, which has become a setback for the efficiency, cost effectiveness, and sustainability of a lignocellulosic biorefinery. Essentially all current bioconversion platforms lead to a lignin-containing waste stream that needs to be further processed into valuable products. Although a certain amount of lignin ( $\sim 30\%$ -40%) is needed for the thermal requirements of biofuel production, a modern cellulosic processing plant will have  $\sim 60\%$  excess lignin. The utilization of this excess lignin-containing residue as feedstock for renewable fuels and chemicals offers a significant opportunity to enhance the operational efficiency, lower the overall biofuel cost, reduce the net carbon footprint, and improve the replacement of petroleum. The proposed research will translate the latest technology breakthroughs into a transformative lignin-to-PHA route.

#### Weighted Project Score: 6.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

This project uniquely addresses the mission and goals of BETO with the following three objectives: (1) process enablement by engineering and optimizing microorganisms to convert biorefinery waste streams to PHA for bioplastics; (2) process development by characterizing biorefinery residues, optimizing lignin treatment and fermentation, and designing the novel bioprocess; and (3) process integration and optimization by biorefinery on-site scale-up, TEA, and life cycle assessment for the lignin-to-PHA upgrading process. During the past two and a half years, we have made significant progresses in all three objectives, including systems biology-guided engineering of *P. putida* to effeciently convert lignin into PHA, the development of new combinatorial pretreatment and coprocessing of lignin and residual saccharides (CLARS) processes to enhance both lignin and carbohydrate processibility, and the integration of TEA to evaluate the impact of the process for biorefineries and the bioeconomy. The technical advances have translated into 30-times increase of PHA titer from biorefinery waste, more than 20-times increase of conversion efficiency for biorefinery waste-to-PHA conversion, and 50-times decrease of PHA production cost from biorefinery waste, all of which leapfrogged the technology to address an important challenge in modern biorefinery development.

The proposed research will address an imminent challenge of biorefineries with a transformational solution. Scientifically, the bioconversion of lignin at a high efficiency has rarely been achieved. The integration of multimodule design enabled the highly innovative lignin-to-PHA route. Besides the significant scientific merits and innovation, successful development of this single-unit process will allow the conversion of a significant amount of renewable biomass to bioplastics to meet DOE's near- and long-term targets for production of low-cost biofuels from lignocellulosics. The process will also maximize replacement of petroleum products, as bioplastics have a rapidly increasing market and represent a sustainable way to replace petroleum-based plastics. This novel platform complements the current technologies supported by BETO to enable the utilization of all structural components of cell wall for better cost effectiveness, overall carbon efficiency, and sustainability for biofuels.

#### **OVERALL IMPRESSIONS**

- The project addresses pretreatment fractionation, strain engineering, and fermentation development to improve overall process streams and enable optimal microbial valorization of lignin to PHAs. Significant progress has been made under lab- and bench-scale conditions. Additional development, scale-up, and refined TEA validation are required to determine whether the process is commercially viable.
- This was challenging work but the team did have some very nice results. Our main concern is they are likely not on scale to meet BETO goals, even if successful at one liter to reach the \$5/kg goal. This is based on the fact that they are two times away from the goal. Many bio projects fail not at the one liter stage but at the pilot- or full-scale stage, making most organism approaches higher risk for commercial-scale success rather than chemical approaches. If PHA remains a niche material, then introduction of increased volumes into market could cause collapse. The only viability I see is if they can go way under PHA current price to drive market acceptance and grow the PHA business/acceptance dramatically.
- By investigating both pretreatment and bioconversion processes, the research team developed the CLARS process. The CLARS process harnesses the value of low sugar levels in lignin-enriched streams to biologically transform the lignin components into bioplastics (i.e., PHA). While the team reports high PHA yield from lignin, corresponding measures are mainly based on depletion of ferulic acid. As a next step, it will be important to determine yields from the total lignin supplied to the engineered *P. putida* strains that accumulate PHA. Notably, the team also demonstrated benefits of using a laccase/mediator system to increase lignin utilization by *P. putida*; however, the robustness of this approach should be confirmed.
- The PIs present a scientifically interesting project that also incorporates the novel concept of biochemical lignin conversion. By optimizing the pretreatment leading to monomers, the PI has been able to improve the yield of *p*-hydroxycinnamates needed for eventual conversion to PHAs. The project would benefit from a clearer description of the economics, a better quantification of the active substrates in the lignin extract, and an improved justification for the choice of PHAs as the target material.

• This appears to be a very broad and ambitious program that has attacked the problem of lignin valorization from a fairly holistic approach to the biorefinery process. The team should be commended for the range of their accomplishments and overall progress. The team needs to be more clear as to how much of the PHA produced is actually from the lignin and how much from residual sugars, and how much of the PHA produced from lignin can be attributed to the improvements achieved in this project.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reveiwer's comment that "significant progress has been made under lab- and benchscale conditions." Indeed, the project achieved >30-times increase on PHA titer, >20-times increase on lignin-to-PHA conversion efficiency, and >50-times decrease on minimal selling price of PHA. We agreed with the reviewer that "additional development, scale-up, and refined TEA validation are required," which are exactly the goals of budget period two of the project. Now that the budget period one validation has just passed, the project is moving to budget period two. In addition, we are working with Altex Inc. and Danimer Scientific on the commercialization and scale-up of the technology.
- We appreciate the reviewer's acknowledgement of "very nice results." The team has two general approaches in addressing the market risks. First, in recognization the market risks, the team has already worked with ICM Inc., Altex Inc., and Danimer Scientific on the scale-up of the technologies. In particular, considering the recent ban on trash import from China, there is a significant increase in demand for biodegradable plastics. Danimer Scientific and other companies are working on significantly increasing the PHA production in the United States to address this challenge. The team is working with these companies to broaden the PHA market. Second, and importantly, the team has also developed multistream biorefinery strategies, where different bioproducts can be developed to avoid the market saturation. These lignin-based products include carbon fiber, asphalt binder modifier, lipid, bioplastics, and other bulk products. The future solution could be that different biorefineries could adapt various bioproducts based on market demands to avoid saturation.
- We appreciate the reviewer's acknowledgement of the CLARS process to harness the low-value sugars. We have evaluated lignin conversion efficiency with both ferulic acid and lignin-based methods. We agreed with the reviewer that even though the ferulic acid-based evaluation is very accurate, the lignin-based evaluation is complicated by the complex substrate. We are identifying a solution for this challenge in budget period two. For laccase-mediator-based fractionation, the recent technology development demonstrates that an efficient factionation can be achieved without laccase. We aim to avoid the laccase-based method due to the potential high cost of laccase.
- We appreciate the reviewer's acknowledgement for improved yield of monomers and eventually PHA conversion. We did include TEA analysis in the "relevance" section, and more thorough TEA analysis of different scenarios are being carried out in budget period two. Both lignin and residual sugars are active substrates in the lignin extracts, along with some organic acids, which complicates the exact contribution of each component to the eventual PHA yield. However, such complication does not impact the economics, as none of these components, including the residual sugars at low concentraction, have other economic values. As aforementioned and shown in the economic analysis, PHA is a perfect target for biorefinery products due to: (1) higher value, (2) large market potential due to the recent wastemanagement crisis, (3) serving as one of the many products for lignin utilization, and (4) funnelling diverse aromatics into single products to reduce the separation challenge.
- We appreciate the reviewer acknowledging the holistic approach. We actually have estimation of how much PHA is from lignin and sugar, respectively, though we do agree that such estaimation needs to be better defined during budget period two. However, as aforementioned, the detailed evaluation of how each component of biorefinery waste contributes to the PHA yield will not impact the overall economics, as none of these components can be isolated for producing high-value products.

# GAS-PHASE SELECTIVE PARTIAL OXIDATION OF LIGNIN FOR COPRODUCTS FROM BIOMASS CONVERSION

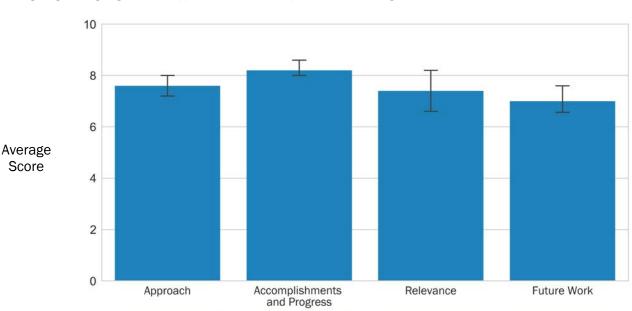
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

This project seeks to develop a catalyst and process that can convert low-value lignin streams from biorefineries into valuable phenolic coproducts by the gas-phase catalytic partial oxidation of lignin pyrolysis vapors. The technology will enable a diversified revenue stream for an integrated biorefinery in which the cellulose and hemicellulose biomass fractions are primarily used to produce a suite of fuels and coproducts, creating valuable phenolic compounds from lignin. The focus on producing simple phenols (phenols that do not contain methoxy functional groups) is due to their high value and market sizes (~1,100 per tonne, 11,400 kT/y phenol; 3,800 per tonne *p*-cresol, 3,400 kT/y *p*-cresol; 6,000 per tonne, 45 kT/y catechol).

| WBS:                      | 2.3.1.501           |
|---------------------------|---------------------|
| CID:                      | NL0033404           |
| Principal Investigator:   | Dr. Matt Yung       |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$800,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$400,000           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

The approach for catalyst development focuses on design of catalysts by varying two parameters known to be important in selective oxidation catalysis: (1) metal-oxygen bond strength and (2) active site density. The activities that were performed and will be discussed include: (1) establishing benchmarks on yield composition for various types of lignin pyrolysis vapors, (2) establishing a benchmark with a commercial catalyst for



#### Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

phenol yield from partial oxidation of lignin pyrolysis vapors, (3) computational guidance on materials selection, (4) synthesis and characterization of catalyst materials, (5) reaction testing of catalysts using both model compounds and the whole vapor stream from lignin pyrolysis, and (6) integration of TEA with experiment results. Recent catalyst and process development accomplishments are highlighted by improvements in the carbon yield to the desired phenolic compounds and the resulting estimated impact on the reduction in modeled minimum fuel selling price will be presented.

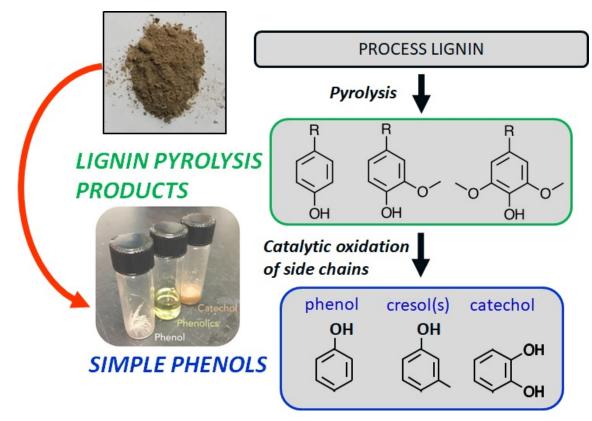


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- The project is on track to develop catalysts and conditions for improved yield of simple oxygenated phenols from lignin pyrolysis vapors. Improvements in yield, catalyst regeneration, and scale-up to demonstrate scalability are on deck. Significant interest from upstream and downstream entities bodes well for commercial interest in a successful project.
- This is a difficult project with many challenges. The project is well managed and well run with clear partnerships and a well-thought-out technical approach. There are two concerns to address in the future, one being the choice of the vanadium catalyst, because vanadium has seen large price increases in recent years due to potential demand in the battery market as well as a reduced supply from a key region in China. Second, the key challenge is the requirement to meet a BETO goal of 25% yield of simple phenolics, which represents a future improvement of 66% yield versus current work results. I believe this could be the most difficult challenge to achieve with the current plan. Still, I commend the team for their excellent collaboration across multiple areas with internal and external partners and their progress to date.
- This appears to be a well-organized program that has made very impressive progress to date. They have made good use of computational modeling to streamline catalyst design and selection. Their future work

plans are targeted at appropriate critical issues for cost reduction and scale-up risk reduction. The team should leverage the interaction with their industry partners to validate the market value of their intended product stream (mixed phenols).

- The PIs have made reasonable progress in their understanding of this pyrolysis process and of the materials that are generated as a result. The project needs more clarity as to the potential markets for mixed phenolics, how a value higher than pure phenol is used in the TEA, and how this project represents a clear improvement over the many literature reports of converting lignin or biomass into phenols.
- This project includes excellent representation of industry partners across the value chain and benefits from a high level of partner engagement. Already, the team exceeded their goal to demonstrate ≥10% yield of phenolics at the lab scale, and developed a catalyst with two-times higher performance than a commercial benchmark. The scalability of the process will be important to demonstrate as a next step.

- We thank the reviewers for their detailed responses. In order to address concerns of the catalyst cost, we are exploring multiple types of catalysts, including non-vanadium catalysts (e.g., perovskites and industrially supplied catalysts from partners) and will use a BETO-developed tool (CatCost<sup>™</sup>) to estimate the scaled-up cost of our catalyst to see if the catalyst cost is a driver and look for opportunities to reduce this cost. The end-of-project goal is to demonstrate a 10% yield to simple phenols on the bench scale, and while this has been demonstrated on the lab scale, improving the overall economics will require additional improvements in the yield to simple phenols, which is why we will continue process/catalyst development throughout the project.
- We are actively working on improving our TEA model to reflect the experimental data and understand the separations costs/requirements. There are existing markets and values for phenol (\$1.10/kg), *o*-cresol (\$2.40/kg), *m*-cresol (\$3.90/kg), *p*-cresol (\$4.00/kg), and mixed *m*-/*p*-cresol (\$2.80/kg). The lower cost of the mixed cresols has the separations costs "built in." There is ongoing work at NREL within BETO projects focused on separation methods and has shown the ability to produce >97% purity fractions of phenol, *o*-cresol, and *m*-/*p*-cresol from the condensed catalytic fast pyrolysis broth from whole biomass. The price of phenol (and all commodities) fluctuates, so we have used a phenol price band in our TEA analyses that is representative of both (1) fluctuations in market prices and (2) fluctuations in the product distribution (i.e., lower-value phenol versus higher-value cresols). Our condensed simple phenols consist of 40% cresols, 30% phenol, and 30% alkyl phenols. We are still determining the appropriate markets/prices for alkyl phenols, but using a weighted average of phenol and mixed cresol values gives us estimated market prices of \$2.10/kg, which is in line with what we used in the analysis (\$1.90/kg).

# **BIOLOGICAL LIGNIN VALORIZATION – NREL**

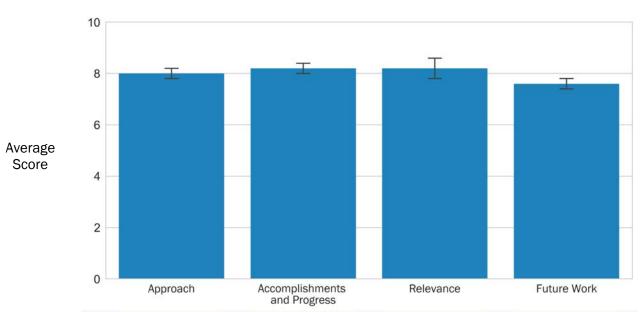
## National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

This project aims to develop robust biological processes to produce novel coproducts from lignin-derived aromatic compounds. In collaboration with the Lignin Utilization project (focused on chemical lignin depolymerization and lignin analytics), this project will directly contribute to the minimum fuel selling price targets of \$2.50/GGE in 2022. The project focuses on the production of three compounds—muconic acid and two other aromaticcatabolic intermediates—that are relevant to large-marketsize, direct-replacement chemicals (such as adipic acid and terephthalic acid) to be able to realistically aid the bioenergy industry. The final project milestone for this three-year project cycle is to produce these compounds at

| WBS:                      | 2.3.2.100             |
|---------------------------|-----------------------|
| CID:                      | NL0026678             |
| Principal Investigator:   | Dr. Davinia Salvachua |
| Period of<br>Performance: | 10/1/2017-9/30/2020   |
| Total DOE Funding:        | \$2,550,000           |
| DOE Funding FY16:         | \$600,000             |
| DOE Funding FY17:         | \$550,000             |
| DOE Funding FY18:         | \$700,000             |
| DOE Funding FY19:         | \$700,000             |
| Project Status:           | Ongoing               |
|                           |                       |

50 g/L and 90% yield. Moreover, this project is among the three collaborative efforts in the BETO lignin portfolio developing the "biological funneling" concept, which aims to convert a heterogeneous slate of ligninderived compounds to a single product—a relatively new concept for the biorefinery. Thus, beyond direct contributions to meeting cost targets through effective lignin valorization, this project is providing foundational scientific knowledge for the burgeoning concept of microbial lignin conversion, which is likely applicable to many types of lignin streams and offers a new approach for the much-needed problem of lignin valorization in an integrated biorefinery.



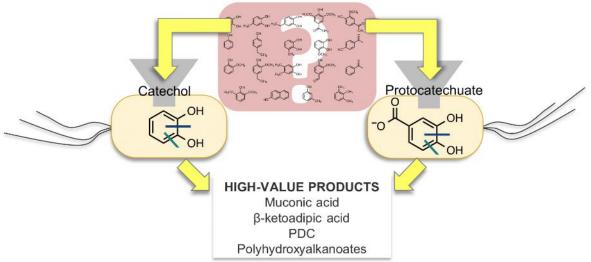
#### Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

The project is distributed across three tasks: the first task focuses on metabolic engineering of a robust aromatic-catabolic chassis microbe, Pseudomonas putida KT2440, to convert aromatic monomers found in lignin streams to targeted intermediates, with muconic acid as the first exemplary product. The second task focuses on closely associated bioprocess development efforts using bioreactor cultivation to control pH, feeding rate, and mode and other associated process variables. The two tasks work closely to optimize key bioprocess performance metrics, including titer, rate, yield, and substrate toxicity tolerance. Recent accomplishments from this effort of the project include the development of robust P. putida strains and associated bioprocesses that are able to convert hydroxycinnamic acids, which are highly prevalent in lignin streams from agricultural residues and grasses, to muconic acid at high titers, rates, and yields. Key activities include overcoming bottlenecks in upper pathways by overexpression of rate-limiting enzymes, cofactor engineering, expression of heterologous genes in place of native genes, deregulation of carbon catabolism, and associated optimization of the bioprocess parameters such as feeding control. Progress has additionally been made in collaboration with the Denmark Technical University on evolving strains for higher toxicity tolerance to both substrates and products. Lastly, the project has engineered both syringate and syringol turnover in P. *putida*, which enables syringyl-type lignin (which is highly prevalent in hardwoods and grasses) to be converted into value-added compounds. All of these learnings are being applied towards other BETO projects, such as a close collaboration with the Metabolic Engineering for Lignin Conversion project at ORNL and the Agile BioFoundry, to deploy bioprocesses to aromatic-catabolic strains engineered in other projects.

The third task in the project focuses, in collaboration with the Biological Lignin Valorization project at SNL, on the cleavage of dimers and oligomers that are not able to be catabolized by native strains. Our project mostly focuses on understanding the native capacity of *P. putida* to cleave dimers and oligomers, whereas the Biological Lignin Valorization project at SNL aims to discover new catabolic capacities for inclusion into a chassis strain. To date, our project has discovered that *P. putida* likely packages enzymes into outer membrane vesicles for extracellular lignin catabolism.



# Lignin Depolymerization Product Slate

Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• This program describes an important strategy to build an organism to valorize lignin-derived compounds biologically. The work is in a good position to benefit from progress in the Lignin Utilization program and appears to be doing so, for example by utilizing model substrates and potentially enabling the building of mock substrate mixtures to focus on limiting compounds as it moves toward authentic

substrate compositions. The Agile BioFoundry is mentioned briefly in the project description but it is not clear to what extent information is flowing and in what direction. Discussion with the Agile BioFoundry regarding *P. putida* development is a clear win-win, as the Agile BioFoundry is working on building a *P. putida* chassis. One could easily see implementation of a Design-Build-Test-Learn strategy (or at least a mini-Design-Build-Test-Learn in the early stages of discovery) for gene dosing (copy number) and stacking of tolerance factors and "on-pathway" substrate utilization/product genes as they emerge, and are likely to add value to move the program quickly. The discovery of a secreted enzyme system is interesting and may provide additional strategies to exploit this for extracellular degradation of potentially cytotoxic compounds such as soluble lignin-derived oligomers. The team is encouraged to further explore the secretome of the organism to determine its potential and limitations, and optimize key enzymes.

- The team has done an outstanding job making progress across many challenges that arose during the project for such stretching goals. This team worked well together, showing solid management of program and good collaboration across the various other teams inputting information and product streams for evaluation. Again, from experience, biological conversion on such complex materials is highly challenging and the team is commended for taking on this challenge and making great progress. This program has a chance to contribute substantially to BETO goals by funneling many products into single key materials when lignin processing produces so many compounds. I would hope this project could find a way to continue beyond the September end date.
- The PIs continue a scientifically excellent project for the biochemical transformation of lignin into muconate, and ultimately adipic acid. High-yield success in this project through biological funneling will be a nice addition to biorefinery development. Demonstration of this approach on a wider range of lignins and a clear TEA will further improve the project's impact.
- This project has made excellent progress towards identifying new enzymes able to cleave the five most relevant linkages in lignin, and then transferring that capability to *P. putida* to increase lignin bioconversion into valued biochemicals. In addition to using lignin model compounds, the team developed *P. putida* strains that can utilize syringyl lignin, transform syringol, and produce muconic acid from base-catalyzed depolymerized lignin. As a next step, strain tolerance to fluctuations in feedstock composition and slight changes in pretreatment conditions will be important to quantify.
- This project fits nicely in the lignin valorization portfolio and is well integrated with other relevant programs. The team appears to have made very substantial progress on titer, rate, and yield performance in model systems, which presumably is carrying over to the performance in "real" lignin streams. It appears that currently the levels of rate and titer they can achieve in these real streams is limited by the upstream processes' abilities to produce a high-enough concentration of addressable carbon.

- We appreciate the positive comments and feedback. Indeed, we will on-board some of the tools developed in the Agile BioFoundry (e.g., biosensors and transformation tools), and much of the work originating in this project has informed engineering in the Agile BioFoundry as well, so synergies will exist in both directions. We are certainly investigating the secretome in more detail as bandwidth permits and also leveraging fundamental discoveries made in the DOE Office of Science-funded and academic efforts.
- We completely agree that this approach needs to be demonstrated on a wide range of lignins. We are actively engineering a *Pseudomonas putida* chassis that is able to convert syringyl (S), guaiacyl (G), and hydroxyphenyl (H)-type lignin monomers, and hence will ideally be useful for lignin samples from multiple upstream catalytic treatments and biomass sources.

- We agree that upstream changes will modify the organism needs and balance. At present, we are attempting to establish a baseline strain that is able to catabolize H-, G-, and S-type lignin monomers that will be produced from a wide variety of biomass samples.
- The comment regarding the upstream process abilities dictating the titers, rates, and yields is absolutely correct: namely, the upstream lignin depolymerization process dictates the amount of "bioavailable" aromatic carbon for the microbe to convert. We are working in close collaboration with the Lignin Utilization project to enable higher amounts of aromatic carbon that is biologically accessible now.

# **BIOLOGICAL LIGNIN VALORIZATION – SNL**

## **Sandia National Laboratories**

#### **PROJECT DESCRIPTION**

Depolymerization of lignin and subsequent upgrading of lignin-derived intermediates to fuels and chemicals is key to meeting BETO's 2022 goal of \$3/GGE; however, utilization of lignin has not been successfully demonstrated in an industrially relevant manner. This is in part due to our limited understanding of both the compounds biological systems produce when they depolymerize either native lignin or lignin coming from a biomass pretreatment process and which of the produced compounds microorganisms metabolize. This project is focused on developing fundamental understandings of microbial and enzymatic depolymerization of lignin and answering several key questions: To what extent can lignin can be

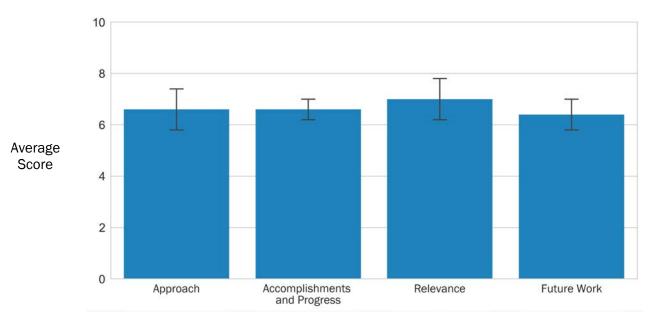
| WBS:                      | 2.3.2.101           |
|---------------------------|---------------------|
| CID:                      | NL0026729           |
| Principal Investigator:   | Dr. Kenneth Sale    |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,231,931         |
| DOE Funding FY16:         | \$300,000           |
| DOE Funding FY17:         | \$229,631           |
| DOE Funding FY18:         | \$452,300           |
| DOE Funding FY19:         | \$250,000           |
| Project Status:           | Ongoing             |
|                           |                     |

enzymatically depolymerized? What intermediates are produced? Which of these intermediates are consumed by microbes? What are the enzymes involved in lignin degradation and metabolism? Answers to these questions will provide insights into the requirements for biological upgrading of lignin, which is critical to the work being done in a companion project at NREL developing microbial strains and bioprocesses to convert lignin-derived monomers and oligomers to products.

Realizing the difficulties of top-down approaches in which lignin depolymerization is studied using either native lignin or lignin from biomass pretreatment processes, in this project we are taking a bottom-up approach

## Weighted Project Score: 6.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

in which initial studies are being performed using model dimer compounds containing the canonical C-O and C-C linkages in lignin. This allows us to develop a fundamental understanding of how lignin-metabolizing organisms modify lignin-derived intermediates, to examine how defined bond types are enzymatically cleaved and to identify the enzymes involved in these processes. The knowledge derived from these studies will be used to guide analysis of studies on mixed bond-type lignin model polymers and lignin coming from process-relevant approaches, such as the BETO-funded Deacetylation, Mechanical Refining, and Enzymatic Hydrolysis project.

We have studied a set of 16 microbes reported to be capable of degrading lignin on a set of commercially available model dimer compounds and a set of newly synthesized model dimers containing a fluorescent reporter group. We synthesized two phenolic and two non-phenolic ether compounds linked to the highly fluorescent 4-methylumbelliferone compound. A versatile peroxidase from the *Bjerkandera adusta* cleaved the C-O bond in the absence of hydrogen peroxide ( $H_2O_2$ ) and at low concentrations of exogenously added maganese(II) chloride (MnCl<sub>2</sub>), suggesting manganese peroxidase activity dominates and the Mn binding site is fully occupied. These compounds have also been used as substrates in the presence of the 16 identified microbes, and several produce enzymes capable of catalyzing C-O bond cleavage in both phenolic and non-phenolic ether compounds.

We also investigated dimer degradation and modification by 16 microorganisms using a panel of C-O (SGE, VGE, GGE) and C-C (DDVA, pinoresinol) bonded dimers. A subset of these microorganisms, including *Exophiala alcalophila, Sphingobium sp.* SYK-6, *Delftia acidovorans, Rodococcus jostii, Pseudomonas putida* mt-2, and *Streptomyces viridosporus*, modified all five compounds, establishing they either secrete ligninolytic enzymes or are capable of incorporating and metabolizing these compounds. Additional studies of the kinetics of GGE and pinoresinol modification by *Sphingobium sp.* SYK-6 were conducted and showed the presence of multiple intermediates expected to be produced based on its published aromatic metabolism pathways. Similar experiments examining the modification of dimer compounds by combinations of the subset of microorganisms that modified the five dimers are ongoing and future experiments will include studies using a commercially available synthetic lignin polymer with defined structure and mixed bond types (two C-C bonds and one C-C bond).

## **OVERALL IMPRESSIONS**

- The project is the bottom-up counterpart to other biological lignin valorization projects, seeking to discover enzymes from a set of organisms showing an ability to work on a set of synthesized lignin dimers. This is an important complement to those programs and may provide valuable leads for heterologous genes and their encoded enzymes that can be levered into potential chassis hosts such as *P. putida*, or perhaps as hosts in their own right (although this seems less likely given resources and stage of development).
- The PIs present a potentially interesting expansion of their *P. putida* work by investigating the reactivity of a broader family of lignin-converting organisms. If successful, the project could identify systems tailored to key structural units in lignin and alternative biochemical approaches to lignin-derived chemical products.
- An important and distinguishing capability of this project is its focus on the synthesize lignin model substrates that facilitate enzyme and microbial screening. The focus on compound synthesis to support enzyme and microbial screens addresses a central limitation to enzyme discovery. To build from the project's success, the team is advised to now focus on the synthesis of lignin model compounds that retain structures that are difficult to transform by known enzymes and microbes (e.g., condensed C-C linkages).
- The team took a sound technical work approach. I do like the approach to look at mixtures of enzymes/organisms that may have synergistic impact. I am concerned that no realistic samples of lignin

or lignin products have been tried and progressed organisms only on model compounds. Testing of realistic samples early is needed to define how far away they are from future goals.

• Overall, this is a meaningful project which fits well in the BETO-funded portfolio of lignin valorization programs. The team has made good progress in developing model compounds that fluoresce to indicate bond cleavage as a means of tracking lignin degradation activity. However, it appears that most of the effort to date has focused on the more tractable C-O linkages, which may not be particularly relevant in technical lignins, which would be the substrate in the context of a biorefinery process. Hopefully in the balance of the project they will make progress on the C-C linkages comparable to the strong progress they have made on addressing the C-O linkages.

- We are taking a "bottom-up" approach, in as much as we are as this project was conceived as an alternative approach to lignin depolymerization by exploring and exploiting the enzymatic diversity present in select microorganisms with reported capabilities for degradation of aromatic compounds.
- We agree and are currently synthesizing a C-C linked model compound. Synthesizing a C-C bonded compound to include a compound that fluoresces upon bond breaking proved difficult, so we are now synthesizing a compound suitable for a flourescence resonance energy transfer-based assay.
- Our plan is to continue to move toward more complex lignin samples. Our current set of model dimers are very useful for identifying new lignin-utilizing organisms and evaluating potential metabolic pathways and associated enzymes. Using more complex lignin substrates will allow us to identify organism that must be secreting enzymes that break down polymeric lignin to fragments. We are working to understand how microbes break down lignin and utilize the lignin fragments produced. We are trying to fill the gap in understanding of the lignin fragments produced during biological depolymerization and of these fragments that are consumed and utilized. This will inform synthetic biology approaches to lignin valorization, but as the commenter suggests does require investigating more complex lignin compounds and polymers.
- Continuing the comments above, our approach is to first tackle C-C bond cleavage by generating a C-C • linked model compound(s) and then move on to investigating more complex lignin polymers containing mixed bond types. While we agree with the comments suggesting we focus future work on C-C bond cleavage and are indeed working on this, we also think  $\beta$ -O-4-containing compounds are relevant. A primary goal of this work is to address gaps in knowledge around lignin products produced from biological depolymerization of lignin and of these products that can be used by microbes to sustain growth and are thus target fragments for use as substrates by microbial hosts engineered to metabolize them into valuable products. It is still difficult to predict if fragments produced from technical lignins lacking β-O-4 bonds will provide fragments amenable for microbial conversion. Control of processes to produce desired targeted intermediates amenable to upgrading may require pretreatment processes that leave  $\beta$ -O-4 bonds intact. Our results have shown that compounds containing  $\beta$ -O-4 bonds (e.g., GGE, SGE, VGE) are metabolized by microbes that have evolved to utilize  $\beta$ -O-4 bond-containing dimers; thus, from a fundamental biology/biochemistry perspective it remains important to understand the enzymatic routes and enzymes involved in  $\beta$ -O-4 bond cleavage. One important component of this work is to determine the effects of the size and structural complexity of different target substrates with different bond types on the degree of bond breakage by biological systems, as well as identifying depolymerization products capable of sustaining microbial growth. This information is key to developing biomass deconstruction processes that optimize valorization of both sugars and lignin, and may conclude that processes producing lignin streams in which  $\beta$ -O-4 bonds are completely cleaved also produce lignin intermediates less amenable to upgrading via synthetic biology and biomass and, therefore, pretreatment processes may need to avoid  $\beta$ -O-4 bond cleavage. For example, biomass pretreatment processes such as ionic liquids solubilize lignin but do not result in  $\beta$ -O-4 or C-C bond cleavage.

# METABOLIC ENGINEERING FOR LIGNIN CONVERSION

## **Oak Ridge National Laboratory**

#### **PROJECT DESCRIPTION**

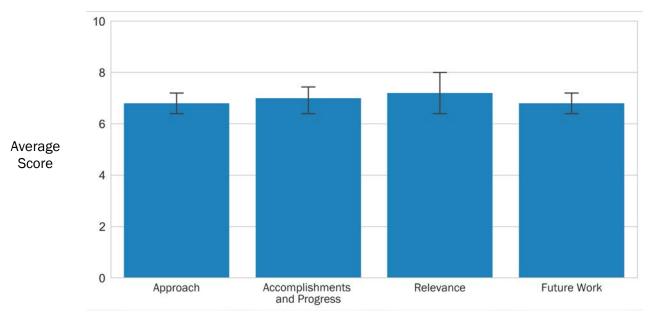
Lignin valorization will be critical for the economic production of biofuels in a biorefinery. Therefore, technologies are needed to convert lignin into more valuable products. However, chemical markets are small compared to fuel markets, so the ability to produce a range of products from lignin would increase the flexibility of biorefineries to meet market demands. One attractive approach for lignin valorization is to engineer microorganisms for the bioconversion of lignin-derived aromatic compounds into products of interest. *Pseudomonas putida* KT2440 is a highly robust bacterium capable of efficiently utilizing a variety of carbon sources, including aromatic compounds derived from lignin, and it

| WBS:                      | 2.3.2.104           |
|---------------------------|---------------------|
| CID:                      | NL0026701           |
| Principal Investigator:   | Dr. Adam Guss       |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$1,452,000         |
| DOE Funding FY16:         | \$350,000           |
| DOE Funding FY17:         | \$350,000           |
| DOE Funding FY18:         | \$402,000           |
| DOE Funding FY19:         | \$350,000           |
| Project Status:           | Ongoing             |
|                           |                     |

has recently been engineered to convert lignin streams from plant biomass into muconic and adipic acids. In this project, our goal is to engineer *P. putida* to convert lignin into products derived from other parts of cellular metabolism, thus demonstrating that we can diversify the portfolio of products that can be made from lignin. One example is medium-chain-length polyhydroxyalkanoates (mcl-PHAs), which are natural carbon storage compounds produced by *P. putida* that can also be used as bioplastics. Through a combination of gene deletions and heterologous expression, we have engineered *P. putida* to increase the yield of mcl-PHAs from both model aromatic compounds and depolymerized lignin. This work is being leveraged to also produce medium-chain-length alcohols (mcl-alcohols) from aromatic compounds, because both biosynthetic pathways

## Weighted Project Score: 7.0

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 ${f I}$  One standard deviation of reviewers' scores

are offshoots of fatty acid biosynthesis. To further increase the compounds able to be made from lignin, we are also exploring production of molecules derived from the tricarboxylic acid (TCA) cycle such as itaconic acid, and current progress will be discussed. Together, this work is a critical step forward in demonstrating microbial approaches for lignin valorization to enable sustainable biorefineries.

#### **OVERALL IMPRESSIONS**

- This project adds to the suite of *P. putida* projects seeking to valorize lignin. The goal of this project is specifically oriented to produce a target molecule from aromatics to a specified titer and yield by on-pathway manipulation, including regulation, deletion, and heterologous gene expression. Initial performance targets are being achieved on both model and lignin-derived substrates; the inclusion of such (more) authentic lignin substrate is greatly appreciated to put the progress into context with conditions more reflective of real-world conditions.
- The PIs are pursuing a relevant project for lignin conversion to itaconic acid (and other chemicals) using novel biochemical approaches in contrast to chemical catalysis. Initial results have shown that discrete chemicals can be derived from lignin, albeit at low concentrations. The future direction of the project should demonstrate the breadth of the conversion with regard to different lignin sources and identify new markets for itaconic that might arise if the cost drops as a result of this research.
- This project applies a carefully designed metabolic engineering approach to increase product yields from lignin substrates, while uncovering general strategies that can be employed to control the performance of engineered organisms. As a result, there is an excellent opportunity to further leverage the outcomes of this work in other BETO projects. In an effort to further utilize TEAs as a research tool, the team could evaluate the impact that improved product yields and costs can have on the market size of the targeted biochemicals.
- The team has progressed the project well and done an impressive job developing this organism for multiple targets. My only concern is that at this stage various BETO sources of lignin from upstream project isolation have not been tested to define the robustness of the engineered organism. Also I suggest, if not already doing so, taking a closer look at past history of LS9, Inc. and current Renewable Energy Group (REG) work in this area, if accessible, to make fatty acids from sugar. This is great project on fatty alcohols and a U.S.-sourced supply could make for an interesting market, if it can be made at current or lower fatty alcohol prices than alcohol made from palm kernel oil.
- This appears to be a strong, well-organized program making good progress, and making good use of TEA to drive metrics and performance assessment. It is encouraging to see what appears to be a good collaborative effort with the NREL team. In addition to the TEA to assess economic impact, it would be helpful to undertake (possibly outside the scope of this project) an assessment of the challenges and key issues to bring a molecule such as itaconic acid in as part of a material substitution versus well-established materials. I suspect that these challenges are underestimated, and they need to be well understood so projects moving forward can be designed with these challenges in mind so they are addressed early.

- Thank you for the positive comments.
- We agree that exploring diverse lignins and market analysis are important directions for the future, so we will continue to collaborate closely with researchers at NREL for both the bioconversion of real lignin streams and for TEA and exploration of market opportunities.
- We agree and plan to continue to work closely with the NREL TEA team to further explore the intersections between performance (e.g., titer, rate, yield), cost, and potential market size.

- Substantial work has already been performed on the robustness of *Pseudomonas putida* in different lignin streams by our collaborators at NREL (and by others), and it will be interesting to explore how our engineered strains perform on these diverse lignin streams. We will also explore any publicly available work on fatty acid production by LS9, Inc./REG to look for lessons learned and potential paths to improvement in our system.
- While the reviewer is correct that exploring the challenges of bringing a molecule to new markets/applications is beyond the scope of this project, we anticipate that we will reach out to potential commercial partners as strain performance (e.g., titer, rate, yield) improves, and that these potential partners could explore new applications. We can similarly reach out to other BETO projects related to downstream processing.

# BIOLOGICAL CONVERSION OF THERMOCHEMICAL AQUEOUS STREAMS

## National Renewable Energy Laboratory

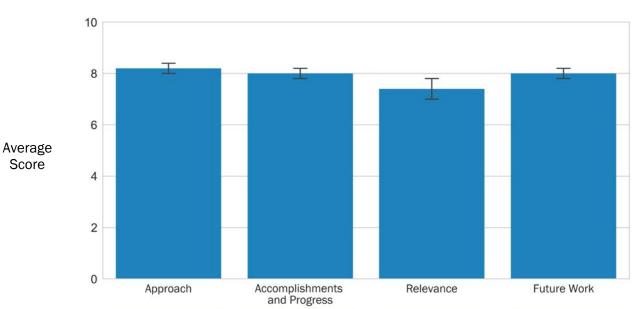
### **PROJECT DESCRIPTION**

The project aims to biologically upgrade compounds in aqueous streams from thermochemical (TC) processing to value-added coproducts. This work will support the BETO mission towards cost-effective TC conversion by producing coproducts (with the exemplary products, mcl-PHAs or muconic acid) that will result in a switch from a \$0.25/GGE cost for wastewater treatment to a revenue stream of a similar magnitude toward lowering the minimum fuel selling price. Utilization of such "waste" carbon is key to the responsive TC biorefinery to produce fuels and chemicals. We predominantly utilize a soil bacterium, *Pseudomonas putida* KT2440, as the organism for this work, as it can catabolize substrates including

| WBS:                      | 2.3.2.301           |
|---------------------------|---------------------|
| CID:                      | NL0026687           |
| Principal Investigator:   | Dr. Gregg Beckham   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$2,305,000         |
| DOE Funding FY16:         | \$750,000           |
| DOE Funding FY17:         | \$750,000           |
| DOE Funding FY18:         | \$485,000           |
| DOE Funding FY19:         | \$320,000           |
| Project Status:           | Ongoing             |
|                           |                     |

some furans, lignin-derived species, and organic acids, and it is tolerant to high concentrations of organic substrates.

This project comprises two tasks: the first is focused on comprehensive analytical method development to fully characterize TC waste streams using mass spectrometry coupled to gas chromatography or liquid chromatography, nuclear magnetic resonance spectroscopy, and molecular weight analyses. The second task



## Weighted Project Score: 7.9

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

focuses on the engineering of *P. putida* for improved toxicity tolerance and expanded substrate specificity. The work will ultimately culminate in a bioprocess development effort at the end of the current three-year cycle that will demonstrate a cultivation strategy for biologically converting a waste stream from *ex situ* catalytic fast pyrolysis to value-added products.

To date, the first task has developed a robust protocol for characterizing TC waste streams from multiple technologies, including fast pyrolysis, *ex situ* and *in situ* catalytic fast pyrolysis, and fast pyrolysis with fractionation approaches. These results have been provided to the analysis projects in the BETO portfolio for rigorous TEAs. Technical accomplishments to date from the second task include engineering of a *P. putida* strain combining chaperone overexpression, dehydrogenase engineering, and membrane modifications that are significantly more toxicity tolerant than the wild-type strain. Additionally, we have engineered the strain to be able to convert over 90% of the carbon found in pilot-scale *ex situ* catalytic fast pyrolysis streams to value-added compounds. Future work includes continued development of *P. putida* towards much higher toxicity tolerance thresholds, additional characterization of *ex situ* catalytic fast pyrolysis pilot-scale derived aqueous streams (including streams from the newly developed platinum [Pt] titanium dioxide [TiO<sub>2</sub>] catalysts), and bioprocess development towards the end-of-project milestone.

It is also noteworthy that this project has larger implications to the BETO portfolio and the synthetic biology and lignin valorization communities more generally; namely, developments in this project will make strides in improving toxicity tolerance of strains to harsh waste streams, and this project will also develop new aromaticcatabolic pathways that can also be harnessed in the context of lignin (as has already been done with discoveries in this project that have translated to the Biological Lignin Valorization at NREL and PET Upcycling projects).

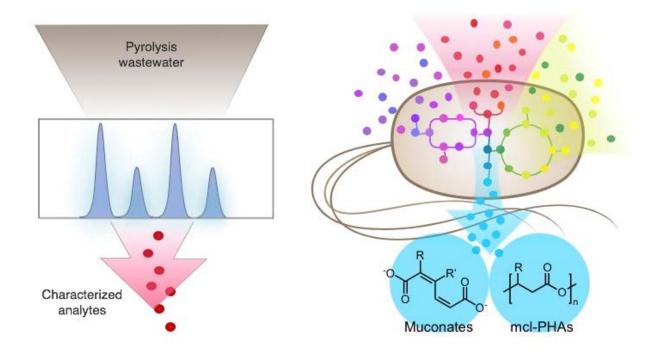


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This is another *P. putida* platform development program that focuses on aqueous thermochemical process waste streams that may have up to 10% waste carbon. Valorizing this level of waste to a useful coproduct, as well as cleaning up the wastewater stream itself, appears to be a worthy target, although it depends on the concentration (a well-developed TEA will bear out the cost-benefit). Strain tolerance is a key issue, and the discovery of a misalignment of substrate composition from TC processing at different scales is key, and presents a challenge. New strategies, strain engineering methods, and potential PABPs have all resulted from this project so far, which is good progress.
- The PIs have presented a scientifically compelling approach to conversion of carbon that would otherwise be lost. The products are reasonable and recognized in the chemical industry. While the specific application of this work to waste streams faces considerable challenges, the broader applicability to lignin conversion is promising, as it is trying to address lignin's structural heterogeneity.
- This project tackles the difficult task to biologically transform low levels of carbon-containing compounds that can be recovered from thermochemical effluents into valuable biochemicals. Although difficult, this objective can reduce wastewater treatment costs incurred by biorefineries, while generating valuable coproducts. This project has made excellent progress. For example, the team has uncovered important differences in aqueous stream compositions as a function of pilot versus bench-scale TC processes. They also made significant improvements to strain tolerance. Codigestion of thermochemical effluents with other industrial process streams represents an important opportunity for future investigation.
- The team has done well coordinating across two very different work programs from analytics to bioengineering and extending the funnel of carbon utilization. Also commended for their ability to work well across different disciplines from process, catalyst team, analytics, and bio team all coordinating well, which speaks to good team management. The project is a success overall, though there is a question as to whether the value return to fuel GGE is sufficient to justify further work, albeit this can contribute learning to lignin bioconversion. Also, there is an interesting development for methyl branched mucconates, which perhaps can be reapplied to lignin programs. Excellent utilization of the waste carbon.
- Overall this is a strong project that has made a number of good technical achievements. I would like to see more explicit statements of the translation of the accomplishments in the basic science, which seem to be numerous, into practical results. For example, what level of carbon utilization has been achieved in bioprocessing of either mock or real catalytic fast pyrolysis wastewater streams, and what is the yield of useful products? How does the performance in these type of tests compare with the necessary targets for commercial viability, and what are the key remaining challenges to be overcome? Maybe all of that is part of future work. This team has done some very solid work to bring the underlying technology along quite far, so it would be good to see their vision as to how that gets translated to a viable, ready-to-deploy technology.

- We appreciate the positive and constructive feedback from the review team overall.
- We have achieved 89% carbon utilization of a pyrolysis wastewater stream. The product yield to muconates is approximately >50% of the carbon. The product yield to PHAs, inherently, will be approximately 30%–40% of the carbon. In terms of developing a bioprocess towards a TEA model, we have just developed a rigorous and comprehensive TEA model, and we are baselining strain performance and bioprocess performance against these targets now.

# LIGNIN UTILIZATION

## National Renewable Energy Laboratory

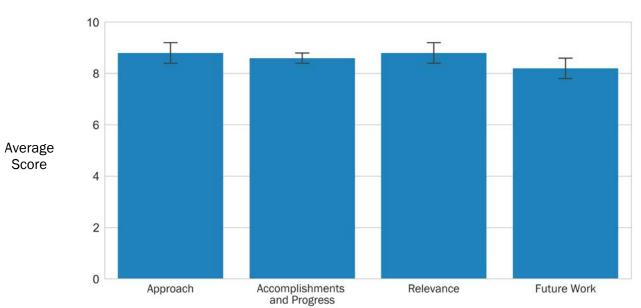
#### PROJECT DESCRIPTION

The project aims to develop industrially relevant processes for lignin valorization with a particular focus on (1) chemical catalysis for lignin depolymerization, (2) chemical catalysis for lignin upgrading in collaboration with the Biological Lignin Valorization at NREL project, (3) lignin analytics applications and development, and (4) lignin model compound synthesis. Through rigorous TEA conducted at NREL by the Biochemical Platform Analysis project, lignin valorization has been shown to be essential for meeting the 2022 BETO minimum fuel selling price cost target of \$2.50/GGE, and this project aims to contribute directly to that effort. The project comprises three tasks: depolymerization, upgrading, and analytics

| WBS:                      | 2.3.4.100           |
|---------------------------|---------------------|
| CID:                      | NL0025416           |
| Principal Investigator:   | Dr. Gregg Beckham   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$5,751,124         |
| DOE Funding FY16:         | \$1,000,000         |
| DOE Funding FY17:         | \$1,500,000         |
| DOE Funding FY18:         | \$1,801,124         |
| DOE Funding FY19:         | \$1,450,000         |
| Project Status:           | Ongoing             |
|                           |                     |

synthesis, and works closely with other BETO projects across the entire conversion portfolio to ensure that the solutions developed in Lignin Utilization are applicable across the spectrum of lignin isolation and biomass-conversion technologies. The end-of-project goal for FY 2019 is to demonstrate a 40% yield of usable monomers from lignin, and to work with the Biological Lignin Valorization at NREL project to show that the monomers can be assimilated in an engineered aromatic-catabolic microbe.

Catalysis strategies for lignin depolymerization focus on aromatic monomer yield and aim to develop methods that are lignin feedstock agnostic. Accordingly, oxidation is a major thrust area aiming at both C-O and C-C



#### Weighted Project Score: 8.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

bond cleavage. The ability to develop catalysts that are able to cleave both C-O and C-C bonds would increase the theoretical lignin monomer yield from many industrially relevant lignin streams, including from acid pretreatment, the pulp-and-paper industry, and the deacetylation and mechanical refining paradigm currently being employed in the BETO conversion portfolio. Accomplishments in this space include the evaluation of alkaline oxidation catalysis across a wide range of conditions and cocatalysts and the development of heterogeneous vanadium-based catalysts. The oxidation catalysis work is culminating with a new catalyst formulation able to cleave both C-O and C-C bonds, which is the major emphasis of the project to complete the current three-year project cycle. This catalyst has been demonstrated to cleave dimers, trimers, and oligomers from reductive catalytic fractionation oil, which is known to contain very few C-O bonds. Deployment of this catalyst system to other lignins is ongoing.

For lignin upgrading, efforts in the current three-year cycle include catalysis and associated process developments to produce the direct replacement, commodity monomers terephthalic acid and adipic acid, both of which are used in very large-market applications. Both of these monomers can be produced from *cis,cis*-muconic acid, which is being made biologically in the Biological Lignin Valorization at NREL project from lignin monomers produced in the Lignin Utilization effort. To date, we have demonstrated greater than 99% yield of adipic acid from muconic acid at high substrate flow rates and with industrially relevant catalysts (in collaboration with the Chemical Catalysis for Bioenergy Consortium project for development of robust catalysts). In addition, we are developing industrially relevant strategies to convert *cis,cis*-muconic acid to terephthalic acid via isomerization, Diels-Alder coupling with ethylene, and dehydrogenation. To date, we have demonstrated isolated steps for each chemistry, achieving 70% terephthalic acid process yield.

Lastly, the project developed a comprehensive library of analytical methods to characterize lignin in the solid form to examine lignin chemistry in the cell wall and in residual lignin solids, as well as methods to characterize depolymerized lignin using advanced mass spectrometry methods. In addition to analytics, the project also produces lignin model compounds for catalysis and biology efforts in support of other BETO projects.

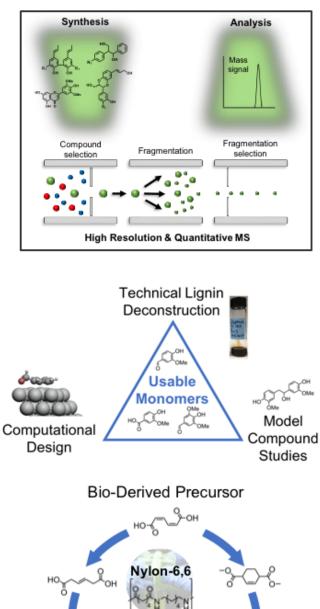




Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

• The Lignin Utilization project is tasked with a wide breadth of work that is actually three projects (described as tasks: characterization, deconstruction, and upgrading). Ultimately, the goal is to recover

the highest possible yield of usable monomers from lignin, to be upgraded either chemically or biologically to value-added compounds (e.g., muconic acid, adipic acid, terephthalic acid), all to be done from an economically attractive process. Each of these tasks performed to date have demonstrated progress on track with expectations. A new catalyst for C-C bond cleavage has been identified, a more recoverable base to replace sodium hydroxide (NaOH), better understanding of structure, analytical development, and synthesis of model compounds, and pathways to adipic acid and terephthalic acid have been demonstrated. There is still a long way to go in terms of yields, such as additional catalyst identification and development, process integration (chemical and biological), and, importantly, proving out the economics. The project appears very well managed and integrated with other projects such as Biological Lignin Valorization, which will continue to be essential to keep on track.

- This is a well-thought-out and organized team effort with a solid technical approach. Model compound synthesis upfront to evaluate and define the approach is a great first principle approach for the project. There are excellent project results to date, and the team is on track to assist the fuel dollars-per-GGE longer term and help other teams by excellent characterization of products formed for use by the bioupgrading team. Excellent progress on the recovery of monomers from multiple feed materials with the easier-to-recover oxidative bases versus sodium hydroxide. There are minor questions around processes to convert muconate to dimethyl terephthalate (DMT), including iodine, which can be a challenge to remove from wastestreams and any traces could carry through causing issues with processes downstream. Has the team considered other isomerization approaches that might be easier to separate, such as solid isomerization catalysts for fixed-bed operations? Also is there a reason why nickel, which is cheaper than palladium (Pd), is not used in dehydrogenation to DMT? Or is it just for initial proof of concept?
- This project tackles a key challenge to higher biological utilization of lignin-enriched streams, namely presence of condensed C-C linkages. The approach builds on NaOH-catalyzed lignin depolymerization, now using bases that can be readily recovered and recycled. To facilitate the analysis of lignin products, the team created a library of model lignin compounds, which represents a unique resource that has been made available to other BETO projects. To further demonstrate the applied significance of a base-catalyzed lignin depolymerization process, it will be helpful to report yields of products from the downstream bioconversion step in terms of amount of product per amount of total lignin consumed. The stability of lignin-derived compounds produced by the base-catalyzed process will also be important to verify.
- This appears to have been a broad, effective program that has made significant progress toward its goals while enabling other projects through expansion of the lignin analysis toolbox. The application of analytics and development of a range of model compounds should be leveraged across multiple BETO lignin-related projects.
- The PIs present an important project with direct relevance to the biorefinery. Their effort to generate a reasonable yield of monomers from lignin depolymerization processes that can be used for further biological processing is valuable and addresses a crosscutting challenge to biorefinery development. Improving the clarity regarding certain process steps and the current status of the model versus real lignin work would be helpful.

- We thank the reviewers for the positive and constructive feedback.
- The question about use of iodine is a good one. Iodine catalysis is used industrially today, but we are working towards other options for the muconate isomerization in parallel as well, including heterogeneous catalysis strategies, as the reviewer suggests. In terms of the dehydrogenation chemistry

to produce DMT, Pd is an initial starting point for this reaction to demonstrate proof of concept, as the reviewer notes.

• We agree on how to report yields. This is indeed a challenge in many lignin conversion processes, but as discussed at the peer review during the questions, we are attempting to achieve comprehensive mass closures to be able to provide these yield data to the TEA teams in a rigorous fashion.

# OXIDATIVE VALORIZATION OF LIGNIN

## Pacific Northwest National Laboratory

#### **PROJECT DESCRIPTION**

Depolymerization of the lignin macromolecule to its monomeric constituents provides an opportunity to generate marketable chemicals or value-added intermediates. However, due to its heterogeneity and compact structure integrity, developing an efficient and cost-effective lignin depolymerization method that also produces selective products has been a well-recognized challenge.

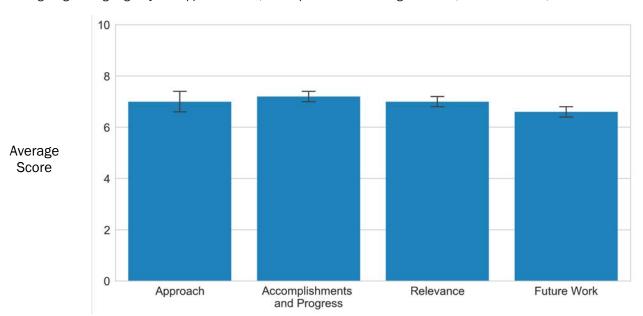
During the last decade, PNNL and Washington State University have developed an oxidative valorization of lignin (OVL) pathway to produce selective monomers, such as monomeric phenolic compounds (MPC) and

| WBS:                      | 2.3.4.101           |
|---------------------------|---------------------|
| CID:                      | NL0033409           |
| Principal Investigator:   | Dr. Xiao Zhang      |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$400,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$O                 |
| DOE Funding FY18:         | \$200,000           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

dicarboxylic acids (DCA), which have promising applications. We have tested OVL on more than half a dozen biorefinery lignin samples, and demonstrated that OVL is an efficient lignin depolymerization technology capable of producing MPC in high yield (i.e., 47% based on initial lignin) under mild reaction conditions (i.e., 1 atm, 60°C).

The specific target of this annual operating plan project is to significantly reduce the cost of catalyst and oxidant (both by 50%) utilized during lignin oxidation while maintaining the product yields and conversion process efficiency.

#### Weighted Project Score: 7.0 Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

The presentation will report progress made in this project to date as well as the future work and potential impact of this project on sustainable biorefinery development.



Photo courtesy of Pacific Northwest National Laboratory

#### OVERALL IMPRESSIONS

- The PIs present good progress on their efforts to convert corn stover lignin into mixed phenols at a specified yield. The primary weakness is that they do not clearly delineate their efforts from the many similar efforts in the literature with regards to improvements and the ability to get mixed phenolics into the chemical industry. A much clearer description of the assumptions used in their TEA would improve the project.
- The OVL project has been successful in demonstrating useful monomer productions in milestonerelevant yields. The process may ultimately be challenged by oxidant and catalyst cost, pending significant further progress on loading or less expensive alternatives to be identified.
- The team has made good progress and has a solid strategy to define the best catalyst systems through high-throughput experiments. The work is at an extremely small scale. I would have liked to see some testing of the current best result at a scale of 100 g or so. Also, there is a big concern over such oxidative processes on a commercial scale, and before scaling the team needs to be clear on potential risks for runaway oxidation reactions unless the lignin itself is a self control for such runaway reactions. The biggest challenge is to reduce cost of catalyst and peracidic levels. One suggestion is to explore self-regenerating peracid or other surface active peracids or aromatic peracids with unique oxidation catalysts that have a high turnover of conversion of acid to peracid regeneration. These may or may not be compatible with the other catalysts but worth exploring from a proof of concept to see if the amount of oxidant loading can be used. See patents by Scheibel et. al. from the Procter & Gamble Company on these iminium ion compounds for use in laundry applications. I cannot say if these materials will be stable to reaction conditions and other cocatalysts. The soils on clothing and dishes are often similar in

challenge to remove, and often aromatic with multiple rings and functionality from the human body, soot from pollution in some countries, polymerized fats/oils, and other complex structures from soil and grass.

- This appears to be a strong project. The team has clearly identified the key challenges and criteria for success and shown very good progress against program milestones. Some high level of assessment of the commercial uses of the OVL products and what a route to commercialization would look like would be additive in defining the key next set of challenges for follow-on work.
- An important development from this project includes a platform to simultaneously screen multiple catalyst formulations. A key aim of this project is to also identify lignin intermediates, which promoted the development of analytical methods for lignin characterization. From a product standpoint, the goal is to increase the phenolic content of lignin to approximately 50%. To reach this goal, it will be important to test selected catalysts on different lignin sources, and evaluate requirements for downstream separation technologies.

- We greatly appreciate the reviewers' comments and suggestion for this project. We strongly agree with reviewers that the oxidant and catalyst are the key cost barriers toward the commercialization of this progress. Based on the suggestions, we plan to include two specific tasks in future work: investigate the regeneration of the peracid and test lignin depolymerization at a larger scale (e.g., 100-g level). We will also conduct a more rigorous TEA analysis in the final year of the project. We also plan to expand the research to test the OVL on other lignin sources and determine the market application/value of monomeric phenolic compounds as the funding will allow.
- We must admit that the TEA assumptions should have been better described. Many inputs were assessed, and the primary cost drivers were oxidant consumption and product yield. Although the dollars-per-GGE fuel value shown above each vertical bar on the waterfall chart was based on an assumed monomeric phenolic compound product value of \$1.00/lb, the value at \$0/lb monomeric phenolic compounds credit is merely the value on the y-axis corresponding to the top of the bar charts. The downward trend in the bar chart illustrated cost reductions against the base case bar at the far left.
- Preliminary TEA shows that oxidant cost is a significant cost driver. Hence, we conducted experiments to better understand peracetic acid decomposition and its interaction with the catalyst and substrate in order to identify less-expensive alternatives. We expect that catalyst cost will also be important and thus conducted a combinatorial study to identify active and less-expensive catalysts.
- Current operating temperature and pressure conditions are low enough that runaway oxidation reactions are not a concern. Indeed, we are excited to find an alternative oxidant and catalyst, as well as applications to selectively produce oxidant reactive species that will produce our desired product and improve oxidant cost and consumption efficiency.

# PERFORMANCE-ADVANTAGED BIOPRODUCTS AND SEPARATIONS

TECHNOLOGY AREA

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# INTRODUCTION

The Performance-Advantaged Bioproducts and Separations (PABP/SEPS) Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place on March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 14 projects were reviewed in the Performance-Advantaged Bioproducts and Separations session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$25,459,273 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 3% of the BETO portfolio reviewed during the 2019 Peer Review. During the project peer review meeting, the principal investigator (PI) for each project was given 30–35 minutes (depending primarily on the funding level) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the PABP/SEPS Technology Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Ms. Andrea Bailey as the Performance-Advantaged Bioproducts and Separations Technology Area Review Lead, with contractor support from Jessica Phillips (Allegheny Science & Technology). In this capacity, Ms. Bailey was responsible for all aspects of review planning and implementation.

# PABP/SEPS OVERVIEW

The PABP/SEPS session covered projects in two areas:

- 1. Projects identifying promising novel bio-based molecules that could offer a performance advantage over existing products, and that are not currently produced through any process.
- 2. Projects that are part of the DOE national lab-led Bioprocessing Separations Consortium (BioSep) that are developing cost-effective, high-performing separations technologies in biochemical and thermochemical processes.

These two areas were combined into a single review session due to the similarities in technology types that were reviewed.

#### PERFORMANCE-ADVANTAGED BIOPRODUCTS

Because bioproducts can be produced from biofuel process residues or at the same facility as biofuels and represent a new revenue stream that could increase consumer and investor interest in bio-based processes, research on bio-based products helps enable bio-based fuels production. BETO funds bioproducts research on both direct replacements, which are identical to products produced through existing processes, and on novel products, which may have potential performance advantages. Projects reviewed in this session focus specifically on these novel products, which are referred to as performance-advantaged bioproducts (PABP). This work involves both predictive modeling of platform molecules and experimental synthesis of the most promising candidates.

BETO's work on PABP spans both independent competitive awards and national lab projects, and a national lab-led consortium of projects working on combining capabilities to identify new products and test their performance attributes.

#### **BIOPROCESSING SEPARATIONS CONSORTIUM**

Developing cost-competitive biofuels and bioproducts requires proven technologies to separate process streams. Today, the cost of separation can represent up to 70% of processing costs. BETO currently funds research and development (R&D) to address these needs through the national lab-led BioSep.

BioSep addresses separations challenges such as impurities in intermediates impeding downstream biological and chemical catalysts, the need for low-cost purification technologies, and recovery and conversion of dilute carbon. The consortium is organized around the two primary process types: biochemical conversion and thermochemical conversion. There is also a crosscutting analysis team, integrated with the two research teams, which conducts techno-economic analysis (TEA) and life cycle assessment (LCA) to inform and prioritize research directions.

# PABP/SEPS REVIEW PANEL

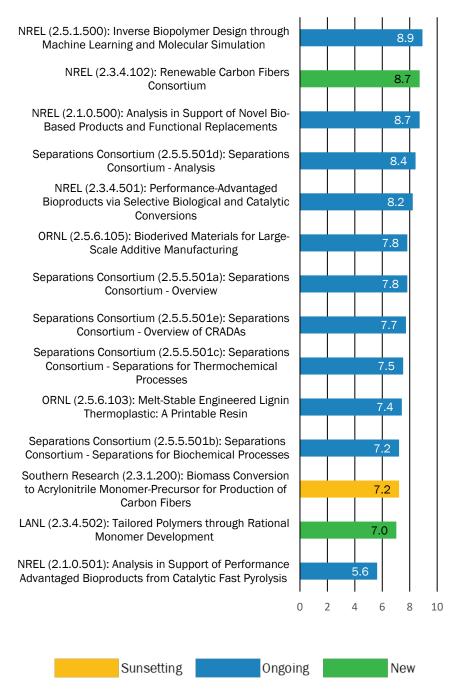
The following external experts served as reviewers for the PABP/SEPS Technology Area during the 2019 Project Peer Review.

| Name             | Affiliation                         |
|------------------|-------------------------------------|
| Joseph Bozell*   | University of Tennessee             |
| Matthew Tobin    | Matthew B. Tobin Consulting         |
| Jeff Scheibel    | J. J. Scheibel Consulting LLC       |
| Melissa Klembara | DOE's Advanced Manufacturing Office |
| Peter Keeling    | Purdue University                   |

\*Lead Reviewer

# TECHNOLOGY AREA SCORE RESULTS

## Average Weighted Scores by Project



# PABP/SEPS REVIEW PANEL SUMMARY REPORT

#### Prepared by the PABP/SEPS Review Panel

Given the space demands of the final report, this write-up can be, at best, only a summary of critical highlights and high-level comments resulting from the panel review. Much more detailed and project-specific information was distributed to the PIs.

Differentiation of the projects resulted primarily from the technical approach and accomplishments presented by the PIs. For example, a strength of the program is that each project demonstrated good relevance to the overall effort. The management plans for all projects contained the pertinent components necessary to carry out the project, with the general exception of adequate risk analysis and mitigation. The program would be strengthened by better inclusion of risk mitigation approaches as part of project management. Future research efforts generally seemed well linked to the results obtained by the PIs.

The panel recognizes that clear communication and alignment between project partners and BETO is essential, but it needs to be as efficient as possible. A potential weakness in program management may exist with regard to the number of meetings, conference calls, reviews, and updates required for the PIs and their teams. A tally of these requirements, especially for PIs involved in multiple projects, would appear to consume a large amount of time. It would be useful for the program to comment on this issue and helpful to technical progress if there was a way to reduce this part of the effort.

#### IMPACT

#### Separations

Separations remain a critical barrier to biorefinery development and operation, as the process streams resulting from biomass conversion offer challenges not seen in conventional petrochemical refining. The PIs presented the very interesting statistic that industrial separations account for as much as 15% of total U.S. energy use, while improved separations could reduce fuel costs by 50%. Thus, success in this area would have a significant impact on overall biorefinery operation.

The efforts underway by BETO's BioSep suggest a number of novel approaches to realizing this potential and, as desired, a route to improve the state of technology with regard to the unique issues that face biomass/biorefinery separations. BETO is supporting efforts in separation research and separation process analysis, which is helping to place the various projects in the context of eventual industrial utility. In parallel, the research activities are closely coupled with a well-organized economic analysis capability within the consortium, which is of particular importance and a true program strength, as it provides the economic basis for project evaluation and direction and crosscuts almost all projects in the portfolio. The team is currently focused on getting bioproducts out of fermentation, separating products from biochemical lignin valorization, and isolating products from pyrolysis mixtures, all key areas to BETO's mission. Further, the more efficient the separation, the more profit one can wring from conversion technology (i.e., improved industrial utility). These issues are well integrated within the program and fully relevant to BETO's broader programmatic directions.

The program faces some issues that may reduce the overall impact. First, as will be described in subsequent sections, a wide range of novel separation techniques are being evaluated with respect to other research in BETO's biorefinery effort. However, there is a gap in understanding whether a separation technology would ever be industrially viable. A given approach might work well, but also might be considered too exotic for industrial application at scale. This data gap, which was acknowledged by the PIs, is an important barrier to address, as the impact of the program is significantly diminished if industry fails to adopt a given technology.

Second, the impact from thermochemical approaches remains unclear. The panel saw an excellent presentation on separation of thermochemical process streams, but more broadly, the scientific challenges underlying pyrolysis may be too large to make an impact on the gallons gasoline equivalent (GGE) regardless of separation. There are simply too many examples of pyrolytic processes in the literature that have been unable to show that pyrolysis can lead to an economically viable process. Generating a complex mixture of low molecular weight compounds simply isn't the way to valorize biomass, and it is not obvious that improved separation methods will overcome this challenge. The program would benefit by a clear description of how these approaches may finally crack these historically intractable issues.

Finally, the panel saw a number of projects displaying an end date of September 2019, making it unclear as to what happens next. Separation research, and particularly the analytical component, is a necessary and evergreen type of effort. But it's not clear what BETO has in mind or how they plan to continue the effort. The presentations described that the time required to complete the steps between an initial concept and its inclusion as a funded effort could take as long as a year, which seems unnecessarily long. The panel recognized that the effort will likely continue, but more clarity around the mechanism would be helpful.

#### Products

The potential impact of this portion of BETO's portfolio is clear. Development of industrially relevant biobased products is at the core of BETO's efforts to achieve their GGE targets. The coupling of high-volume biobased fuels with high-value bio-based chemicals will lead to a biorefinery operation that is overall economically viable and able to compete with the petrochemical industry. To achieve these goals, BETO has constructed a promising and innovative program that couples solid scientific research with rigorous economic analysis and computation. By understanding the properties and performance (which are, in reality, the true products sold by the chemical industry) of bio-based chemicals and defining the technology needs to derive these properties from biomass, the program will demonstrate that the biorefinery can be as important to the chemical industry as the petrochemical refinery.

Economic analysis of the chemical product space is central to the program. In the last two years, the program generated an initial white paper describing product opportunities and is now moving to develop a more comprehensive evaluation, which will be useful in providing a context for broader research. This new report is fairly early stage, and thus its overall impact is somewhat more difficult to assess. However, the PIs appear to be using a market-driven approach. This will be useful as it avoids efforts to "pick winners" by focusing on broad-based conversion technology rather than targeting single products.

The program has demonstrated several successes that can be directly linked to eventual industrial utility:

- Of particular importance is the Carbon Fiber Consortium. By building on some initial, elegant science, the team has moved from the lab to larger scales, has assembled industrial partners, and is ready to generate bio-based acrylonitrile (bio-ACN) at a scale necessary for industrial testing and deployment. The project has followed a trajectory fully in line with BETO's definition of success: initial concept ⇒ lab demonstration ⇒ initial scale-up ⇒ transition to industrial use.
- The program includes work at Oak Ridge National Laboratory (ORNL) that has successfully generated several new lignin-based polymers. The final materials are elastomers made from a polyethylene glycol (PEG) derivative and ACN-refined lignin. This approach appears to have considerable breadth as acrylonitrile-butadiene-lignin polymers give shape memory and 3D-printable composites. Further, the lignin could be mixed with nylon and carbon fiber to give new polymers that meet and exceed automotive strength requirements, which is an important potential application market.
- The program also includes an effort targeting materials production rather than discrete chemical entities. This work at ORNL is markedly different from the other projects in the BETO portfolio but nonetheless is interesting. The project does no real conversion of the biomass; instead, biomass is used as a

component of a plastic in 3D printing. The PIs have been able to make a wide range of fully bio-based materials, shapes, and structures at the ORNL manufacturing facility from 3D printing of polylactic acid reinforced with bamboo fibers and are targeting the use of other natural fibers in future work. The strengths of this concept include an approach that is straightforward, easily understandable, and gives final products with utility easily perceived by a wide audience. The wider goal is to test the use of natural fibers as a replacement for carbon fibers in certain 3D-printing applications. This is a strength, as it helps define a different range of market segments where the strength of carbon fibers may be overkill. This project is on the "applied" end of the BETO project spectrum but demonstrates a balanced program that will lead to greater impact.

#### **INNOVATION**

#### Separations

Several of the presentations on separations were more overviews than detailed research summaries, making it more difficult to evaluate the program's potential level of innovation. Nonetheless, the panel was presented with a scientifically solid program that employed what appear to be a number of cutting-edge technologies. The presentations further emphasized separation technologies identified as uniquely suited for projects generating bioproducts from fermentation and lignin. The recognition of these opportunities across the whole biorefinery process chain and the effort to tailor separations to these needs is a strength. More broadly, the incorporation of these more fundamental efforts needs to remain at the core of BETO biomass research, as it couples basic scientific knowledge to successful biorefinery development and bridges fundamentals with applications. The willingness of BETO to include such efforts (in contrast to efforts supported by earlier incarnations of BETO) is a real strength of the program. The program's cooperative research and development agreement (CRADA)-lite effort with industry (detailed below) is a nice example of an innovative approach to industrial engagement.

The program's innovation would be strengthened, however, with a clearer discrimination between the potential of the different approaches. That is, all projects seemed to be given approximately equal importance and priority, even for processes that would be considered by industry as exotic. Examples include:

- The program has developed a phosphate oil/aqueous-based two-phase separation process for organic acids. It works, is scientifically interesting, and has led to publications. But is it industrially relevant? Issues around the lifetime of this material, its expense, and the impact of entrained impurities at higher levels remain unaddressed. Moreover, mineral oil + tri-*n*-octylphosphine oxide (TOPO) + undecanone could be expensive. It is not clear that the separation improvement justifies a higher cost than alternative separations.
- Two separation paths are described for two methods of lignin conversion, but neither is shown to be better than the other, nor are they categorized as to their potential for industrial utility.
- All projects are shown to have a positive impact on the GGE goals, show success, and are well organized and managed. But they can't all be equally good, or alternatively, they can't all be incorporated into the biorefinery. Are electro-separation methods currently used within industry at the scale necessary to meet GGE targets? Where? If yes, does this represent an improvement? If no, why would industry adopt them? These questions apply to each of the technologies described in the presentation. Surprisingly, several of these approaches have been under investigation for 2–3 years but have not yet been subjected to a comparative analysis.

As such, it would be helpful if the PIs could cite large-scale examples where such approaches are used for commodity chemicals as targeted in the program. The examples need not be direct, step-by-step analogies, but rather approaches that have a similar level of complexity. Alternatively, examples of ultrasonic separations, or two-phase extractions with chemicals of similar complexity and expense would be useful in generating greater

justification for the effort. Presenting examples of how (or whether) a project was working with entities in the commercial separations sector to identify, improve, and innovate technology, such as membranes, materials, and equipment development would lend additional credibility to the technology choices. Further, application of TEA (or even a literature search targeting examples of larger-scale use of these processes) against some kind of industrial baseline will be very important. The panel noted that the relative significance of the projects may be indicated by the funding allocated by BETO.

#### Products

The level of innovation within the program is high. A particular example is the National Renewable Energy Laboratory (NREL) project carrying out computational evaluation of new biopolymers. The foundation for this project is straightforward and important. Computational analysis will be used to define easily obtained biobased starting materials that can serve as monomers in polymer production and offer advantages over petrochemical materials. This is a novel concept and a strength of the project. Overall, the project will query a set of polymer properties (e.g., glass transition temperature and stiffness). A hypothetical bio-based monomer, which will exhibit these properties when polymerized, will be predicted computationally. The potential impact of this project is clear and presents a new means of addressing the questions of what makes a good PABP. It incorporates the considerable computational strength of the NREL team and directs it toward developing a powerful means of defining those products that could be made most easily in the biorefinery. This is a terrific new effort that could be significant for the overall BETO program. The project would benefit from incorporating readily available molecular weight data or polydispersity in their database. Molecular weight is likely one of the most important properties in polymer production, and one of the most widely reported properties of a new material. Polydispersity, directly calculated from the molecular weight data, gives an indication of the polymer's homogeneity. The ability to tell a manufacturer that structure X, because of a computational evaluation, would be able to give a new polymer with molecular weight Y would be a real coup. If that information could then be overlaid with a credible prediction of performance properties, a tool of broad applicability would result.

The program's efforts in bio-ACN production within the Carbon Fiber Consortium and at Southern Research are both based on innovative and scientifically interesting approaches. The PIs in both projects did an excellent job of linking their innovation to the potential impact of their technology. If made less expensively, carbon fiber can replace heavier materials in different segments of the U.S. manufacturing sector. For example, increased use of carbon fiber in automobiles will lead to light-weighting of the fleet and a significant improvement in vehicle efficiency without loss of strength. Based on their research, the PIs have identified clear metrics that define success in their upcoming efforts. The Southern Research effort has operated their process at batch scale for several hundred hours and have achieved the ability to make relatively large amounts of bio-ACN. This would appear to be a significant success.

The program is also supporting innovative early-stage projects. Efforts at Los Alamos National Laboratory (LANL) target the production of new polymeric materials from novel and unique bio-based building blocks. The expected outcome is the production of new materials with new properties, which is a good fit with the BETO conceptualization of PABP. A particular strength of this project is the development of degradation paths in parallel to the synthesis paths, where the choice between biodegradability versus recyclability might be determined by the practical ability of the product to be reclaimed versus recycled. Given the current level of concern over plastics in general, incorporating end-of-use ideas into new polymer development is important. The PI has chosen polycarbonates as a target, addressing a large market with multiple applications. Their effort also incorporates specifications from industry in order to determine targets for these new materials.

#### SYNERGIES

#### Separations

The development of a multi-lab consortium to address the cross-cutting issue of separations is a strength of BETO's efforts and demonstrates clear synergies within the laboratories. The management structure is

appropriate for a multi-institutional effort such as this. The PIs presented a clear impact statement associated with the challenges of running this organization and did a good job of emphasizing the strengths within this cross-cutting support function. The current partners in this effort are terrific (NREL, LANL, Lawrence Berkeley National Laboratory [LBNL], and Argonne National Laboratory [ANL]), well-coordinated, and integrated across multiple labs. This is an excellent means of leveraging DOE facilities to solve a common problem and reduces unnecessary lab competition around a technical challenge that can negatively affect all the scientific effort.

#### Products

The overall program has a current focus on bio-based polymers, and as a result, there is considerable opportunity for interaction between projects. Longer-term work at NREL based on their biochemical funneling approach has led to the production of a number of new polymeric materials based on compounds such as beta-ketoadipic acid as a starting monomer. In parallel, the NREL team has commissioned a new polymer characterization lab that will offer important capacity for evaluating the performance of new bio-based materials generated by BETO research. The NREL project included some nice examples of how new monomers from biomass can be incorporated into new polymers, leading to some examples of performance advantages, in the sense of being able to modify performance and properties through inclusion of bio-based structural units. The new NREL effort in computational prediction of polymer properties is particularly interesting in this regard. If the team is able to develop a robust *in silico* approach for evaluating bio-based monomers, it will have direct and immediate applicability to multiple projects within the BETO portfolio.

Synergy should also exist between the parallel carbon fiber projects from Southern Research and the Carbon Fiber Consortium in the portfolio, but there did not appear to be a connection between the efforts. When compared, the consortium's approach seemed to have a much better chance of succeeding. A better understanding of the interaction/competition between this project and the one underway at Southern Research would be helpful. Will there be a downselection at some point?

#### FOCUS

#### Separations

It is critical to understand the intent of the comments that follow. First and foremost, BETO's willingness to support multiple projects and approaches to biorefinery separation is a real strength and must remain a driver in future work—the technology for biomass conversion still requires a broad-based and flexible effort to define the best approaches, even if it takes longer to reach an answer. If the choice was between supporting multiple, diverse projects and trying to choose a single winner at this point, the undeniable recommendation would be for the former. To this point, the consortium has developed and is investigating eight different base cases requiring separation as a key component. These analyses help identify the most important barriers to overcome for a successful conversion process. This, in turn, helps the researchers focus their efforts where they will do the most good and provide credibility to industrial stakeholders regarding the potential utility of a given separation process.

The separations effort for thermochemical processing offers a nice example of a well-focused investigation. The panel was presented with three well-defined purification methodologies (removal of impurities, capturing carbon from aqueous streams, and intensifying separation processes) designed to make downstream catalytic upgrading of pyrolysis vapor more effective. This project addresses a high-cost component in the generation of bio-based products, and as a result, has the potential of making a large impact on overall economics and GGE goals. Hot gas filtration successfully removes certain interferences and components that lead to coking and is able to use industrially accepted filtration systems to achieve the results. This is a strength, as it will ease the transition to commercial deployment. Further, the PIs were able to show that char, an interfering component in pyrolysis processes, is effectively removed and eliminated from the system using their separation technologies. Finally, their processes can extract acetic acid to give fairly high concentrations in aqueous solution, and at a level that could be economically viable. The project was unique in the separations portfolio, as it included

quite a bit of intellectual property that will be helpful in tech transfer efforts. This is a key strength for this technology as it transitions to industrial use.

There are areas where the program focus would benefit by a little tightening. Several examples of different separation technologies under investigation were described, but they all exhibited a similar weakness. The following is illustrative: for an ongoing algae project, ultrasonic filtration was employed and led to the successful achievement of a technical separation goal. But it is less clear when the next step comes in, which is to evaluate the economic feasibility of separation itself, and more importantly, whether industry would ever use it on the scale necessary to achieve GGE targets. Ultrasonics would seem to be exotic and expensive. Thus, while the technology offers a way to meet a technical goal, understanding whether it is affordable at the scale necessary for a biofuel project would be important. The industrial baseline used in biochemical separations is the simulated moving bed. Are there others that would work? The same questions exist for other separations methodologies included in the presentation.

To their credit, the PIs showed a block diagram comparison of how an analysis is set up. One of the strengths of the program is the existence of a well-defined template for analysis. However, the presentation did not include illustrative results. It would be useful to know for each project where analysis is pointing the researchers when there are several separation technologies under consideration, for example in the lignin and pyrolysis projects. Of the multiple separation approaches described in the presentations, none appeared to have been subjected to TEA, despite having been under investigation for some time. Can the PIs point to actual use of such approaches in industry at the scale needed to meet BETO goals? At what point does BETO look at the various comparative analyses and decide to focus on the lowest-cost approach? It was not clear when such prioritization takes place or how such a process would be carried out. In the absence of any prioritization, the overall focus of the program suffers. Drawing on the expertise of the industrial advisory board (IAB) members could also offer some insight into this question. Indeed, it was stated that the IAB may have seen these approaches. What comments and suggestions were received and did they/will they impact future research directions?

Overall, this perceived lack of focus may diminish the program's relevance. The work coming out of the consortium is scientifically great, but it is more basic than typical BETO projects; it looks more like a DOE Office of Science effort—basic science projects with an "applications" wrapper may not meet BETO's goals. Please do not misinterpret these comments; the approaches are scientifically interesting, and the work is being carried out well. The concern is whether they can make the transition to commercialization, which is a key part of the overall philosophy within BETO.

TEA would be an important contributor to improving program focus, but again, it is critical to understand what is meant. TEA needs to be applied with discretion, and its level of detail must be commensurate with the current state of development of a given project. There is a big opportunity to develop a "TEA-light" so that a promising program wouldn't be missed because sufficient data weren't yet available. This type of evaluation would be a "best-case" scenario for low-technology-readiness-level projects where the cost of an effort could be evaluated assuming each step went in the maximum possible yield (i.e., a simple demonstration of broad economic possibility), but more importantly, an initial demonstration of where the greatest impact of research would be on the cost of a process.

#### Products

Overall, the focus in this part of BETO's program appears quite good. One could argue that research is currently limited to bio-based polymers (several projects), materials (ORNL), and bio-ACN (the Consortium and Southern Research). This is a strength, as these activities address key components of BETO's overall goals: large market opportunities (polymers), bio-based materials (direct use of biomass), and transition from the lab to commercialization (bio-ACN/carbon fibers). As with the Separations program, the inclusion of these multiple efforts is to be applauded. Further, it appears that early-stage projects are being given sufficient funding and time to demonstrate principle without being too heavily burdened with economic evaluation.

Projects are incorporating efforts to understand fundamental molecular-level interactions, which will be critical to process control and operation and tailoring of product properties for performance. As an example, the ORNL effort in developing a printable resin did an excellent job of placing the work in the context of molecular-level interactions within composites.

The focus of the BETO products effort is always challenged by the huge number of product opportunities available. As a result, the crosscutting analytical work at NREL will be an important component of the overall program. As the analysis proceeds, it will be most effective if it maintains a broad technology development focus and does not become an effort driven by identifying specific compounds for study. Further, analysis will benefit by carefully defining how a new report/analysis differs from the many similar analyses now in the literature, and from those that have been done by DOE itself. The presentation on product analysis identified the understanding of performance traits as highly important. In actuality, one could argue that the industry has already defined these traits within their well-defined market segments: coatings, resins, surfactants, etc. Additionally, polymers also have well-defined property and performance specifications. The bigger challenge, which did not seem to be emphasized, is a definition of technology opportunities, and identification of the products that can be most easily made from that technology. This concern is particularly acute with regard to the PABP concept. Identifying key compounds that come from biomass is good, but many of the compounds described in the presentations exhibited higher molecular complexity than is normally generated by the chemical industry. The PIs might consider looking at the literature on quantitative scales for molecular complexity to see if their materials fall within indices representative of what the industry currently makes.

It would be useful if the analysis could also describe the strengths and weaknesses of the current prototype targets in other parts of the program. For example, the panel saw descriptions of butanediol (BDO) and adipic acid in the design cases of the biorefinery and GGE calculations. But what if other products were substituted? Do the assessments change if 2,3-BDO (a biochemical with little or no current market) is substituted with 1,4-BDO, a known material with known markets? These types of evaluations are needed for multiple families of chemicals to assure interface with the chemical industry. Otherwise, the project runs the risk of becoming internally consistent, but having less utility when compared to existing markets.

As with Separations, TEA will help focus the program on the most promising opportunities. For more advanced projects, presentations in several sessions presented a well-organized TEA template developed at NREL. However, this methodology was not employed uniformly. Some projects used these techniques, while others used internally developed analyses or employed TEA carried out by the project PI that was not well supported. Several examples illustrate this issue:

- The ORNL effort in 3D printing targeted a composite cost of \$3.00/lb, or 50% of the carbon fiber cost. Can the PIs show that even with a reduction to \$3.00/lb, the industry would use such a material? How/where do the PIs see these materials fitting into the market and for what applications? Are these markets of sufficient volume to make a difference? Are there data on these potential uses? In addition, many of the other projects in this portfolio describe the cost impact with regard to its impact on GGE, and thus it would be helpful if the PIs did the same thing here, projecting the reduction in GGE as a result of producing these materials within the current state of technology.
- During a question and answer (Q&A) session on the ORNL effort to develop a printable resin, it was indicated that the TEA was carried out by the PI and not by any of the TEA experts within the BETO organization. Further, it became clear that the assumptions used and conclusions resulting from their analysis were murky and difficult to understand. One was left with the impression that good science had been accomplished but the costs could be too high for the project ever to make the leap to commercialization. The PIs did not include the cost of lignin extraction and isolation, which could be significant. The milestone slide indicates a goal of increasing lignin's "value," but the meaning is not clear. The implication is that the lignin must have a certain minimum value in order to meet GGE goals, which is an odd way to describe how TEA is being used. It would seem that the more appropriate goal

would be to minimize the product cost so that it could be economically competitive. If the lignin cost is too high, the new composites will also be expensive and of limited market. Greater clarification of these arguments would be helpful.

• The NREL effort to generate monomers from pyrolysis oil was also not convincing. The relevance (as acknowledged by the PIs) of this project is hampered by the potentially small amounts of material that could be derived from pyrolysis oil. To better assess the approach, the PIs would benefit by completing a rough mass balance diagram that indicates (under optimum conditions): 100 g biomass ⇒ XX g oil ⇒ XX g phenolics ⇒ XX g starting monomer ⇒ XX g of a "performance-advantaged" biopolymer. The numbers will likely be very, very small, thus bringing the viability of this approach into question. Using some of the PI's own numbers, and starting from 100 g of biomass, one might get 25 g of pyrolysis oil. Of that, one might obtain 3.5% of cyclopentenone even before the start of a multistep polymerization. In a 2,000-tonnes-per-day biorefinery, that's a very small amount of polymer. They would further benefit from a clear description of the separation technology needed to get fully purified cyclopentenone (for example) from the pyrolysis oil mixture.

### TECHNOLOGY DEVELOPMENT PIPELINE

#### Separations

The Separations program demonstrates high scientific quality nicely coupled with analytical evaluation. However, the path to commercialization was less clear. This may not be a weakness at this stage—optimal separations for biomass and biorefinery process streams are not yet developed, and the effort to carry out more fundamental research is worthwhile. Such research should be given sufficient time to reach fruition without being fully driven by efforts to reach commercialization. Nonetheless, the PIs described a clear interest in presenting capabilities within the consortium to potential industrial partners. That shows a balance between internal separations development and access to facilities for external partners, which is a strength.

The listening day (and the industrial outreach, more generally) is interesting and potentially useful. A particular strength is that in this outreach it appears that these activities are coordinated more at the management/program level, rather than making it the responsibility of the individual PIs, as seen in other programs. A further strength of the program, and useful for engaging stakeholders, is the consortium's website describing the capabilities of the consortium.

The panel was impressed with the innovative "CRADA-lite" effort funding short-term screening efforts in separations with industrial partners. This is an interesting approach for engaging industry and offers an opportunity to examine a focused concept for a short period of time to see if it has promise and could contribute to BETO's goals. The concept of seed grants to increase industrial participation in BETO projects is useful and could serve as a model for other portions of the program. The panel felt that the total number of interested applicants could have been larger, and that future rounds of CRADAs should be planned sufficiently in advance to provide continuity of effort and use of resources. Such modifications to the program could serve as positive advertisements for future CRADAs. Overall, the presentation demonstrated that the PI's approaches are reasonable and are addressing one of the larger goals of the subset of the BioSep presentation—industrial participation and outreach.

Technology development could be strengthened in some areas. For example, the CRADA-lite funding levels seem low, and BETO would benefit from limiting the number of partners that could be involved on any single grant. For example, the Kalion and HelioBioSys CRADAs have \$200,000 with three national lab partners spread over two years. It is not clear that this is an effective use of funds given the costs at the labs. A better description of how the industrial partnerships "speed-dating" process operated would be helpful in understanding how the partners were chosen and invited to participate in the program. The review panel expressed mixed views on partnering choices. Some thought it a clear benefit to partner with smaller entities to provide missing expertise, equipment, and bandwidth, while others on the panel felt that the lack of chemical

companies like DuPont or BASF, for example, could be perceived as a weakness, as they would bring greater industrial credibility than a small startup. The Q&A revealed that some larger industries were in the proposal mix but did not make the cut.

A stronger description of how the listening day differs from standard BETO road-mapping workshops would be helpful, as would a description of whether this approach is any more successful than others. There are many historical examples of putting the lab researchers and industrial representatives into a room for a day in order to "find out what industry wants." They're often quite valuable for industry, as they get a sense of what's going on in the labs, but much less useful in the other direction, as industry is slow to reveal what they're working on and what problems they need to solve.

#### Products

The Renewable Carbon Fiber Consortium is a great example of science being translated to commercial use. It appears that the team has moved to precommercial scale and testing, and presumably has the economics to make it work. What is presented is an excellent example of good science and good application following a well-laid-out path to a potentially important product. The weaknesses are minimal, in that the route to bio-ACN has been demonstrated, and initial work in scale-up is also showing success. The project has a clearly defined goal and is therefore directly understandable to a wide audience (i.e., "we will make cheap carbon fiber"). A real strength of the project is its identification of the key members of the team needed to carry out each of the steps in production and evaluation. Overall, all the steps, partners, and planned work is exactly what is needed to move this program to the next phase. All important questions are being answered and all challenges have appropriate plans in place to make it work. The handoff from one partner to another is really well laid out. They have experts on each step in place. Bigger picture, this is a really nice organization addressing exactly the needs necessary to prove out the overall approach. Good science has led to good applications that attract industry and offer opportunities for commercial deployment.

As the effort proceeds, the program will need to continue their close organization of a number of partners to make sure that problems with one do not impact the overall plan and schedule. It would be helpful to have more detail on how the partners were vetted. For example, it is interesting (and surprising) that the PIs are using an external producer of their carbon fiber, given the availability of the carbon fiber manufacturing facility at ORNL. Finally, catalyst deactivation seems important, and the team has identified it as a key issue. Getting a sense of whether there might be multiple solutions to the issue would also be useful to know. This could be a showstopper, so some insight as to what's going on would be helpful.

A primary opportunity for improving the potential for technology transfer would be a deeper analysis of whether a given project has a chance of being industrially relevant. The panel saw several projects where this question was of concern:

- The LANL effort to generate new polymers begs the question of whether the industry would adopt compounds of this complexity, especially when they require multiple steps for their synthesis. The answer may eventually be yes, but the project would benefit from industrial examples that might have an equivalent number of steps from raw material, to monomer, to polymer, and which exhibit similar structural complexity.
- The Southern Research effort in bio-ACN would benefit from a better understanding of the dependence of ACN cost on propylene glycol sales and a clearer delineation of TEA assumptions. Industry tends to avoid coproduct schemes, and thus understanding how the PIs will avoid this problem would be helpful.
- The industrial utility of the ORNL effort to make printable resins would be strengthened with a better understanding of the true target cost of these composites, and whether it will be low enough to compete would be useful. For example, the presentation suggested competition with resins at \$1.12/lb. But the complexity of the process suggests that the cost may be significantly higher for this process. Thus, a

clear, simple presentation of targets and economic assumptions is needed. The process requires lignin preprocessing (for example, extraction of the initial lignin with acetonitrile) to get a refined lignin for the 3D and composite applications. The lignin is then mixed with a polymer under high-shear melt mixing to give the final product. As the presentation proceeded, the number of steps and actual yields became a concern with regard to final lignin cost and process complexity. The PIs did not indicate the amount of material derived from their extraction process. Is it 10% of the starting input? 50%? Further, the use of acetonitrile for extraction would seem to be an overly complex process for an industrial plastic. In the BETO context, do the costs establish a credible case for industrial adoption?

- More broadly, the program's interest in bio-based polymers needs to face the reality of the polymer industry: introducing new polymers into the market is a real challenge. The current polymer industry has a huge amount of experience in formulation and process modification to introduce properties of interest. In fact, the last polymer to be introduced at a large scale was probably DuPont's 1,3-propanediol polyester. And before that, it would have been years and years between introductions. The polymer market is particularly tough to crack, and thus simply because something is polymerizable doesn't mean that it can be commercialized. To that end, the PIs need to describe how a new material might make it to market, and answer questions regarding comparisons between the candidates and the existing market (e.g., "bio-based polymer X is most like polystyrene, or polypropylene..."). It is not clear that improved properties alone are sufficient to make a difference and generate the revenue needed to meet GGE targets. Can the program make a credible argument that a new structure would have a reasonable chance of becoming commercial?
- NREL is carrying out efforts to isolate specific compounds from pyrolysis oil for the purposes of generating new polymers. The general concept of extracting greater value from pyrolysis oil is laudable, and the PIs describe some approaches that are reasonable on paper. However, this program faces the considerable challenges of trying to extract a very small amount of their starting chemicals in purity sufficient to drive downstream conversion. The further complexity in their process may make it difficult to get the project transitioned to industry. The PIs acknowledge the most critical challenge of this project: pyrolysis oil contains dozens of identified products, and maybe hundreds unidentified. It is not at all clear how this complex mixture can be a reasonable source of polymer starting materials. Further, the proposed synthetic sequence to monomers from cyclopentenone is not convincing if considered in an industrial context. The approach is scientifically interesting, but hard to accept as a reasonable way to make barrier materials. In the BETO context, it is not clear that such an approach could ever be commercial. If the PIs are using this simply as a demonstration of principle, they also need to present some idea of how it could be improved. Unfortunately, the yields do not seem to be sufficient even at a lab scale. These weaknesses are all considerable barriers to technology transfer.

#### RECOMMENDATIONS

- Continuing the multifaceted approach by supporting multiple separation and product development efforts will be critical in understanding the technology space needed for optimal biorefinery separation processes
- The integration of science and molecular-level understanding with industrial applications should continue, as this will form the best foundation for process development and control
- There are opportunities to improve the focus of the program, but they must not be done at the expense of promising but unproven separation or product development approaches.

# PABP/SEPS PROGRAMMATIC RESPONSE

# INTRODUCTION/OVERVIEW

BETO would like to take the opportunity to thank the reviewers for their time and careful review of the portfolio. The program recognizes that this was a difficult review process because additional projects relevant to this area presented in other sessions due to time constraints. BETO agrees with the review panel that these two areas have strong potential for helping their office meet future GGE targets and appreciates the detailed feedback across both areas. The recommendations from the review panel will be discussed and taken into consideration when working on future project selection and program design, as future appropriations allow.

For each recommendation, BETO provided a general response followed by some specific examples of how they will be integrated into the two technology areas covered in the session.

#### Recommendation 1: Continue multifaceted approach.

BETO is committed to continuing support for a diverse slate of separations and PABP as appropriations allow. The program agrees that a strength of their approach to both of these areas is the ability to fund a number of different technology types across a broad range of funding recipients. BETO also recognizes that part of funding such a large number of technologies is the ability to identify those that are not likely to be successful or those that no longer are at a stage requiring government funding, and either downselect or graduate those technologies. Moving forward, BETO will work on communicating how different projects, as well as their office as a whole, goes about those processes. Further, we agree with the review panel comment that researchers can be overburdened by coordination efforts, and BETO staff will be cognizant of this moving forward.

*Separations:* After the review completed, BioSep conducted an internal review of the existing projects and reprioritized some of their work in response to feedback from the panel, as well as selected work in new areas. BETO is committed to this kind of exercise, which will allow the consortium to integrate new separations technologies and move on from those that are either ready to transfer to a higher technology-readiness level or that do not appear likely to be economically viable in a commercial biorefinery setting.

*Products:* The PABP Technology Area is relatively new to BETO, and several of the projects that presented were only selected in the last review cycle. BETO is committed to investigating a wide range of options for PABPs, and the projects that presented in this session will be joined by additional national labs and competitively selected projects over the coming fiscal years. Several projects selected in FY 2018 competitive solicitations had not completed enough work to participate in the full review but did present in the poster session. The two Renewable Carbon Fiber Consortium efforts were specifically cited by reviewers as an example of projects that could use either additional collaboration with each other or consideration from BETO for a future downselect. Both of these projects were selected from the same FY 2014 funding opportunity, and due to the structure of competitive awards would not specifically be considered for collaboration with one another. BETO will, however, consider how to best integrate their results into new work in this area moving forward, as appropriations allow.

#### Recommendation 2: Continue to integrate science with industrial applications.

BETO agrees with the reviewers that a crucial piece of both of these areas is the commitment to interacting with industrial entities and will continue to focus on linking research to industrially relevant goals. To help facilitate this process, BETO is committed to the continuation of soliciting feedback from external stakeholders on the portfolio through listening days, workshops, and requests for information. Generally, road-mapping workshops are specifically designed to answer a set of questions about how BETO can provide value in an area of research over a set timeframe, whereas listening days are used to gather more general feedback on a broader number of topics. BETO has found both are useful depending on the final desired outcome. Feedback from a public workshop in the summer of 2017 led directly to the creation of the national lab PABP Consortium, and

feedback at other similar events has resulted in BETO moving into new work on different types of potential PABPs, including novel plastics.

*Separations:* The CRADA-lite projects that BioSep presented on were launched in FY 2019, and BETO appreciates that the reviewers found these projects promising. BETO will track the progress of these projects and the other similar efforts funded throughout other parts of the portfolio and hopes to fund additional projects in this space as appropriations allow. Additionally, BioSep will continue their work with their IAB.

*Products:* The national lab consortium PABP projects appreciated the reviewers' suggestions to consolidate under a single IAB and have started efforts to combine their industry contacts. This work should continue throughout FY 2020.

#### Recommendation 3: Improve focus while still investigating novel approaches.

As with Recommendation 1, BETO agrees that a strength of both of these areas is the ability for researchers to investigate a number of different approaches, some of which are often too novel and/or risky to likely be funded through other means. BETO also understands that a result of funding work like this is that these projects are often less likely to be economically viable in an industrial setting, and that once this becomes clear, it is not an impactful use of funding to continue work. To help identify points where certain pieces of these larger consortia projects may no longer be successful, BETO is committed to continue to require all projects to use feedback from external reviewers and TEA results to help adjust research priorities and keep them relevant. BETO is also committed to finding an appropriate level of TEA for more novel technologies, as recommended by the reviewers, and will continue efforts to make sure TEA is applied appropriately going forward.

*Separations:* As the BioSep moves into a new three-year funding cycle, they have developed milestones and decision points focused on using property-based differences to provide insight into relative advantages and disadvantages of bioprocessing separations approaches. The consortium is committed to developing a standardized and transparent process for making decisions about R&D priorities. They will also continue to incorporate TEA into each technology area that they work on.

*Products:* As the national lab PABP work matures, BETO is committed to integrating more TEA and LCA with the existing work, as appropriations allow. Due to time and availability constraints, the same teams cannot always perform the TEA for each project, especially across different national labs, which has led to some of the discrepancies identified by reviewers. BETO will continue to make an effort to standardize TEA and make sure different project teams share their assumptions. BETO will also continue to work with competitively selected projects to monitor results based on TEA approaches. BETO recognizes that most current work in this area is focused on polymers and agrees with some of the limitations identified by the review panel in focusing on this product type. As BETO generates more data in the area of PABPs, their office expects to expand focus into other promising products, as well as be able to better identify what will give a polymer or any other product a better chance of industrial uptake.

# ANALYSIS IN SUPPORT OF NOVEL BIO-BASED PRODUCTS AND FUNCTIONAL REPLACEMENTS

# National Renewable Energy Laboratory

# **PROJECT DESCRIPTION**

The production of chemicals is a major driver of the U.S. economy, as it has accounted for roughly 2% of the U.S. gross domestic product over the past several decades and has a growth rate projected by the industry to produce well over one million new jobs. Therefore, producing chemicals from biomass has the opportunity to significantly impact the future growth of the chemicals industry and the U.S. economy overall. In fact, recent reports by the U.S. Department of Agriculture have concluded that there are roughly 1.5 million jobs in the United States directly associated with the production of bioproducts.

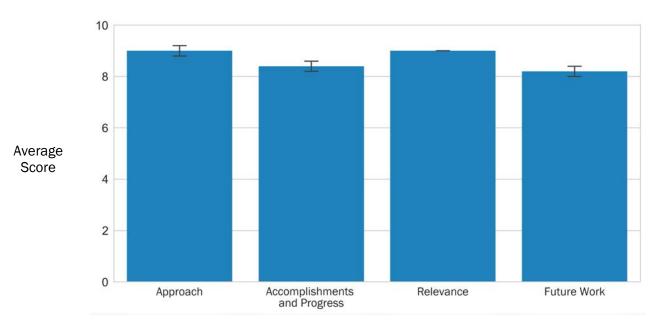
| WBS:                      | 2.1.0.500           |
|---------------------------|---------------------|
| CID:                      | NL0033392           |
| Principal Investigator:   | Dr. Mary Biddy      |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$500,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$250,000           |
| DOE Funding FY19:         | \$250,000           |
| Project Status:           | Ongoing             |

Two primary approaches have been adopted to produce

chemicals from biomass. One option is to produce chemicals that are identical to those currently derived from fossil feedstocks and are often referred to as direct or drop-in replacements. Such bio-based chemicals are indistinguishable from their fossil-derived counterparts in terms of their chemistries, compositions, purities, and properties. The other option is to produce chemicals that are different from fossil counterparts, but that have unique properties or improved performance. These bio-based chemicals are thus referred to as PABPs. While a number of examples of performance-advantaged bioproducts are produced commercially, one of the

# Weighted Project Score: 8.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



biggest challenges facing growth in manufacturing and research and development activities in this area has been understanding what specific characteristics and performance traits are desirable for these chemicals.

The NREL project on analysis in support of novel bio-based products and functional replacements aims to fill this information gap. The objective of this project is to understand and outline the value propositions and potential drivers for producing PABPs. Within this analysis effort, the team is working to outline specific properties needed for a wide range of end-use applications. The result of this three-year analysis effort will be a guiding document that can be used by industrial and academic researchers to focus their R&D on PABPs with the biggest potential to impact and grow the U.S. bioeconomy.

#### **OVERALL IMPRESSIONS**

- The project must filter down choices quickly to focus on few chemicals to move forward. Two years seems long to filter down. Suggest that they should group materials together in terms of similar functionality to target mixtures that could replace things like chelants, aqueous viscosity modifiers for consumer products, or even lower molecular weight, water-soluble-type oligomers may be easier targets for functional materials in the 20,000 molecular weight average range or lower. This could avoid costly separation of single materials in some cases while providing a bigger cost reduction to fuel cost/GGE and a bigger chance to be successful overall.
- This has potential to be a very valuable publication when completed. Would be good if it could somehow identify pointers to next-generation molecules.
- The project is addressing a core goal in biorefinery development—understanding the properties and performance that are the true products of the chemical industry. Incorporating this understanding with a definition of the technology needs to derive these properties from bio-based building blocks will need to be a key component of any report or white paper resulting from this work.
- The project aims to generate a list of desirable bio-based targets, differing from prior work by including more performance and characteristics criteria to prioritize performance-advantaged bioproducts. With the pressing need to improve biorefinery economics via better valorization of streams, this effort is of strategic importance and, if successful, can be a guiding decision tool to focus valuable R&D time on better target choices.
- Great integrated approach to share information, results, and resources. Very well presented and the explanation of the framework for analysis of evaluating performance-advantaged bioproducts was clear. External advisory panel with eleven advisors provides a wide variety of industry perspectives. This is very thorough research and analysis to outline the value proposition and market pull.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their helpful feedback and comments. We will work to incorporate these suggestions in the project going forward.

# ANALYSIS IN SUPPORT OF PERFORMANCE-ADVANTAGED BIOPRODUCTS FROM CATALYTIC FAST PYROLYSIS

# National Renewable Energy Laboratory

# **PROJECT DESCRIPTION**

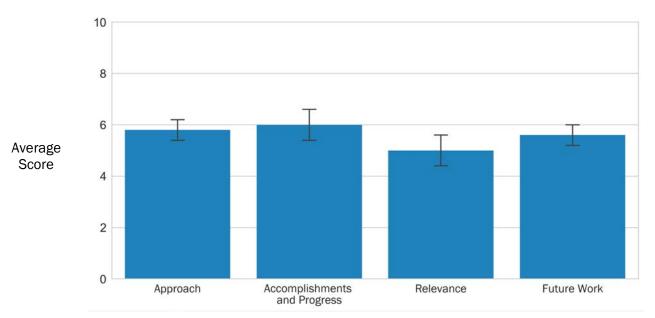
The high oxygen content in biomass (40%–50%) enables the production of oxygenated molecules that can be used to produce novel polymers that often have superior properties over existing materials. Synthesis of these same molecules from nonoxygenated fossil fuels is often expensive and requires hazardous and environmentally damaging transformations. Thus, there are clear potential advantages for biomass-based polymers in terms of performance, cost, energy use, and environmental impact. Catalytic fast pyrolysis (CFP) of biomass offers an inexpensive, highthroughput route to deconstructing the biopolymers found in plant cell walls, but there is a knowledge gap concerning how to use this technology to produce novel and

| 2.1.0.501           |
|---------------------|
| NL0034074           |
| Dr. Mark Nimlos     |
| 3/31/2018-9/30/2020 |
| \$400,000           |
| \$0                 |
| \$0                 |
| \$200,000           |
| \$200,000           |
| Ongoing             |
|                     |

performance-advantaged polymers that preserve the unique chemical structure and composition of biomass. In this project, we bridge that gap by providing experimental work that shows pathways to performanceadvantaged polymers from CFP-derived monomers. Novel polymers are synthesized using the oxygenated molecules found in CFP biocrude, and their properties (glass transition temperature, permeability, Young's Modulus, etc.) are measured to identify performance enhancement needed to meet industrial specifications.

# Weighted Project Score: 5.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



The results of this work will help advance the bioeconomy by providing pathways to high-value coproducts that can increase the commercial viability of biorefineries.

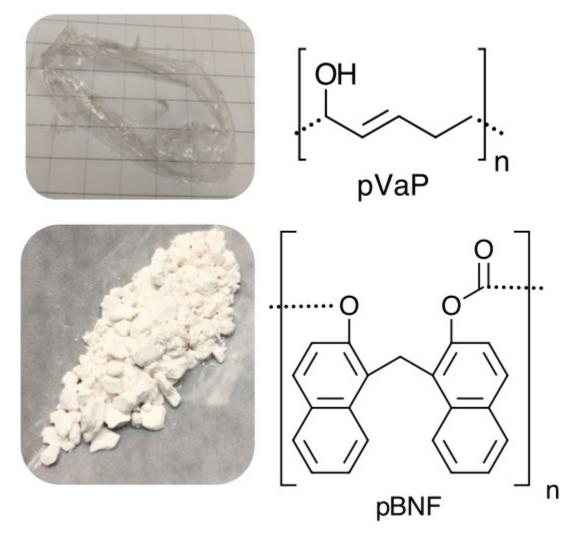


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• Great work to produce a variety of polymers for potential evaluation using various identified CFP lignin products. This work result could be valuable in general outside of the BETO projects by identifying new classes of polymers for commercialization in the near term. However, there is concern over the level of these monomers in the CFP process and isolation of these individual compounds appears to be of low probability for use. My main feedback would be to group together a number of distillation products in similar boiling ranges to see if the total weight percent in lignin products could reach a reasonable amount of, say, 10%–15% total. Next, see what chemistry can be done similarly to that group to form monomers of use, which perhaps could also be copolymerized to make new polymers or isolated at this stage to feed to different processes. Simplification is key to this project success. The more consolidation that can be done to simplify the isolation and number of process steps and volume of material converted, the better the economics and viability could be.

- It was not clear what the number of processing steps is for a TEA to be attractive. The fraction of the biomass to products seems extremely low to capture a meaningful market share. It would have been good to understand the value proposition here from industry.
- The general concept of extracting greater value from pyrolysis oil is laudable, and the PIs describe some approaches that are reasonable on paper. However, this program faces the considerable challenges of trying to extract a very small amount of their starting chemicals in purity sufficient enough to drive downstream conversion. The further complexity in their process may make it difficult to get the project transitioned to industry.
- Potentially useful. Products look challenging.
- The overall approach of deriving value by synthesis of PABPs from CFP seems very challenging due to the complex mixture of chemicals (and hence product streams) that are likely to result.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate this valuable feedback.
- As we acknowledged in our presentation material, the selectivity of individual molecules from CFP is low where this conversion is currently being studied. These studies (at NREL, RTI International, Chemical Process Engineering Research Institute [CPERI]/Centre for Research and Technology-Hellas [CERTH] in Greece, and VTT Technical Research Centre of Finland) have focused exclusively on producing biofuels, where organic yields, not selectivity, are important. However, there are examples in the literature and industry where selectivities of individual molecules are much higher. For instance, levoglucosan, levoglucosenone, furans, some phenols, and aromatic molecules have been produced at concentrations ranging from 5%–30%. Aromatic molecule production for chemicals is being commercialized by Anellotech, Inc. and BioBTX.
- Given that there is literature and industrial precedent for higher selectivity of molecules from CFP, the goal of this project was to identify novel, performance-advantaged polymers that could be produced from CFP biocrude. We have started with molecules identified in CFP biocrude from a biofuels processes and used these to synthesize and test novel polymers. Once we have identified performance-advantaged polymers and their molecular precursors based upon their properties and industrial need, that is the point where increasing selectivity should be improved. There are other projects in the BETO portfolio that are working on ways to improve selectivity and separations and they have the capability and means to address this.
- This is exactly the approach that was used for many polymers such as polycarbonates. They were discovered in spite of the fact that phenols were found in low concentrations from coal tars, etc. It wasn't until the commercial importance of polycarbonates were established that the Cumene process was discovered for making phenol. We propose to establish the importance of new materials and then find a way to improve the production.
- The idea of attempting to use 10%–15% of the CFP biocrude as a class of compounds is an excellent one, and there is work in other projects to do just that.
- TEA efforts for coproducts is an ongoing effort in parallel projects, and we agree with the challenge of economic coproduct production.
- The polymers that we are investigating use biomass-sourced molecules and thus, due to their elemental composition, have a shorter pathway to products. For instance, commercial polyvinyl alcohol (PVA) is synthesized from ethylene, which comes from the cracking of petroleum and vinyl alcohol, which is made from acetic acid and ethylene. Acetic acid is made by the carbonylation of methanol, which is

produced by the gasification of natural gas and catalytic synthesis. There are five steps from the raw materials and a number of separations processes required:

- Natural gas  $\Rightarrow$  syngas  $\Rightarrow$  methanol  $\Rightarrow$  acetic acid [+ ethylene]  $\Rightarrow$  vinyl acetate
- petroleum ightarrow ethylene ightarrow ethanol
- $\circ$  ethanol + vinyl acetate  $\Rightarrow$  PVA
- Our process to make a novel polyvinyl alcohol propene (PVAP) is when biomass is converted with CFP, the cyclopentenone is reduced, and the product is polymerized. There are three steps fewer in the separations processes:
  - Biomass  $\Rightarrow$  cyclopentenone  $\Rightarrow$  cyclopentenol  $\Rightarrow$  PVAP
- Market share alignment is part of current TEA efforts. The value proposition is creating value from materials that cannot be achieved through conventional petrochemicals.
- As discussed above, we recognize the problems associated with low selectivity, but other projects are addressing these issues. Our goal is to prepare and test PABPs.

# BIOMASS CONVERSION TO ACRYLONITRILE MONOMER-PRECURSOR FOR PRODUCTION OF CARBON FIBERS

#### **Southern Research**

# **PROJECT DESCRIPTION**

Polyacrylonitrile (PAN)-based, lightweight, high-strength carbon fibers are receiving great interest from the automotive industry, particularly in their bid to improve fuel efficiency of vehicles. However, widespread application of carbon fibers is presently deterred by high manufacturing cost (greater than \$10.00/lb). Ninety percent of the world's carbon fibers are PAN based, derived from an ACN monomer and commercially

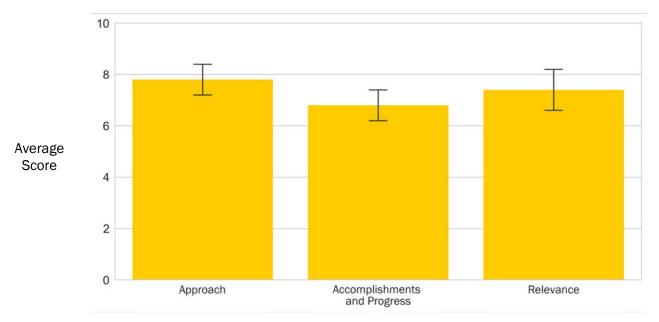
| WBS:                      | 2.3.1.200          |
|---------------------------|--------------------|
| CID:                      | EE0006781          |
| Principal Investigator:   | Dr. Amit Goyal     |
| Period of<br>Performance: | 2/1/2015-2/28/2019 |
| Total DOE Funding:        | \$5,981,713        |
| Project Status:           | Sunsetting         |
|                           |                    |

produced from petroleum-based feedstock (e.g., propylene). Propylene prices are volatile, and its production is decreasing in the United States. In order to effectively reduce the cost of ACN (to less than \$1.00/lb), an alternative feedstock available at scale, commercially viable with a sustainable conversion process and a high-purity product are desired.

Southern Research has developed a multistep catalytic biomass-derived non-food sugar-to-ACN process under a cooperative agreement with DOE. The catalytic steps are the hydrocracking of sugar to glycerol (R1), dehydration of glycerol to acrolein (R2), and ammoxidation of acrolein to ACN (R3). Southern Research has successfully completed the phase one part of the study where novel high-performance catalysts have been developed and tested at laboratory scale. Based on the Phase I results, significant reductions in ACN production cost (\$0.70-\$0.80/lb) and greenhouse gases were predicted from preliminary TEA and LCA. The

# Weighted Project Score: 7.2

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



produced bio-ACN from Phase one was validated by a commercial carbon fiber manufacturing partner (Solvay) for drop-in quality and was subsequently polymerized.

Following the Phase I study, the Phase II scale-up study has been initiated. For this part, three bench-scale skids for the three catalytic steps (R1, R2, R3) have been fabricated for decoupled operation. Design and fabrication of these skids include critical safety and operational controls. From lab scale (Phase I) to bench scale (Phase II), up to 1,000 times scale-up has been targeted. A continuous run on the first skid (R1) using commercial sugar hydrolyzates has been completed for more than 500 hours. The scaled-up catalyst did not show any sign of deactivation in the testing duration. Parallel to this study, impacts of various process-derived impurities on polymerized ACN (PAN) properties have been studied in a small-scale one-liter reactor. From this study, the allowable limit of these impurities has been determined, which will guide the purification steps of produced bio-ACN.

In the next few months, continuous runs on the remaining two skids (R2, R3) are planned. Southern Research will produce 200–250 kg of bio-can, which will be used by Solvay for polymerization and spinning. The TEA and LCA will also be updated with Phase II results.

#### **OVERALL IMPRESSIONS**

- Outstanding program and progress towards the BETO goals contributing to overall reduction in renewable fuel cost. I could find no major weaknesses in the program, which was well managed with clear milestones and achievements throughout the program. I expect the last phase of the project to achieve the goals with no major issues.
- The PIs have made progress on a challenging project to lower ACN costs for the production of carbon fiber and are trying to transition to larger scale. A better understanding of the dependence of ACN cost on propylene glycol sales and a clearer delineation of TEA assumptions would improve the presentation. Industry tends to avoid coproduct schemes, and thus a clearer description of how the PIs will avoid this problem would be helpful.
- Potentially promising technology. I am concerned about waste streams and economics.
- This project has made significant progress on each of the process steps to produce bio-ACN from nonfood sugars. It would be interesting to see how the process scales, and how it performs on different substrates. It was refreshing to see a project that laid out incumbent product specifications as criteria for success. Some attention should be given to side products and the number of steps where yield losses can stack up and disadvantage the route.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# RENEWABLE CARBON FIBERS CONSORTIUM

# National Renewable Energy Laboratory

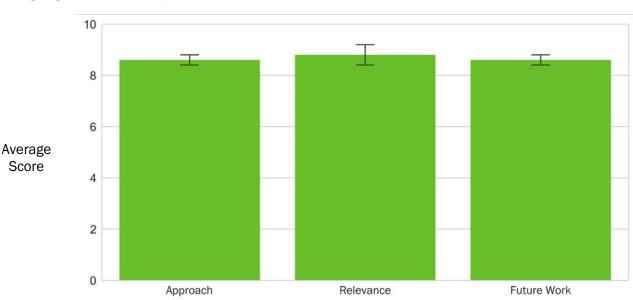
# **PROJECT DESCRIPTION**

The Renewable Carbon Fibers Consortium project goal is to demonstrate cost-effective production of renewable carbon fibers through bio-ACN. The final product will be 50 kg of ACN converted into a carbon fiber component for performance testing, with a modeled cost of less than \$1.00/lb. This work will identify bioenergy product and coproduct opportunities for industry evaluation with associated TEA and LCA, as well as industrially relevant improvements for bio-ACN and carbon fiber production via 3-hydroxypropionic acid (3-HP) pathway. The project leverages knowledge from a previous funding opportunity announcement, building on existing work.

| WBS:                      | 2.3.4.102          |
|---------------------------|--------------------|
| CID:                      | NL0033912          |
| Principal Investigator:   | Dr. Mary Biddy     |
| Period of<br>Performance: | 1/1/2018-9/30/2020 |
| Total DOE Funding:        | \$2,864,600        |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$0                |
| DOE Funding FY18:         | \$2,300,000        |
| DOE Funding FY19:         | \$564,600          |
| Project Status:           | New                |
|                           |                    |

Carbon fiber produced from renewable sources has many advantages. In addition to environmental benefits from renewable sugars as a feedstock source, the use of bio-based sources can potentially level out historically volatile acrylonitrile prices. The final report for the project will detail the process design to meet economic and sustainability metrics, document assumptions, and present R&D for further improvements via the bio-based route.

The bench-scale portion of the work focuses on improvements to the catalyst performance during the conversion of 3-HP to acrylonitrile. Catalyst deactivation during this stage is undesirable and adds to the cost of production. The goal will be to understand how critical process variables (reactant feed concentrations,



# Weighted Project Score: 8.7

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

temperature, etc.) affect catalyst deactivation and ACN production. We will perform design of experiment studies to determine optimal reaction conditions to mitigate deactivation rate, as well as investigate the addition of chemical dopants to alleviate deactivation.

The scale-up component of the project is the largest portion and involves several external partners. The production route is 3-HP production  $\Rightarrow$  bio-ACN production  $\Rightarrow$  carbon fiber productin  $\Rightarrow$  carbon fiber production  $\Rightarrow$  carbon fiber production  $\Rightarrow$  ca

- Cargill, with extensive experience in strain engineering and fermentation optimization around 3-HP, will generate 3-HP from first-generation sugars (i.e., sucrose) via fermentation.
- The 3-HP will undergo esterification and nitrilation, converting it into bio-ACN at the Mid-Atlantic Technology, Research, and Innovation Center (MATRIC), which has extensive experience in development, testing, and scale-up of catalytic processes and handling reactive monomers. Johnson Matthey will provide the nitrilation catalyst to MATRIC.
- The bio-ACN will be converted into polyacrylonitrile and carbon fiber at Fisipe. Fisipe has experience in polymerization, polymer solution preparation, acrylic fiber extrusion, and carbon fiber production. Finally, the carbon fiber will be manufactured into a carbon fiber component by Ford Motor Company, where it will be performance tested. Ford has wide experience in this area.

This project directly supports BETO's mission to "develop industrially relevant bioenergy technologies to enable sustainable, domestically produced bioproducts." It will provide a renewable route to ACN, as well as project metrics and technical targets driven by TEA. By leveraging previous work, the goals of (1) a complete single carbohydrate to carbon fiber product demonstration run with industrial partners and (2) continued bench-scale work are both possible to meet the goal of cost-effective production of renewable carbon fibers through bio-based ACN.

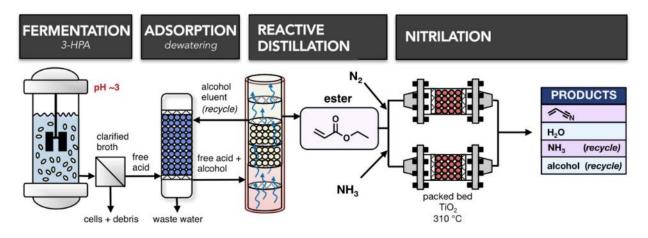


Photo courtesy of National Renewable Energy Laboratory

# **OVERALL IMPRESSIONS**

• Outstanding achievement on conversion from 3-HP by the team with existing catalyst on all processing steps. However, concern over commercial-scale activity time frame before regeneration could be a project killer. An additional concern is whether even reaching \$1.00/lb (~\$2,200/ton) can be sufficient to compete with the propylene process to ACN. Market dynamics have been lower as of late and only a few years ago the ACN price was in the \$2,400.00/ton range. Some think the price will go down further. Thus, to have market pull, I believe the price target must be much lower than \$1.00/lb, which their

current economics indicates as \$0.78/lb. If they can truly meet this price at scale, they can have a robust competitive price for bio even without a bio premium, which may be add on. Also, I am surprised that they did not include information on previous commercial-scale plants using sugar to glycerin glycols production. The company in China, Global Bio-Chem Technology Group, was making its corn-based propylene glycol since 2007 at its 200,000-tonne-per-year plant (total production of this and other chemicals) in Jilin Province and was big news in 2013 around the collaboration on a catalyst with Archer Daniels Midland Company. I believe they are no longer producing and believe it was due to the price of sugar increase around 2014 or so. This information would have to be confirmed, but perhaps a discussion with them could help the team understand real challenges commercially.

- This project is an excellent example of what BETO wants to do with the science and lab-scale investigations being carried out by their labs. Good science has led to good applications that attract industry and offer opportunities for commercial deployment.
- Looks very promising. Industry partners are a plus.
- The techno-economic advantage of this project is in a minimal unit operation, the chemocatalytic conversion process from 3-HP to bio-ACN, which should help mitigate yield losses. Very high yield has been demonstrated previously, although catalyst deactivation was an issue. This, along with scale-up, and subsequent carbon fiber and composite production and testing are areas for future work. Although apparently out of scope for this project, codevelopment of a highly efficient fermentation organism and process to 3-HP is going to be a prerequisite for a non-food sugar process to achieve success, so cross-talk with projects that may be working on this component is critical. Assuming success, this has the potential to be a highly advantageous process route.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the panel for their helpful review and suggestions. Going forward, we will work to incorporate these suggestions into the project.

# PERFORMANCE-ADVANTAGED BIOPRODUCTS VIA SELECTIVE BIOLOGICAL AND CATALYTIC CONVERSIONS

# National Renewable Energy Laboratory

# **PROJECT DESCRIPTION**

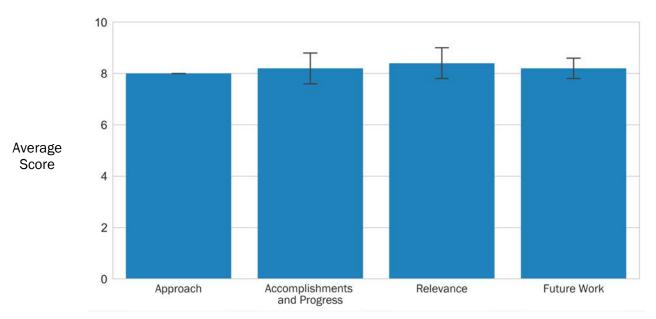
This project began in FY 2018 as one of four projects in the PABP mini-consortium. The goal of this project is to develop PABPs that employ intermediates derived from atom-efficient and selective biological and catalytic conversion of biomass and other waste oxygenated feedstocks. Given the slate of monomers that can be derived from sugars or lignin-derived aromatic compounds through selective biological and catalytic conversions, in combination with the vast chemical space available for polymer synthesis and formulation, the possibilities to derive new bio-based polymers are immense. This project (1) leverages a portfolio of selective biological and catalytic processes in the BETO portfolio to produce novel

| WBS:                      | 2.3.4.501           |
|---------------------------|---------------------|
| CID:                      | NL0033411           |
| Principal Investigator:   | Dr. Gregg Beckham   |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,000,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$600,000           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

bio-based monomers, (2) synthesizes new polymers from combinations of bio-based monomers targeted to specific materials classes across a broad suite of polymeric materials, and (3) measures critical material properties to ascertain if these bio-based materials are performance advantaged over their petroleum counterparts. "Performance advantage" is measured relative to a petroleum-derived counterpart synthesized in the laboratory in the same manner as the bio-based product. The goal of the project in the three-year project cycle is to produce 50 new bioderived polymer formulations for multiple applications at the gram scale and to

# Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



develop ≥10 materials that are considered performance advantaged relative to petroleum-derived materials. This work is done in close collaboration with multiple projects, including the Inverse Biopolymer Design through Machine Learning and Molecular Simulation, Performance-Advantaged Bioproducts from Catalytic Fast Pyrolysis, and Tailored Polymers through Rational Monomer Development.

The first major accomplishment in this project was the establishment of a small-scale polymer synthesis and characterization laboratory at NREL that is used by all three experimental projects in the PABP miniconsortium. Up to 30 polymerization reactions can be conducted in parallel, and thermal, mechanical, and barrier properties can be measured for polymer formulations at the gram scale. Additionally, industry engagement is an important part of this project, and to date, over 50 companies have been contacted, with multiple in-depth customer discovery interviews conducted. This activity has directly informed what industry considers performance-advantaged across a wide range of materials and will be conducted continuously throughout the project. In terms of new polymer formulations, new nylon formulations have been produced through the use of  $\beta$ -ketoadipic acid, which has been used in place of adipic acid in nylon-6.6. The resulting material exhibits significantly lower water uptake properties and dramatically improved thermal properties, both of which are considered performance advantaged. Additional results include the use of other aromaticcatabolic intermediates, such as pyrone-dicarboxylic acid (PDC) in place of isophthalate in multiple formulations; PDC exhibits a lactone functionality, which in turn imparts ease of chemical recyclability at the end of the material lifetime. Multiple lignin-derived compounds have also been tested in place of bisphenol A in polycarbonates and epoxy resins, which exhibit similar or improved mechanical and thermal properties. Endocrine disruption tests relative to bisphenol A demonstrate essentially zero toxicity. Multiple additional examples are under active development.

Future work includes the use of new monomers that encompass heteroatoms (e.g., nitrogen and sulfur), monomers from other bioderived sources (e.g., fatty acids), and new material formulations that enable expansion into other materials markets (e.g., rubber, coatings, nitriles, thermosets, and applications beyond polymers such as lubricants and surfactants).

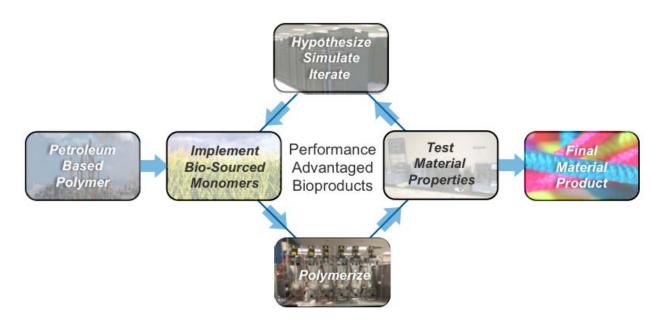


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- Excellent work results and progress on polymers. I would have liked to see some end uses that are water-soluble oligomers potentially useful in many consumer goods products and industrial applications; however, I'm glad to see future work on other applications. β–ketoadipic acid work is exceptional and I'm glad to see results here as I feel this may be a first work moving forward in industry. Don't rely on weak links and biodegradability of polymers. Better to focus on recyclability because the European Union may in the future ban weak-link polymers and U.S. policy usually takes time to adjust, but often follows stiffer guidelines in the future.
- It seems like bioproducts do have great potential to deliver better properties. The question becomes how does this reach an innovation level great enough to bring sufficient investment to make a commercialized product.
- This is an interesting project to build and test new polymers from bio-based monomers and measure their properties. Very good progress on synthesis of new formulations have been reported, some of which exhibit enhanced properties. This program has received extensive input from industry on worthwhile performance characteristics and is nicely synergistic to the inverse learning program, as it will generate novel information to augment databases and improve predictive tools for new polymers.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the positive comments from the reviewers. We agree that it would be ideal to expand beyond the current applications to include others, which additional funding would enable to increase bandwidth. The comment regarding biodegradability is excellent and we fully agree. We are attempting to make polymers that can be more easily chemically recycled.
- We agree that the bio-based materials need to reach a level of innovation to catalyze industrial investment. To that end, we are in close coordination with industry regarding the innovations coming from this project to offboard them as we reach a sufficient technical readiness level.

# TAILORED POLYMERS THROUGH RATIONAL MONOMER DEVELOPMENT

# Los Alamos National Laboratory

# **PROJECT DESCRIPTION**

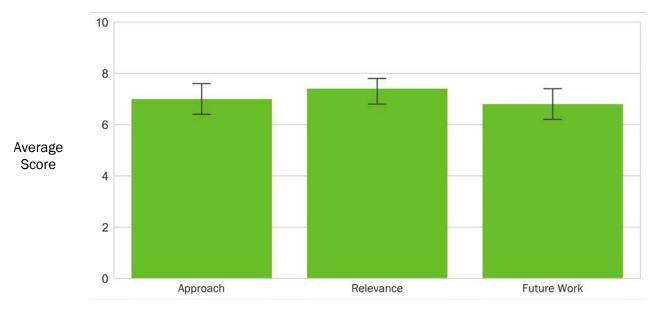
Plastics are synthetic polymers that are constructed of repeating subunits of a variety of petroleum-based monomers. The judicious choice of the monomer and its polymerization method enables the fine tuning of strength, stiffness, density, heat resistance, and biodegradability of the resultant polymer. While there has not been widespread market penetration of bioplastics, one example of a biodegradable thermoplastic found in single-use packaging products is polylactic acid. However, the low strength, durability, and heat resistance of polylactic acid currently limit its widespread utility. Our approach to developing a new bioplastic will apply a retrosynthetic analysis; monomers will be synthesized from bioderived building

| WBS:                      | 2.3.4.502           |
|---------------------------|---------------------|
| CID:                      | NL0034401           |
| Principal Investigator:   | Dr. Andy Sutton     |
| Period of<br>Performance: | 10/1/2018-10/1/2020 |
| Total DOE Funding:        | \$225,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$225,000           |
| Project Status:           | New                 |
|                           |                     |

blocks with inherent chemical and environmental safety. Thus, the materials engineered herein will not degrade to toxic or harmful molecules (such as bisphenol A [BPA]). By incorporating the ability to degrade into these benign intermediates, the long-term accumulation of plastics in the environment and the elaborate recycling pathways used for traditional plastics and polylactic acid, which often require a specialized reprocessing facility, can be avoided. A durable and fully recyclable bioplastic would reduce our dependence on a nonrenewable carbon source, eliminate hazardous processes that use toxic materials (such as phosgene), and produce a plastic that has no long-term environmental impact. The utilization of biomass to generate new

# Weighted Project Score: 7.0

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

polymers provides us the unique opportunity to produce materials with improved performance over current technology by taking advantage of the variety of functional groups in bioderived molecules as structural and electronic handles to tune the properties of the monomers and their resultant polymers. This project will synthesize bio-based monomers and the corresponding polymers with a focus on engineering a rational decomposition pathway to yield environmentally benign decomposition products. If successful, this work will help significantly reduce the amount of plastic that is discarded or incinerated and help pave the way for a circular carbon economy.

#### **OVERALL IMPRESSIONS**

- Good initial progress towards program goals. No major inputs or questions except for perhaps some nearer-term goals versus the broader quarterly goals would have been nice to have but not significant enough for a new program.
- The project performers clearly described how their project contributes to meeting PABP/BETO's goals and objectives. The project performers considered applications of their expected outputs. The project performers have presented the relevancy of this project and how successful completion of this project will advance the state of technology and impact the viability of commercial biorefinery concepts.
- The PIs present a scientifically interesting route to new polymeric materials that addresses the BETO PABP concept. The primary issue is whether industry will accept and commercialize materials of this complexity, which require multiple steps for their synthesis. The project would benefit from industrial examples that might have an equivalent number of steps from raw material to monomer to polymer, and which exhibit similar structural complexity.
- Early-stage seed project at this time.
- Creating polymers that can be reversibly degraded into nontoxic components is an intriguing idea. It will be interesting to determine how the balance between product performance versus degradation plays out and directs these polymers into various application areas.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

We thank the reviewers for the constructive and thoughtful feedback, which is especially useful to this project as it is a new start and receiving this guidance at such an early stage will help focus our efforts for the remainder of the project. The main concerns raised by the reviewers include the current multistep synthetic pathways to our current monomers, the complexity of the monomers, and the potential position of our polymers in a very competitive and cost-driven marketplace. The current synthesis was performed to provide an initial proof of concept for the project to demonstrate that at the three-month mark of the project we could use our approach to construct polymers from our proposed building blocks and subsequently deconstruct them. With this achieved, we can further refine and optimize the synthesis in collaboration with TEA. This will identify costly unit operations and allow us to determine the economic feasibility and potential price point we could achieve via this strategy. In collaboration with the machinelearning project, we will iterate through molecular structure variations that have the potential to both simplify the monomer structure and enhance performance of the materials we can prepare. We are very aware that a simple approach would be more amenable to scaling and we thank the reviewers for reminding us of this. The polycarbonate market will be challenging to compete in, and we are currently performing customer discovery interviews to identify niche applications or other market opportunities that would be more amenable for this kind of approach.

# INVERSE BIOPOLYMER DESIGN THROUGH MACHINE LEARNING AND MOLECULAR SIMULATION

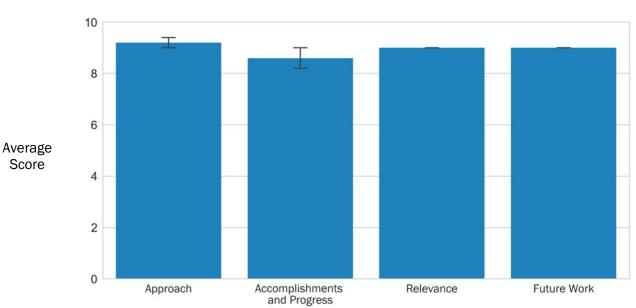
# National Renewable Energy Laboratory

# **PROJECT DESCRIPTION**

An economically feasible bioeconomy will require producing value-added coproducts alongside fuel replacements. Deconstructed biomass offers a wide range of chemical functionality that can likely be harnessed to create inexpensive and high-performance biomass-sourced polymers. A key challenge in commercialization of biomass-derived compounds is deciding *a priori* which functional replacements have the highest potential for displacing incumbent materials. In this project, we develop an integrated approach to reverse-design materials from biomass-derived compounds. This ultimately increases research efficiency, reduces time to market, and creates new opportunities for advanced biomaterials.

| WBS:                      | 2.5.1.500           |
|---------------------------|---------------------|
| CID:                      | NL0033412           |
| Principal Investigator:   | Dr. Mike Crowley    |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$850,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$400,000           |
| DOE Funding FY19:         | \$450,000           |
| Project Status:           | Ongoing             |
|                           |                     |

In contrast to the traditional approach where applications for a polymer are researched post synthesis, inverse material design starts with desired properties and works backwards to a suitable starting monomer. This field of computer-assisted material design exploits the tendency for many polymer properties to be correlated with molecular structure. The vast majority of methods for inverse design are focused on homopolymers with a high degree of polymerization and low macromolecular complexity. Existing databases and literature will serve as a



# Weighted Project Score: 8.9

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

basis for the proposed work; however extending the information in these databases through guided atomistic modeling and experimentation can bridge the information deficiency associated with biomass-derived polymers. Additionally, advanced synthesis methods for performance-advantaged bioproducts aim to control macromolecular complexity to optimize properties through structure. The resulting polymers often feature complex chain branching, block copolymer structures, or controlled tacticity1-2 complications omitted from simple monomer-based group-contribution design algorithms. Models necessarily need to extend beyond basic considerations of monomer chemistry for quantitative structure-property relationship to be effective for biomass-derived polymers. This project leverages atomistic simulation to magnify experimental effort and use *in silico* experiments to help determine optimal approaches for polymer learning.

Molecular modeling and simulation have the ability to approximate physical characteristics of molecular systems in silico and provide two valuable functions to this study: (1) avoid the time-intensive process of synthesizing and characterizing polymers and (2) provide deep insight into the molecular and mesoscale causes of polymer behavior. The ability of polymer simulations to produce experimentally measurable properties, such as glass transition temperature, has been established for some polymer systems and is the basis for the work in this project. The modeling data have the potential to produce a fast turnaround in the development of the machine-learning cycle, where predictions can be made and tested in silico. Our direction is to develop systematic approaches to attaining accurate polymer properties from all available methods and inferring molecular understanding of the source of the polymer behavior as a function of monomer composition, polymer composition, branching characteristics, polymer length, and dispersity of polymer length. These methods are a key part of developing a machine-learning algorithm and tool, a deeper understanding of how polymers get their properties, and how we can more efficiently tune polymers for desired properties. The breadth, accuracy, and precision of properties from simulation will be less than what is possible from actual synthesis and characterization but will be a huge advantage due to the fast turnaround of learning, prediction, and testing when it replaces synthesis in that process. The algorithmic tuning is independent of the accuracy or precision of the data and can be refined very quickly as simulation data are replaced by experimental data over time.

# OVERALL IMPRESSIONS

- Great modeling plan and work results, from my own experience working with modeling teams using state-of-art modeling on much simpler systems than this team. I'm curious why the focus is on high molecular weight polymers first, when it might have been easier to start with lower challenges like small molecule properties such as stated before in future work (i.e., viscosity modifiers/additives to lower plastic melt properties for mold blowing bottles). The current market uses widely fluctuating chemicals that are renewable, like ricinoleic oils, but have limited volume supply and even shrinking volume supply from India as the focus on food crops such as soybeans are causing market issues as growers have stopped growing the plant for ricinoleic oils. Unique, high-performance, water-soluble polymers-like the kind companies like BASF, Dow/DuPont, and others make for consumer goods-which are water soluble and a lower molecular weight, might be another focus area not currently being covered in these programs. Examples might be bio, hydrophobically modified polyacrylates, sulfonated variants used in industry today, or polyethylene glycol-grafted polymers and potential chelant replacements for today's petrol amine-containing chelants, which could be another set of targets to model and develop and perhaps easier to model. Commercialized bio-based chelants from the likes of Dow/Dupont are developed from other processes but not from aromatics like lignin monomers. Another area is solvent modeling for potential replacements for petrol derived.
- Very innovative. I have high hopes for a promising outcome.
- This is a terrific new start for the BETO program that has the potential of answering many questions around PABPs and defining the types of materials that a biorefinery might consider. It could also provide the basis for new, broad-based technology development within the labs. The project will be strengthened

by inclusion of molecular weight data and providing information supporting the possibility that the predicted polymers are able to make the leap to industrial use.

- This is a valuable approach to optimize the search for new PABPs by creating *in silico* high-throughput screening and prediction tools. If successful, its value will be crosscutting and substantial in terms of research efficiency and hit rate.
- This project is doing great and groundbreaking work to enable inverse design of new bioproducts and using a high-throughput method for predicting polymers with advantageous properties. They are developing databases for large classes of products and targeting ten new polymer materials.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their suggestions and insights. We appreciate the time and effort of the reviewers to understand our project and to provide valuable constructive comments, insights, and suggestions. We will be looking into moving into these new directions the reviewers suggest as we successfully complete the initial stages of this work. Our machine-learning prediction tool and consolidated polymer databases will be made available when they are sufficiently reliable and usable. We welcome and seek out collaborations with any industrial and research groups with an interest in these research directions.

# **BIOPROCESSING SEPARATIONS CONSORTIUM – OVERVIEW**

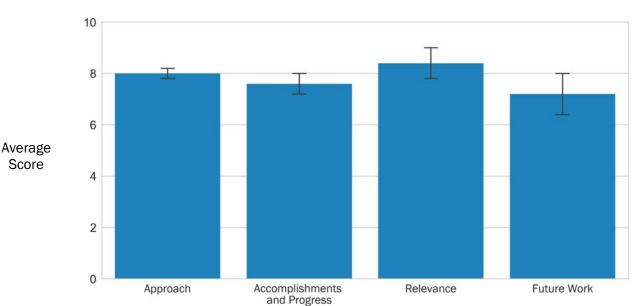
# **Bioprocessing Separations Consortium**

#### **PROJECT DESCRIPTION**

The Bioprocessing Separations Consortium (BioSep) develops cost-effective, high-performing separations technologies through coordinated separations research that targets industry-relevant bioprocessing separations challenges. As a result, biofuels and bioproducts industries will have new, high-performing, low-cost separations technologies available to them. This consortium was formed because BETO industrial stakeholders have long raised separations challenges as a major barrier to costcompetitive biofuels and bioproducts. BETO analyses indicate that separations steps can constitute up to 50% of processing costs. The consortium approach coordinates and brings to bear breadth and depth of national laboratory expertise, capabilities, and resources on this foundational challenge.

| WBS:   | 2.5.5.501a          |
|--|---------------------|
| CID:   | NL0031310a          |
| Principal Investigator:  | Dr. Jennifer Dunn   |
| Period of<br>Performance:  | 10/1/2016-9/30/2019 |
| Total DOE Funding:   | \$11,085,000*       |
| DOE Funding FY16:  | \$0                 |
| DOE Funding FY17:  | \$0                 |
| DOE Funding FY18:  | \$0                 |
| DOE Funding FY19:  | \$0                 |
| Project Status:  | Ongoing             |
| *This total reflects the summation of funding for all<br>projects contributing to the Bioprocessing Separations<br>Consortium. |                     |

The consortium consists of a steering committee, a crosscutting analysis team, and biochemical and thermochemical separations teams. The consortium also has an IAB with eight members that include companies that focus on biochemical and thermochemical processing, as well as separation technology providers. The board helps the consortium maintain an industry-relevant focus and knowledge of recent technology advances and challenges. It also provides advice, reviews results and progress in comparison with



# Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

work plans, provides feedback regarding prioritization of research projects (experimental and analytical), and informs development of the consortium's strategy for out years.

In the first two years of BioSep, the steering committee has had the objectives of guiding the consortium, coordinating external communications, and managing consortium business. Particular achievements in this timeframe include establishing the IAB and coordinating meetings with them twice annually; holding an industrial listening day (May 2017); creating and expanding the website to inform stakeholders of consortium capabilities, managing consortium reporting, and organizing; participating in bioprocessing separations sessions at targeted conferences; planning and monthly communications; and coordinating a directed funding opportunity, which is the subject of another presentation in this session. As a result of this interaction with external stakeholders, BioSep has developed a more complete understanding of bioprocessing separations challenges that will inform its plans for future work.

The consortium is in its third year and has an end-of-project goal to demonstrate the consortium's value to BETO and the biofuel and bioproduct communities through documentation of technical advances, influence on process economics, and potential industrial applications of consortium technologies.



Remove catalyst poisons from feedstocks and fermentation broth

Recover carbon from dilute aqueous streams

Lignin fractionation and valorization

**Process integration** 

Poisons and foulants like carbonyls, furfural limit the lifetimes of upgrading catalysts and biocatalysts. Selective removal strategies to eliminate them will extend catalyst life and decrease processing costs.

Increasing carbon efficiency of processes from recovery of valuable co-products can lead to improved process economics.

Lignin fractionation enables conversion to valuable co-products that can enhance process economics and sustainability.

Reducing the number of processing steps associated with separations, including through reactive fermentation and in-situ product recovery, reduce process energy intensity and costs.

Photos courtesy of Bioprocessing Separations Consortium

# **OVERALL IMPRESSIONS**

• Great technical approach. Provided a thorough background of how they ended up where they are, informed by very robust IABs. The project management plans included are well defined and similar across all projects. It was unclear what the technical targets and cost targets are for the highest-impact separations technologies. There is potential for the number of coordination meetings and conference calls to be onerous. It was mentioned several times that separations can be upwards of 50% of the manufacturing costs, but the underlying analysis for this was not presented and it was not clear how much that was for each of the areas/pathways they chose to focus on for separations. It was unclear what technical targets would be needed to achieve the reductions in the areas/pathways they chose to focus on for separations.

- Team has done great job organizing the work and progressing program. One suggestion: the list of engagement parties excludes fuel companies such as Valero, Royal Dutch Shell, BP, Chevron, etc. This would go a long way to provide sound input and evaluation of the technologies, as many are engaged in their own bio-renewable programs and may even provide some insights from their petrol experience. Other suggestion for an IAB member would be a firm such as LyondellBasell.
- Economic evaluation of the different separations' projects going on at the labs and with industrial partners is a crucial part of the overall program and should be continued. It provides needed credibility to potential stakeholders that the lab research effort also understands the needs of their partners. More clarity about BETO's plans for continuing the project after September would be helpful.
- Enabling technology always has the potential to be impactful. Separations companies need to get involved.
- BioSep is a worthy approach to developing a heretofore underserved focus on separations technology and effectively engaging across national laboratories. Working together with separations technology and equipment providers is advisable so that each can learn from the other regarding emerging needs.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# BIOPROCESSING SEPARATIONS CONSORTIUM – SEPARATIONS FOR BIOCHEMICAL PROCESSES

# **Bioprocessing Separations Consortium**

# **PROJECT DESCRIPTION**

In support of BETO's minimum fuel selling price target of \$2-\$3/GGE for biofuels, the team at BioSep aims to enable cost-effective integrated separation solutions to meet these targets in biological conversion processes. We are tackling two of the cost-driving separations challenges in bioprocesses: (1) recovery of products from fermentation and (2) separations relevant to lignin valorization.

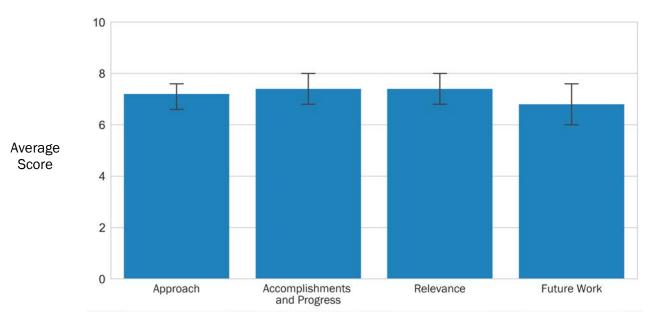
The recovery of bioproducts from fermentation is a wellknown cost driver in biorefining that can account for greater than 50% of the minimum fuel selling price. Several challenges exist in fermentation product recovery,

| WBS:                      | 2.5.5.501b          |
|---------------------------|---------------------|
| CID:                      | NL0031310b          |
| Principal Investigator:   | Dr. Gregg Beckham   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$4,765,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$1,605,000         |
| DOE Funding FY18:         | \$1,575,000         |
| DOE Funding FY19:         | \$1,585,000         |
| Project Status:           | Ongoing             |
|                           |                     |

including dewatering (products are approximately 5–10 wt % in water), removal of trace impurities, and handling of large volumes of fermentation broth at scale. To address these challenges, four projects are ongoing wherein new separation technologies are being developed that reduce the energy and cost associated with classical post-fermentation recovery methods. First, an *in situ* product recovery (ISPR) system is being developed based on continuous liquid-liquid extraction (LLE) of bio-carboxylic acids. Key results of this project include demonstrated ability to increase fermentation titers tenfold over fed-batch titers, direct recovery

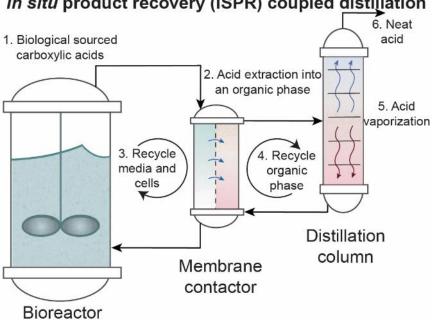
# Weighted Project Score: 7.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



of carboxylic acids as neat products via distillation of the organic phase, and an energy consumption less than 20% of the heating value of the product. Second, wafer-based electrodeionization technology is being developed for the *in situ* recovery of bio-based carboxylic acids. Key results of this work include >90% acid capture into a tenfold concentrated permeate using <1 kWh/lb of acid recovered. Both of these ISPR systems represent an advance from traditional post-fermentation recovery schemes in their nonthermal dewatering capabilities that lower energy requirements and ability to reduce fermenter size by approximately tenfold. A third project involves the design of advanced materials for selective adsorption of fermentation products. New nanomaterials with tunable surfaces are being developed to bind target products. The materials are unique in their ability to be regenerated mechanically, allowing for novel process-intensified separations systems with nonthermal dewatering abilities. Finally, a recent project focuses on the recovery of alcohols, namely 1,4-BDO, from fermentation. This project utilizes a hybrid extraction-distillation system driven by membrane pervaporation.

The valorization of lignin in a biorefinery is an important step towards meeting BETO's \$2-\$3/GGE biofuel target. However, lignin-rich process streams are often difficult to handle and present several separation challenges given the broad range of molecular weight components, fines, and debris present. Four projects are aimed at developing technologies to address these challenges. First, ultrasonic separations are being applied to lignin depolymerized streams to remove fines and debris present that make the solution difficult to filter. This project has shown success in removal of fines and debris in a continuous manner, which is promising given that membranes often foul rapidly when applied to lignin-rich streams. With fines and debris removed, molecular weight fractionation of the lignin material is being investigated. Polymeric membranes in tangential flow filtration (TFF) cells are being developed to recover low molecular weight (LMW) lignin monomers, and in another effort, ceramic membranes in TFF cells are being investigated. Both membranes are effective at recovering LMW monomers from the complex solutions and can be regenerated. Finally, we are applying electrochemical separations to simultaneously recover sodium hydroxide from a black liquor while separating LMW acids. This technology has shown 99% sodium hydroxide recovery and 95% carboxylic acid recovery, representing an important advance in recycling caustic deconstruction catalyst.



# In situ product recovery (ISPR) coupled distillation

Photo courtesy of Bioprocessing Separations Consortium

#### OVERALL IMPRESSIONS

- Did the team exploring fines filtration explore filter technology that is used for removal of fines from Raney nickel in processing glucose to sorbitol? These filters have a unique design of multiple layers to retain larger particles, and at a later stage the fines can be removed to avoid pressure buildup and clogging. This could be useful for the issue with fouling of lignin fines. Also, due to the physical properties of 2,3-BDO, did the team explore freeze fractionation since it was mentioned as an alternative? The melting point of the material is 66.2°F, and as such may lend itself particularly with salt also present. I am curious as to why the team did not attempt this well-known approach to chemical purification prior to the others. Indeed, chilling adds energy input to the process, but this may be one way to simplify the recovery. Ultrasonic separation has always been challenging to do in any field of recovery. I also have concern over the scalability of this approach.
- BioSep has the potential to be a vital, crosscutting component of the overall BETO effort in biorefinery development. Separations will always play a key role in the efficiency of a process and will help determine whether it can make the leap to commercialization. The program would benefit by greater focus and differentiation of its stable of approaches so that the observer has an idea of which methods hold the greatest promise.
- This is a potentially important project that is progressing well. Needs connecting to valuable applications.
- The project has made good early-stage progress on innovative and scientifically interesting separation approaches, focusing on high-value impact areas for fermentation recovery and lignin valorization. The scalability of these approaches needs to be critically evaluated.
- There is a significant amount of interesting science and research being performed in a highly relevant area (separations). Project performers have identified a project management plan that includes well-defined milestones and adequate methods for addressing risks. Critical success factors were well defined. It was not clear why these technologies were chosen versus other options. It was not clear what their potential performance is relative to the current state of technology. It was not clear how and if the program would downselect from the technologies being investigated.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We did not investigate the filter technology used for fines removal from Raney nickel in the glucose-tosorbitol process as a technology for fines removal from an alkaline pretreated liquor stream. Prior to discussion with this reviewer at the peer review we were unaware of this technology. We will follow up with this and explore potentially repurposing this technology for removing fines from lignin-rich process streams.
- Regarding 2,3-BDO, we have internally discussed examining a crystallization/remelt-type strategy for isolating this product but have not pursued it in this three-year cycle. This is a possible approach we have proposed within our next planning cycle.
- Regarding the challenges of ultrasonic separation and its scalability: the challenges posed in general by ultrasonic separation of particles originate in the particle response to ultrasound and the ability to trap particles in the acoustic field, the creation of particle-free channels whereby liquid can pass through the field while particles are held in place, the creation of large aggregates in the acoustic field and their ability to remain intact while settling or floating from the field, and the ability to reach a steady operation, which demands the removal of particles at the same rate as they are entering the acoustic field. These elements depend on the particle properties, the solids content in the feed material, and operating conditions such as the flow rates of input and output streams and power input to the acoustic field. These are the primary factors being investigated in this study. The approach taken to meet any industrial

operating scale requires a practical length for the standing wave to be set based on needed power delivery, and then scaling out the technology to meet the requisite flow rate. In this way, ultrasonic separation can be manufactured to fit a broad range of operating scales. Given the simplicity of ultrasonic hardware, there is no intrinsic feature that would preclude the technology from operating competitively at a large scale.

- As detailed in the subsequent analysis presentation, rigorous TEA was performed to inform decision making on the technology selection.
- The technologies developed in this consortium are aimed at reducing separations costs within the biochemical conversion process to meet the \$3/GGE minimum fuel selling price target. For example, valorizing lignin is predicted to contribute a \$2-\$3/GGE cost reduction. However, in the case of lignin, there is no state of technology and thus these projects are aimed at developing that separation process to recover valuable chemicals from those lignin-rich streams from the ground up. For fermentation intermediate recovery (carboxylic acids), separations are known to account for >50% of the processing costs and thus these new *in situ* product recovery technologies are aimed at reducing that cost by avoiding the expensive post-fermentation separations that are typically employed.
- Many of these technologies were developed within this consortium and as they develop are moved into other projects for scaling and demonstration. For example, the LLE-ISPR system is now being moved into a waste-to-energy task wherein it is undergoing scaling to generate pilot-level data for more detailed TEA.
- Regarding why these technologies were chosen versus other options, we are working internally to develop a presentation format that more effectively communicates metrics of both our technology targets and conventional technology performance and will include this information on the BioSep website. The subsequent analysis presentation included rigorous TEA that detailed performance of the technologies compared to the current state of technology, where available (lignin separations do not have a state of technology), and provide context to how the downselect process occurs.

# BIOPROCESSING SEPARATIONS CONSORTIUM – SEPARATIONS FOR THERMOCHEMICAL PROCESSES

# **Bioprocessing Separations Consortium**

# **PROJECT DESCRIPTION**

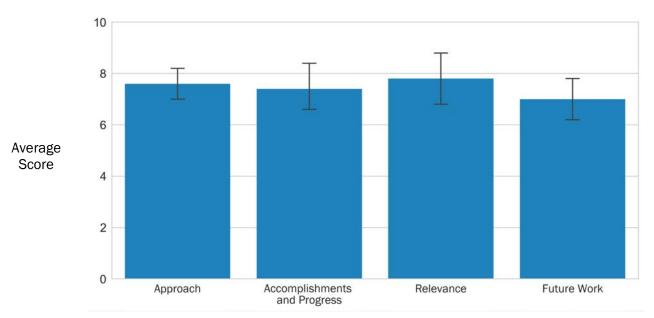
BETO's stakeholders identified energy-intensive, challenging separations as a hurdle to cost-competitive biofuels and bioproducts. A critical technical barrier is impurities in intermediates impeding downstream biological and chemical catalysts and the need for low-cost purification technologies. Additionally, recovery and conversion of dilute carbon can cut the cost per GGE of renewable fuels. Other opportunities to increase use of renewable carbon to maximize carbon conversion and efficiency in BETO pathways include capturing and converting carbon in the aqueous phase after pyrolysis and tapping lignin produced in biochemical pathways as a feedstock for fuels or chemicals.

| WBS:                      | 2.5.5.501c          |
|---------------------------|---------------------|
| CID:                      | NL0031310c          |
| Principal Investigator:   | Dr. Kim Magrini     |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$4,130,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$800,000           |
| DOE Funding FY18:         | \$1,645,000         |
| DOE Funding FY19:         | \$1,685,000         |
| Project Status:           | Ongoing             |
|                           |                     |

Within BioSep, the thermochemical team's three tasks are Molecular Removal Technology for Preprocessing of Liquid Bio-Oils and Biocrudes (Task C.1), Integrated Membrane Separations Technology for Hydrothermal Liquefaction Aqueous Streams (Task C.2), and Catalytic Hot Gas Filtration for Vapor Chemistry Tailoring (Task C.3). These tasks target significant capital expenditure and operational expenditure cost savings, as estimated by TEA, through catalyst preservation and process-intensification strategies. Technical performance

# Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



is measured by removal effectiveness (wt %) of target foulant molecules from bio-oil biocrude, biogenic carbon recovery efficiency from the hydrothermal liquefaction (HTL) aqueous fractions, and catalyst lifetime and/or reaction yield enhancement.

Task C.1 develops molecular removal technology using adsorbents (functional polymers, inorganic materials), to address a major technical and economic challenge in HTL biocrude upgrading: high nitrogen content. The ORNL-Pacific Northwest National Laboratory (PNNL) teams are developing sorbent separation technology for the removal of light heterocyclic nitrogen-containing species (such as indoles, pyridines, piperidines, pyrazines, pyrroles, and pyrrolidines) from wastewater sludge HTL biocrude, and, potentially, amines ammonia from fatty acid amides in the biocrude. It will enable downstream hydrotreating with reduced hydrogen consumption and improved throughput and has the potential for recovery of nitrogen-containing species as higher-value products.

Task C.2 addresses recovery of organic acids and ammonia from HTL aqueous streams that impact process economics. Organic acids are recovered by integrating: (1) ANL's ion-exchange polymer wafer and membrane to extract carboxylic acids from an HTL aqueous stream to greater than 30 wt % (with simultaneous ammonia separation), followed by (2) ORNL's dehydration dewatering membranes to achieve an overall greater than 90% removal of the water with improvement of membrane material stability at higher acid concentration. Another effort seeks to extract individual organic acids from mixed acids in the HTL waste without additional separations steps. The combined ANL-ORNL process could produce higher concentration of target carbon components, beyond what any single separation process could achieve.

Task C.3 couples NREL expertise in hot gas filtration and pyrolysis vapor upgrading with NREL's and ORNL's catalyst capabilities to develop catalytic hot gas filtration (CHGF) for tailoring vapor chemistry for downstream catalytic upgrading to produce upgraded bio-oils that can be used for fuel and chemical production. This task develops and assesses the use of hot gas filtration to remove reactive alkali and char particles from biomass pyrolysis vapors to improve vapor composition and protect downstream upgrading and hydrotreatment catalysts from fouling. Adding a catalyst to the filter (CHGF) provides chemical tailoring (such as deoxygenation) of the feed vapors before they are upgraded to hydrocarbons; catalysts will be assessed for improved product specificity and yield. Approaches include rare earth oxide catalysts to ketonize vapor-phase carbonyls to more upgradeable species, tuning heteropoly acid acidity for alkylation selectivity, and using fractional condensation of vapors to remove coke-forming heavy species prior to upgrading.

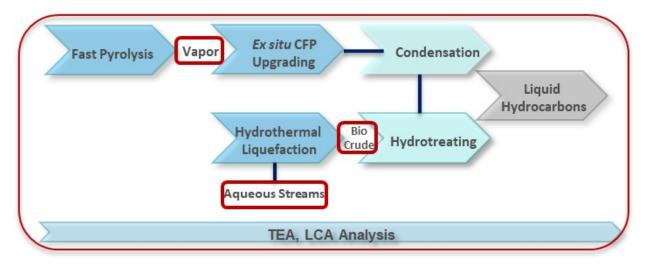


Photo courtesy of Bioprocessing Separations Consortium

#### OVERALL IMPRESSIONS

- Team is well organized and focused on needs of BETO. The only question here: is it worth diluting efforts on the main product stream separations by spending effort now on waste treatment filtration recovery of carbon? However, when considering the environment, this approach is the right thing to do.
- The thermochemical efforts of the BioSep have presented several viable methods for purification of thermochemical process streams. Further, it is more focused than the biochemical effort. More specifics on which technologies hold the greatest promise, or alternatively, a rationale for why multiple processes are needed, would be helpful.
- Project is making good progress but needs a link to valorizable outcomes, which at this time look challenging.
- The removal of low-level contaminants from thermochemical processes is a highly sensible strategy to improving downstream operations. Progress is on track and some piloting work has been performed successfully. A more thorough discussion is needed to ascertain the scalability and commercial acceptability of the technology.
- Really great, thorough, and clear presentation with lots of details on the approach of the R&D. Very clearly explained. Well-organized project management plan and clear understanding of risks. Critical success factors were well defined and the description on commercial relevance and viability was well understood by the research performers. Focusing on catalyst preservation, feed cleaning, and carbon valorization are the three challenges that seem appropriate.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

We thank the reviewers for their insightful and useful comments. The comments for the three thermochemical separation projects that address contaminant removal from biomass-derived process streams (cleaning and conditioning biomass fast pyrolysis vapors through CHGF and removing bio-oil contaminants via selective sorbents prior to hydrotreating or valorizing carbon from aqueous waste streams via selective membrane separation) were insightful and focused on three areas, including more closely tying each project to a valorizable outcome, assessing process scalability and commercial potential, and developing defined progress measures for the sorbent and membrane projects. The CHGF project currently is focused on producing enhanced vapors for downstream upgrading to fuels and chemicals. Future work will focus as well on vapor phase separation of valuable monomers (cresols). Bio-oil cleaning valorization will produce clean feed for hydrotreating to biogenic fuels with demonstrated improvement in catalyst lifetime. Aqueous stream valorization comprises capturing and concentrating acetic acid and ammonia from biomass waste streams. Waste handling from each approach was also identified as a potential significant cost component that is/will be included in each TEA. The IAB review of scalability was suggested and this will be included in the next BioSep meeting with the IAB. The process for downselecting projects is discussed in the overview presentation summary and will be used for the thermochemical separations projects.

# **BIOPROCESSING SEPARATIONS CONSORTIUM – ANALYSIS**

# **Bioprocessing Separations Consortium**

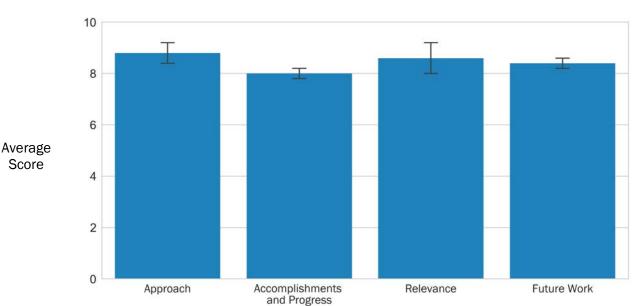
# **PROJECT DESCRIPTION**

Research in the BETO-supported BioSep is leading to new separation strategies designed specifically to address the challenges and scales of biorefinery technologies. This collaborative project integrates eight national laboratories, bringing a broad range of separation techniques to address biorefinery needs, including reducing impurities in intermediates that impede downstream biological and chemical catalysts to the recovery and conversion of dilute carbon. All strategies are developed by targeting highefficiency processes that are both economically viable and sustainable.

| WBS:                      | 2.5.5.501d         |
|---------------------------|--------------------|
| CID:                      | NL0031310d         |
| Principal Investigator:   | Dr. Mary Biddy     |
| Period of<br>Performance: | 5/1/2016-9/30/2019 |
| Total DOE Funding:        | \$1,190,000        |
| DOE Funding FY16:         | \$500,000          |
| DOE Funding FY17:         | \$400,000          |
| DOE Funding FY18:         | \$175,000          |
| DOE Funding FY19:         | \$115,000          |
| Project Status:           | Ongoing            |
|                           |                    |

The goal of the integrated analysis project in BioSep is to

provide an analysis-based foundation to support and guide the research strategies being pursued. The collaborative team from NREL, PNNL, and ANL are developing TEAs and LCAs for each of the strategies being pursued under the integrated consortium. The analysis project works closely with the research teams to develop process designs for each strategy and supports each team by outlining cost and sustainability drivers, as well as key metrics that must be achieved for process scale-up that are critical to the ultimate success of the integrated consortium. One of the biggest challenges the analysis team faces is that the novel technologies being developed are significantly different from the off-the-shelf designs common in industry such that information on capital costs and scale-up performance are often limited. To overcome this challenge, the



# Weighted Project Score: 8.4

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

analysis team works closely with the IAB to review the analysis approach and to vet the results of the designs, economics, and sustainability assessments.

The overview of this project will provide examples of how TEA and LCA have been integrated to support the R&D of novel separations technologies in the consortium and how these analyses inform research directions and highlight key strategies to enable the production of bioderived fuels and chemicals. Future work plans for this analysis project, including publications, will also be outlined.



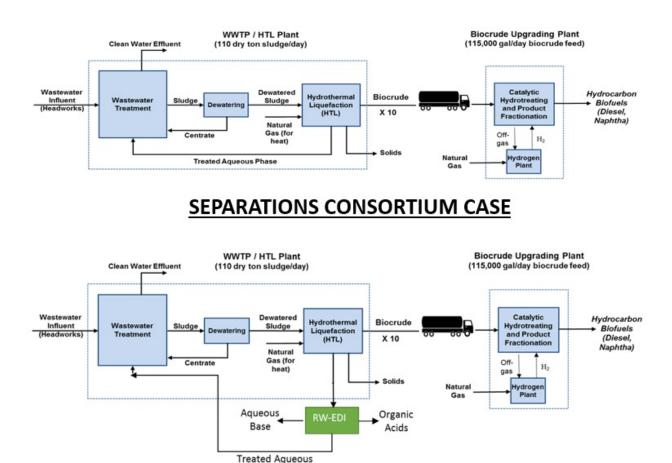


Photo courtesy of Bioprocessing Separations Consortium

#### OVERALL IMPRESSIONS

• This team provided excellent work results. This type of analysis in industry is routine and often starts early in large projects. The value of such analysis work at early-, middle-, and late-stage projects is critical to BETO programs. These analyses increase dramatically the speed of development, providing information on where to focus future efforts to drive down cost or where to stop working when further refinement is not impactful. The only question is, can BETO provide some level of techno-economics to even smaller start projects to make sure that the original strategy has the ability to succeed? The only other comment is that funding for plant capital for new technologies typically, from my experience, is not a 20-year payout but more like 10 years, thus only true for the n<sup>th</sup> plant. Also, I've never known a

plant to come in on original capital cost estimates. Some confidence on calculation information (i.e.,  $\pm x\%$ ) would be helpful as well for reviewers.

- This part of BioSep is the most important.
- The analysis team provides a critical service function to the entire BETO effort. Although this presentation focuses on separations, the broader contributions to the BETO program and the researchers is also vital to the success of the research in an industrial context. Better understanding of actual industrial benchmarks and the viability of different separation techniques at scale will be important as this effort proceeds.
- This project makes the case for baselines, design cases, and meaningful TEAs and LCAs to focus separations projects on high-value strategies as a critical steering tool across BioSep.
- This work is highly relevant to inform how the program/technology area is meeting the objectives of BETO, as cited in the *Multi-Year Plan*. The project performer considered applications of the expected outputs, which are informed by an IAB. The project performer presented the relevancy of this project and how successful completion would advance the state of technology and could have a significant positive impact on the viability of commercial biorefinery applications.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

Reviewer comments on the overview of the consortium were very helpful and focused on three main
points. First, reviewers suggested additional members be added to the IAB such that the board covered
more ground with expertise in separations materials, petroleum refining, and existing separations
technologies. The consortium will seek to enhance the expertise on its board through addition of
members with these areas of expertise. The second set of suggestions centered around the importance of
crosscutting analysis towards a defensible evaluation of reducing the contribution of separations costs
below 50%, which is the case for some pathways based on literature sources, including by the PI.<sup>1</sup> The
final group of comments regarded how the consortium selects projects. BioSep selects projects based on
identification of separations in industry based on input from industry and BETO's existing research into
bioprocessing. Input from industry is obtained through mechanisms such as listening days, special
sessions at conferences, and the directed funding opportunity. Subsequently, we evaluate whether the
consortium has the expertise and capabilities to address the challenge. We then leverage existing
analyses or evaluate anew the possibility of the project to reduce overall bioprocessing separations costs.
If these factors are favorable, the project is a strong candidate for inclusion in the consortium.

<sup>&</sup>lt;sup>1</sup> Biddy, Mary J., Ryan Davis, David Humbird, Ling Tao, Nancy Dowe, Michael T. Guarnieri, Jeffrey G. Linger, et al. 2016. "The Techno-Economic Basis for Coproduct Manufacturing to Enable Hydrocarbon Fuel Production from Lignocellulosic Biomass." ACS Sustainable Chemistry & Engineering 4(6): 3196–3211. http://doi.org/10.1021/acssuschemeng.6b00243.

# BIOPROCESSING SEPARATIONS CONSORTIUM – OVERVIEW OF CRADAS

#### **Bioprocessing Separations Consortium**

#### **PROJECT DESCRIPTION**

A key component of the BioSep is to engage with industry for both stakeholder input and to develop collaborative projects. To achieve the second aim, the consortium team solicited project proposals in an open call. One million dollars in funding was made available by BETO to be spent at the labs in support of industry collaborations.

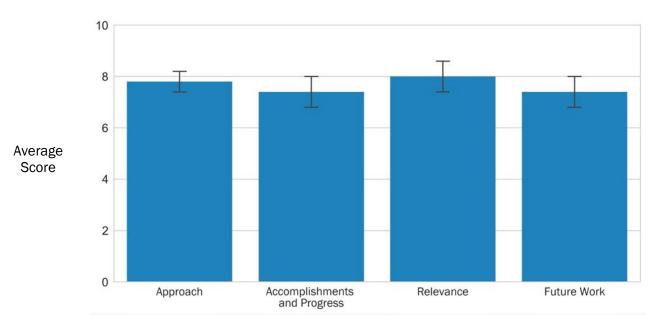
Potential industry participants teamed up with different national lab partners from BioSep. Ultimately, five collaborative projects were selected to be awarded after review by external subject-matter experts. Proposals were scored based on the following criteria: Challenges Addressed and Research Approach (30%); Impact of

| WBS:                      | 2.5.5.501e          |
|---------------------------|---------------------|
| CID:                      | NL0031310e          |
| Principal Investigator:   | Dr. Todd Pray       |
| Period of<br>Performance: | 10/1/2018-9/30/2019 |
| Total DOE Funding:        | \$1,000,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$1,000,000         |
| Project Status:           | Ongoing             |
|                           |                     |

Proposed Research on the Biofuels and Bioproducts Industry (25%); Benefit to Bioprocessing Community (10%); Key Personnel, Resources, and Bioprocessing Separations Consortium Capabilities (20%); and Requested Budget, Milestones, and Appropriateness of Government Funding (15%). The consortium's steering committee also provided input on the proposals related to topic area diversity, capability diversity, relationship to existing annual operating plan (AOP) work, national lab diversity, collaborative projects across national labs, and industry partner diversity.

### Weighted Project Score: 7.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

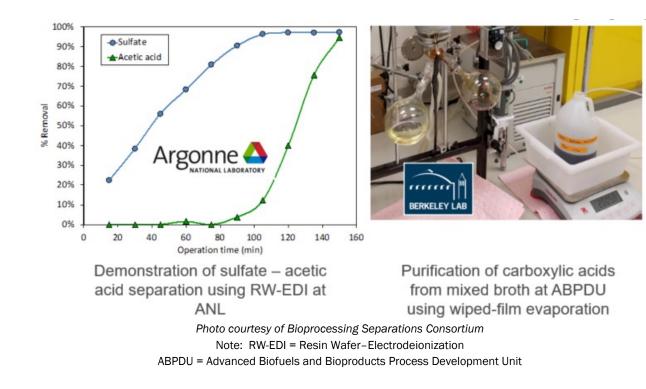


 ${\mathbb T}$  One standard deviation of reviewers' scores

The funds from these projects—\$200,000 each—are being deployed at the national labs to utilize their unique capabilities. The industrial participants are providing in-kind cost share and expertise to help achieve project goals. The awarded projects are with the following organizations:

- DMC Biotechnologies is partnering with a team led by ANL along with LBNL. The goal is to maximize production of high-value terpenoids from microbial fermentations through an adsorptive product recovery process.
- HelioBioSys is partnering with a team led by LBNL along with Sandia National Laboratories [SNL] and NREL. The goal is to develop a cost-effective and efficient protocol for separation and purification of extracellular polysaccharides from marine cyanobacterial culture broth.
- Kalion is partnering with a team led by ORNL along with NREL and ANL. The goal is to develop novel, low-cost means of water removal in Kalion's glucarate glucaric acid purification process.
- Mango Materials is partnering with the team at LBNL. The goal is to dewater lysed cells produced from waste biogas and recover the biopolymer, polyhydroxyalkanoate, using industrial-relevant equipment to help the company reach commercial-scale production.
- Visolis is partnering with a team led by ANL along with LBNL. The goal is to determine the efficiency and viability of extracting their hydroxy acid product from fermentation broth while minimizing the ionic contaminants in the captured aqueous stream.

Each of the above projects will be contracted under a CRADA with the participating national labs. The consortium's steering committee and BETO will monitor progress toward milestones and provide input to help achieve project goals, as stated in the overall consortium.



#### OVERALL IMPRESSIONS

- Program work results were excellent. My only question was that the project only has small-scale industry partners, albeit highly relevant to the biomass type project separation arena.
- Early-stage interactions with real-world ideas are good. The costs are relatively modest in relation to a diverse set of challenges.
- The concept of seed grants to increase industrial participation in BETO projects is useful and could serve as a model for other portions of the program. The funding levels seem low, and BETO would benefit from limiting the number of partners that could be involved on any single grant.
- The selected proposals represent a good diversity of topic areas, feedstocks, products, and separation technologies that are under development. The selection of earlier-stage companies and projects is high risk, but of significant mutual benefit to the innovation cycle because it provides an early process development opportunity that small companies cannot otherwise implement on their own.
- Amazing job putting together such a strong consortium and CRADAs with industry in some innovative areas with such little funding.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The consortium team appreciates the general overall positive feedback from the reviewers. The small companies that were awarded as part of this first cohort of industry partners will hopefully set the stage for larger partners as well in later years. During the selection process we focused on developing a diverse and robust set of partners, and the early-stage companies ended up submitting the most meritorious proposals.
- Moving forward, the BioSep team will work to expand the pool of applicants and potential funding for these CRADA projects. By expanding industry outreach efforts and demonstrating successful outcomes from the first cohort of projects, we expect to attract more and larger corporate partners with relevant technical challenges.
- An added approach to generating a larger and even more robust applicant pool, which the team will work with BETO to prioritize, will be to expand the capabilities and process and materials R&D approaches that the team develops as part of its core BETO pathway and product work. The team will also work with BETO to attempt to find additional resources to support more and larger CRADA projects.

# MELT-STABLE ENGINEERED LIGNIN THERMOPLASTIC: A PRINTABLE RESIN

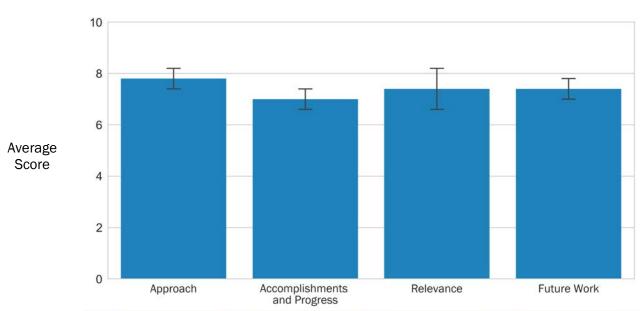
#### **Oak Ridge National Laboratory**

#### **PROJECT DESCRIPTION**

The proposed research develops a novel family of commercial-ready, lignin-based thermoplastic polymers and polymer composites suitable for high-volume applications, specifically those that are inherently recyclable, high-speed moldable, and 3D printable, with the capability to retain their exceedingly high mechanical properties after repeated thermal processing. The objective of this research is to produce and commercialize ligninderived, industrial-grade polymers and composites with properties, including printability, exceeding current petroleum-derived alternatives. Technologies that enable high-value uses of lignin—a biorefinery waste stream—are important to enable the cost-competitive production of biofuels.

| WBS:                      | 2.5.6.103           |
|---------------------------|---------------------|
| CID:                      | NL0031314           |
| Principal Investigator:   | Dr. Amit Naskar     |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$1,860,000         |
| DOE Funding FY16:         | \$500,000           |
| DOE Funding FY17:         | \$500,000           |
| DOE Funding FY18:         | \$460,000           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

We are developing a green processing technology using various lignin fractions. A new fractionation method is introduced in this research to separate functionally graded lignin. High lignin contents in the polymeric products have been aimed at incentivizing biorefining process.



#### Weighted Project Score: 7.4

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- Outstanding project with great learnings and milestone. One suggestion would be to provide some initial stabilization of a small amount of sodium borohydride. I have seen polymeric materials with reactive end groups that can often be treated with low levels of sodium borohydride to stabilize them to color formation and degradation. Lignin-reactive parts are external and the most sensitive to heat and processing because most of the lignin is H-bonding internally to form structures, as discussed. This applies to other teams working on lignin. This may only cost on order of a few cents per pound for low-level pretreatment for initial stabilization if it has not already been tried.
- The project looks promising. What are the key/best target opportunities to hone in on?
- The PIs present an interesting project that is well based in science, but also has a clear target market and potential impact. The project would be greatly strengthened by a better description of the overall yields during lignin extraction, the assumptions underpinning the economics, and an indication of which polymers have the greatest opportunity.
- The use of lignin as a copolymer has significant merit and market potential, especially given that the investigators have demonstrated that advantaged properties can be accessed. The fact that several licensing deals have been closed speaks to significant product pull from industry. It will be important to receive input back from industry to continue to formulate copolymers with desirable properties, protect them (e.g., with patents), and get them into the hands of partners.
- This project is gaining a better understanding of the different lignin characteristics and their potential impacts on properties of lignin-based thermoplastics that can outperform commodity automotive-grade polymers and other petrochemical-derived plastics.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- This is a great suggestion! Sodium borohydride will be able to reduce the carbonyl chromophore, which was shown to be prone to induce photo yellowing and degradation. Although our product is already colored (originates from lignin's brown color), we can use it to enhance the stability of the product. We are glad that the reviewer recognizes the cost issue associated with this and a minimal dosage can be used. We will follow the recommendation.
- Although we find promise with several types of lignin-based polymers (printable plastics, thermoplastic elastomers, self-healing rubber, and adhesives), we may find immediate applications of lignin-based thermoplastic elastomers in automotive interiors. Organosolv lignin will not have an odor issue for such applications. We also recognize a penetration in the automotive market is difficult and currently we are reaching out to several industrial partners on that goal.
- In the future, we will present more details about yield. Our ongoing work not only focuses on yield increase, but also on the application of the extraction residue. We envision complete utilization of lignin. Functional fraction of lignin will deliver the toughest and strongest thermoplastic elastomer and self-healing rubber that will have higher value (≥\$5,500/t). Non-fractionated lignin can go to printable plastics with polyamide or acrylonitrile butadiene styrene. Intermediate-value materials such as elastomers can be made from extract residues. Fibrous residues can be used in a common plastic matrix that are used for low-cost composite applications.
- This is a great suggestion! We are religious about intellectual property protection and feedback from licensees. Also looking forward to the long-term joint development program for targeted industrial products.
- Glad to see this comment. We are indeed targeting automotive-grade polymers. This suggestion itself answers one of the earlier comments.

# BIODERIVED MATERIALS FOR LARGE-SCALE ADDITIVE MANUFACTURING

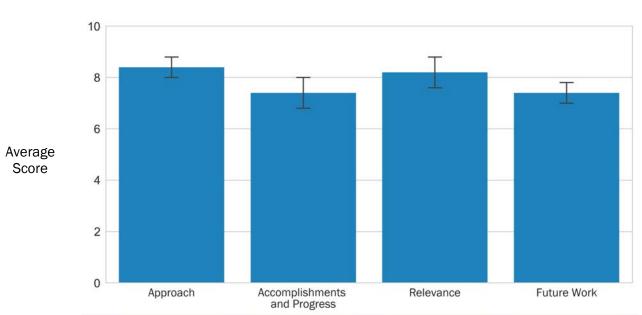
#### **Oak Ridge National Laboratory**

#### **PROJECT DESCRIPTION**

This project will improve economic viability of the biofuels industry by adding a new high-value revenue stream for biomass supply chains—bioderived composites for the rapidly expanding large-scale additive manufacturing industry (i.e., 3D printing). With recent innovations in printer technology and materials development, large-scale 3D printing has transitioned from a prototyping method to an advanced manufacturing technique. The market for 3D printing with polymers is growing rapidly. Among polymer 3D-printing approaches, large-scale additive manufacturing is 200 times faster than conventional desktop 3D-printing equipment and can reach deposition rates comparable to today's high-volume

| WBS:                      | 2.5.6.105           |
|---------------------------|---------------------|
| CID:                      | NL0033558           |
| Principal Investigator:   | Dr. Erin Webb       |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$692,960           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$346,460           |
| DOE Funding FY19:         | \$346,500           |
| Project Status:           | Ongoing             |
|                           |                     |

production methods such as injection molding. The most common material for large-scale 3D printing is a composite consisting of acrylonitrile butadiene styrene (ABS) plastic resin impregnated with roughly 20% carbon fiber (CF ABS). Carbon fibers provide the necessary overall strength and dimensional stability for the composite structure. Priced around \$6.00/lb, CF ABS plastics for large-scale 3D printing are limited to high-value products that require the superior strength of carbon fiber.



### Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${f I}$  One standard deviation of reviewers' scores

A large untapped market exists for 3D printing with composites that are less expensive than CF ABS to enable expansion of the additive manufacturing industry. The current market price of carbon fiber is \$15.00/lb. With current biomass prices in the range of \$100.00-\$250.00/dry ton, composites with biofiber reinforcement can meet this demand. In fall 2016, ORNL printed a pavilion and seating designed by Shop Architects of New York City for the prestigious Design Miami show using a composite of polylactic acid and bamboo particles. Bamboo has very desirable printability properties, but it poses some sustainability concerns as it is not domestically produced at scale. Growing bamboo in the United States is a challenge because most varieties are invasive species and others do not exhibit high yields in U.S. conditions. Rather, in this project we are using domestically sourced bioenergy feedstocks with a positive environmental footprint and rural economic development potential to create a flexible feedstock-to-product stream that optimizes the economic feasibility of both feedstock-to-fuel and feedstock-to-manufacturing pathways.

The central hypothesis of this project is that minimally processed biomass fibers can be used in large-scale additive manufacturing as a low-cost, sustainable alternative to carbon fiber reinforcement. Successful completion of this project will provide a new, high-value feedstock coproduct stream that reduces biofuel costs by sharing feedstock supply-chain resources, and thus costs, with bioenergy feedstocks. Much like conventional refineries can alter their product ratios based on current market prices, flexible biomass-processing strategies (milling and particle size separation) developed in this project will allow for optimum profit from biomass feedstocks.

In printing tests to date, we have produced poplar polylactic acid composites with a tensile strength of 75% CF ABS with superior printability. In future work we plan to test additional feedstocks (namely pine and switchgrass), optimize and scale up feedstock size reduction and fractionation operations for larger-scale printing tests, and match biocomposites with the best applications. Currently, we are targeting tooling—specifically molds—for manufacturing. Current estimates of the U.S. tooling market value are billions of dollars annually. While the cost of 3D printing is not feasible for mass production, it is ideally suited for producing molds that are notoriously expensive and time intensive to construct. 3D printing reduces production time of molds from years or months to weeks. Bioderived composites are well suited for tooling as they do not require the superior strength of carbon fiber and could reduce the costs of molds even further.

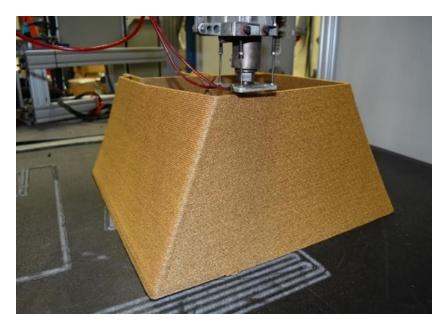


Photo courtesy of Oak Ridge National Laboratory

#### **OVERALL IMPRESSIONS**

- Excellent team effort to make value-added construction material for footprint reduction. Question: has the team tried to connect with companies like ICON who are looking at and claiming 3D-printed homes for \$4,000.00 in 24 hours and working with charity organizations already? I am skeptical about the price of their printed homes currently, but this could fit with the larger DOE goal around the social aspect talked about as an overarching impact on the United States through providing homes for the homeless in cities with homeless population challenges. One concern to address is that the density of the material prepared was quite high versus standard lumber materials, as this cost per cubic foot could be a project killer when trying to compete in the market with other moldable materials from petroleum.
- It's not clear how this project is following a scientific approach. It was not clear who they are working with in the building material space to further develop products. Surface coatings would need to be added to the product, but it was not clear how this was included in the cost analysis. Specifically, how do we know the industry would use this material? Could this project have an IAB similar to other projects? It was not clear what the market size is of these desired end products. It was difficult to connect their research results back to the highest impact application areas.
- The PIs present an interesting, straightforward, and easily understandable project that has the potential to affect a number of markets by the 3D printing of formed materials made from biofibers and polylactic acid. Moving forward, a greater understanding of interfacial interactions and molecular-level investigation could further improve the properties—and thus the areas for application—of their products. A better connection between the potential and reality of eventual industrial use would be helpful.
- This is a very encouraging project. It would be timely to get investors involved.
- This project represents a low-intensity process for valorization of lignin, using minimally (mechanically) processed lignin as an additive for manufacturing. Polylactic acid-lignin mixed polymers have been demonstrated to have structurally useful properties, perhaps best suited for applications where the full strength of carbon fiber is not needed and lower cost is desirable, such as in the 3D printing of manufacturing molds. The work needs to focus on optimization of particle size, testing other feedstocks to improve yields, and matching biocomposites with other applications. This project is an excellent effort, especially for the relatively low amount of funds currently dedicated to it.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The project team would like to thank the review panel for the encouraging and highly constructive • feedback. The reviewers noted our trial-and-error discovery approach employed thus far in this project. We acknowledge that characterization of our approach in the first 18 months of the project was designed to answer two questions: (1) can biomass be a suitable replacement for petroleum-derived carbon fiber reinforcement in large-scale 3D printing, and (2) can this new biomass coproduct reduce biofuel feedstock costs? Now that we have proved both to be true, we are eager to delve into the science of how and why biomass works in this application. We appreciate the reviewer suggestions to explore the molecular interactions between polylactic acid and biomass fibers and to better understand how these interactions determine strength, dimensional stability, and printability. The reviewers also noted that this project would benefit from industry interaction to assess and develop "market pull" for large-scale, bioderived materials. We agree and are optimistic that our success thus far will be useful in capturing the interest of industry partners. Other observations by reviewers were that aligning the scale of biomaterial and biofuel supply chains and scale-up of the biomass processing for biomaterials could be a challenge. We agree with this assessment and are considering how to better address these questions in year three of this project.

# WASTE-TO-ENERGY

**BioMetics** 

TECHNOLOGY AREA



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## INTRODUCTION

The Waste-to-Energy Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place on March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 15 projects were reviewed in the Waste-to-Energy session by four external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$22,750,283, which represents approximately 2.6% of the BETO portfolio reviewed during the 2019 Peer Review. During the project peer review meeting, the principal investigator (PI) 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 approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the Waste-to-Energy Technology Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. David Babson as the Waste-to-Energy Technology Area Review Lead, with contractor support from Dr. Mark Philbrick (Allegheny Science & Technology). In this capacity, Dr. Babson was responsible for all aspects of review planning and implementation.

## WASTE-TO-ENERGY OVERVIEW

Historically, the concept of "waste to energy" (WtE) has referred to any of a number of highly mature technologies (e.g., incineration or anaerobic digestion [AD]) utilized as a means to decrease waste volumes. Landfill capacity scarcity, coupled with increasingly stringent disposal regulations, necessitates novel wastemanagement solutions. In particular, the notion that waste streams represent valuable feedstocks for the production of biofuels and bioproducts is gaining currency. Conversion of feedstocks such as inedible fats and greases, biogas from landfills, dairies, wastewater treatment plants, and the organic fraction of municipal solid wastes into renewable natural gas, diesel, and aviation fuels is just beginning to gain market traction and represents a significant opportunity for additional expansion.

While there are advantageous market and policy factors unique to these feedstocks, they are subject to significant compositional, geographic, and temporal variability. This variability creates unique challenges and requires conversion technologies that are tailored towards particular families of feedstocks. In essence, the technologies need to go to the feedstocks, rather than the other way around.

Projects reviewed in the WtE session included hydrothermal liquefaction (HTL) and other conversion possibilities for both wet and gaseous feedstocks at a wide variety of technology readiness levels (TRLs), as well as analysis projects crucial to understanding the contexts in which these putative technology deployments would occur.

In the end, these feedstocks could comprise a relatively low-cost option that simultaneously solves currently existing disposal problems.

## WTE REVIEW PANEL

The following external experts served as reviewers for the WtE Technology Area during the 2019 Project Peer Review.

| Name          | Affiliation                  |
|---------------|------------------------------|
| Phil Marrone* | Leidos                       |
| Lucca Zullo   | VerdeNero, LLC               |
| Gary Vanzin   | Colorado School of Mines     |
| Tim Olson     | California Energy Commission |

\* Lead Reviewer

# **TECHNOLOGY AREA SCORE RESULTS**

| Average Weighted Scores by Project   |         |    |     |      |
|--|---------|----|-----|------|
| PNNL (2.1.0.113): Waste-to-Energy: Feedstock Evaluation<br>and Biofuels Production Potential - PNNL        |         |    |     | 3.6  |
| NREL (2.3.2.108): Reversing Engineering Anaerobic<br>Digestion of Wet Waste for Biofuel Intermediates and  |         |    | 8.2 | 2    |
| NREL (2.1.0.112): Waste-to-Energy: Feedstock Evaluation<br>and Biofuels Production Potential - NREL        |         |    | 8.2 | 2    |
| LLNL (5.1.3.104): Modular Microbial<br>Electromethanogenesis Flow Reactor for Biogas                       |         |    | 8.1 | •    |
| PNNL (2.1.0.301): Analysis and Sustainability Interface  |         |    | 8.1 | •    |
| NREL (2.3.2.107): Separations in Support of Arresting<br>Anaerobic Digestion                               |         |    | 8.0 | (    |
| PNNL (2.2.2.302): Bench-Scale HTL of Wet Waste<br>Feedstocks   |         |    | 8.0 |      |
| NREL (2.3.2.102): Biogas to Liquid Fuels and Chemicals<br>Using a Methanotrophic Microorganism             |         |    | 7.9 |      |
| PNNL (1.3.4.101): Thermochemical Interface   |         |    | 7.6 |      |
| NREL (2.1.0.104): Waste-to-Energy System Simulation<br>Model   |         |    | 7.5 |      |
| NREL (5.1.3.102): Biomethanation to Upgrade Biogas to<br>Pipeline Grade Methane                            |         |    | 7.4 |      |
| NREL (2.1.0.111): Analysis in Support of Biofuels and<br>Bioproducts from Organic Wet Waste Feedstocks     |         |    | 7.2 |      |
| ANL (5.1.3.105): Production of Methane From Organic<br>Waste Streams with Novel Biofilm-Enhanced Anaerobic |         |    | 7.1 |      |
| NREL (2.3.2.201): Biogas Valorization: Development of a<br>Biogas-to-Muconic Acid Bioprocess               |         |    | 6.5 |      |
| ANL (2.2.4.100): Arrested Methanogenesis for Volatile<br>Fatty Acid Production                             |         |    | 6.4 |      |
|  | 0 2     | 4  | 6   | 8 10 |
| Sunsetting   | Ongoing | Ne | ew  |      |

# WTE REVIEW PANEL SUMMARY REPORT

#### Prepared by the WtE Review Panel

The WtE session that was reviewed at the 2019 Project Peer Review meeting contained a total of 15 projects. This was almost double the number of projects reviewed at the previous meeting in 2017, which was the first appearance of this session title. This report summarizes the main observations, thoughts, and suggestions of the review panel members with respect to the session as a whole. More detailed and specific comments on each project can be seen in the individual project reviews later in this section.

While the concept of WtE and associated technologies are not new, it has been only in recent years that BETO has included this area in its technology portfolio. A workshop held by BETO in June 2016 at the National Renewable Energy Laboratory (NREL) helped to initially identify the potential for energy extraction from wet and gaseous wastes with respect to available feedstock and conversion technologies. Using the resulting report *Biofuels and Bioproducts from Wet and Gaseous Waste Streams: Challenges and Opportunities* as a basis, BETO began a more formal research focus in the area of WtE. The first dedicated session of WtE at a peerreview meeting was in 2017, and the number of projects has grown considerably in 2019, as stated above. Though currently limited to projects involving wet wastes and biogas (itself derived from AD of wet wastes) feeds, the attention now being given by BETO to WtE feedstocks and conversion technologies has been long overdue and is a welcome addition to BETO's research efforts.

The biggest challenge to most renewable energy technologies is not technical achievement but economic viability, especially in the face of conventional, fossil-based technologies that enjoy incumbent advantages. The overall feedstock and production cost of renewable fuels and chemicals is captured in the projected selling price, typically denoted by BETO as the cost per gasoline gallons equivalent (GGE). The current goal is to develop technologies for drop-in biofuels that have a cost of \$3/GGE. Since this goal is currently a challenge for most renewable energy technologies, the developmental focus needs to be on identifying and utilizing every cost advantage possible. Some of the most promising ways to achieve this are to: (1) utilize feedstocks that have a neutral or negative cost (i.e., don't have to be grown or purchased), (2) use conversion technologies that are compatible with the feedstock (i.e., involve minimal operations or steps), and (3) use conversion technologies that utilize as much of the feed composition as possible and recover as many high-value products as possible. Waste materials are the best example of satisfying the first option of neutral or negative cost and is why WtE is an important addition to BETO's portfolio. Eliminating the cost of feedstock growth and/or purchase can have a huge impact on reducing the overall cost of biofuel or bioproducts generation. Aqueousbased conversion technologies, such as hydrothermal processes and digestion, used in conjunction with wet wastes are excellent examples of ways to satisfy the other two options for minimizing costs. Unlike firstgeneration or more conventional processes, which require expensive drying of the feedstock and/or extraction of only certain components, hydrothermal processes and digestion utilize all of the feedstock and perform the necessary conversion reactions in water or a wet environment.

For all of the above reasons, the choice of wet wastes as part of BETO's initial foray into the field of WtE is an excellent start, and the particular focus on aqueous-based conversion (e.g., hydrothermal) and productenhancement (e.g., biomethanation, arrested methanogenesis, biogas-to-liquid) technologies for use with wet wastes makes sense. The parallel support effort by BETO in modeling the availability and distribution of the most common wet-waste feedstocks (e.g., manure, food waste, wastewater sludge) is also a wise investment and helps guide and improve technology development for processing these wastes.

Yet despite this logical start with wet wastes and derivative products, BETO needs to expand its efforts in the WtE field to include more diverse types of waste. Municipal solid waste (MSW), or at least the organic fraction of MSW, represents a much larger potential feedstock and source of carbon that is currently being underutilized. As a waste, it carries the same potential benefits of neutral or negative cost that, with the right conversion technology, can be converted to fuels, chemicals, and/or power. Along with MSW recycling,

research into technologies that can convert plastic waste into useful products would solve longstanding issues on waste reduction (both diversity and mass) while possibly lessening geopolitical issues around the longevity of plastic waste. BETO appears to recognize the value of this next-step expansion of WtE to include a broader definition of wastes based on future efforts outlined during several of the plenary talks at the 2019 Peer Review meeting. It is also encouraging to see mention of future work that includes more than just wet wastes in some of the current WtE projects (see, for example, the Waste-to-Energy: Feedstock Evaluation and Biofuels Production Potential project). This review panel strongly supports this effort by BETO to expand its focus on WtE to include a wider range of waste materials beyond just wet wastes.

#### IMPACT

In general, this review panel believes that all of the projects reviewed are relevant to BETO's mission and are having or promise to have a meaningful impact in the WtE field. While some projects may be more successful than others, all are providing valuable information to collectively advance the state of technology (SOT) for WtE. The achievements demonstrated to date justify further support by BETO of these WtE technologies. If anything, BETO should, in fact, expand its focus to include a more diverse source of waste materials as discussed above.

Of particular importance to note is the work on HTL for conversion of wet wastes to biocrude oil. This technology is a good example of what can be achieved when a process is paired with the right feedstock. The use of a water-based HTL technology is ideal for processing high moisture feeds because it avoids the significant cost of both drying the feed and having to chemically or physically isolate a specific feed component such as lipids. When the wet feedstock is also a true waste (i.e., having a negative cost), such as wastewater sludge, the cost benefits are further enhanced, making the technology even more attractive to potential industrial or commercial users. In light of this, as well as when considering the demonstrated biocrude yield values, it is not that surprising to see that associated modeling efforts have shown HTL as coming the closest to achieving BETO's fuel dollar-per-GGE goal. Despite its achievements, however, HTL technology is at a point in its development where its potential has been fully demonstrated at the research level but not yet at the commercial scale where industry finance is ready to step in. Further support by BETO at pilot scale is necessary for HTL technology to achieve its full potential and bridge the so-called "valley of death" with respect to process funding and development.

Another example of particularly impactful work in the WtE session is represented by the modeling-based projects. The resource modeling projects are performing an exhaustive yet essential task in collecting and organizing wet-waste feedstock quantity, location, and cost data down to a regional level. This information is critical to the development of the WtE industry. Other projects focus on techno-economic analysis (TEA) work in parallel with associated experimental-based projects in either HTL or arrested AD. The concept of using a TEA model fed by the latest experimental data to in turn predict key economic indicators and identify variables to explore further in subsequent experimental work for cost or performance optimization is a brilliant way to maximize research efficiency. The results of the modeling work help drive and direct experimental research, which then in turn feeds new and more accurate iterations of the model. System dynamics-based modeling is innovative and helps provide WtE industry performance and behavior over long-term periods. Taken together, the modeling projects play an important role and are having a significant effect on the development of WtE technologies.

One more example of projects having a notable impact are several that are focused on converting relatively low-value biogas to higher-value liquid chemical products (e.g., organic acids). This is a strategy that many renewable technologies have employed to help become economically viable, which is consistent with the options for maximizing cost advantages discussed above. By generating chemical species that have a high market demand as products or chemical intermediates, the resulting higher selling price helps offset the production cost more than the price that a liquid or gaseous fuel could command. The projects in this WtE session use different approaches to upgrading biogas (e.g., arrested methanogenesis or genetic engineering of microbes), and as exhibited by the attempt to generate muconic acid, success is not always guaranteed. Further,

not all products chosen (e.g., volatile fatty acids) may command a high enough price to justify this approach. However, all of this work is providing valuable lessons learned that future work can build upon. Continued efforts at developing pathways to upgrade fuels to higher-value chemicals is therefore encouraged.

#### **INNOVATION**

Most of the projects reviewed in the WtE session have demonstrated some innovative aspects, whether in equipment design, materials used, and/or technical strategy/approach. The use of HTL technology to process wet wastes seems intuitive from a purely technical perspective but is innovative when one considers how long it has taken BETO to recognize its potential. Previous approaches for processing wet feedstock such as algae involved an elaborate effort to genetically modify the algae to produce high quantities of lipids. These lipids would then have to be chemically or physically extracted after first drying the algae before one could start processing into fuel or chemicals. In light of this background, the use of a water-based technology that utilizes all of the feed biomass is refreshingly innovative.

Several projects have developed innovative reactor designs. In particular, the microbial electrochemical reactor for biogas upgrading is a unique combination of microbial electrosynthesis biology with advanced materials for electrodes in a compact concentric cylinder design that allows a higher electron density and minimizes mass-transfer issues. Similarly, the 3D-printed scaffold design for biologically mediated biogas-to-liquid reactions (muconic and succinic acids) represents a novel design that has shown improved performance and mass transfer relative to the more traditional stirred tank reactor. Several projects also discussed a focus on modularity in design, which is good foresight with respect to future ease of scalability.

The resource-modeling projects are using innovative approaches in their attempts to quantify domestic sources of wet wastes down to the regional level. The overlaying of various categories of spatially based data to identify optimal locations (i.e., "hotspots") with respect to these feedstocks for placement of conversion technologies is particularly valuable. The future focus of these resource-modeling projects on potential feeds, beyond just wet wastes, is an encouraging sign that BETO is beginning to look at tapping into the much wider range of wastes that are available as potential feedstocks. However, the current lack of inclusion of any project with innovative conversion technologies for use with wastes such as MSW represents the most notable area missing from this WtE session.

#### **SYNERGIES**

Identifying and exploiting synergies that exist among individual projects is important for maximizing efficiency with respect to use of BETO's limited funds. There are several examples of project synergies in the WtE session that can be seen and are benefiting the projects involved considerably. The relationship between the experimental and modeling projects associated with the Pacific Northwest National Laboratory (PNNL) HTL technology and the NREL and Argonne National Laboratory (ANL) arrested AD technologies stand out as excellent demonstrations of project synergies. The experimental projects provide data for the modeling projects. The modeling projects then use the experimental data to validate TEA models and identify key variables via sensitivity analysis that have the biggest impacts on cost projections. This information then gets fed back to the experimental projects, which use the TEA results to plan future experiments focusing on these key variables, repeating the cycle. By directing resources to the variables that have the largest impact, one should, in theory, be able to get the maximum production cost reduction in the shortest time.

While it is one thing to set up this relationship on paper, in reality there is no guarantee that the interactions between the experimental and modeling groups will work as planned. It is therefore encouraging to see that the synergistic relationship described above appears to be working well for the PNNL and NREL groups. For example, identification of heat exchanger designs and ammonia removal costs as being significant HTL variables has led in turn to experimental work to better understand heat transfer coefficients for more efficient design and methods of ammonia removal from the aqueous product. Even the resource assessment models and system simulation model have provided useful data for the HTL experimental teams through economic

comparisons to other technologies. Though not as far along as the HTL projects, the modeling effort associated with arrested AD has identified separation efficiency and minimum volatile fatty acid (VFA) product titers for the experimental groups. BETO should do all that it can to support the synergies that are evident among these projects and use the relationships demonstrated in these projects as a model to encourage similar production among experimental and modeling teams in other areas.

The NREL arrested AD experimental effort is itself an example of good synergy between two groups that have divided the work into the biology research and downstream VFA separations research. To make this technology viable, the two very different challenges of biologically stopping the digestion (i.e., methanogenesis) process at the acid production point and subsequently removing these acids from the digestion medium must both be optimized in an integrated continuous system. Conducting both lines of research separately but in parallel generates synergies that should help both areas of research.

While taking advantage of synergies among projects is essential, there is a fine line between project synergies and duplicated efforts. Among projects that focused on the same general technology, it was not always initially clear how the projects differed from each other and what made each one unique. In the future, this review panel feels that it would be helpful if each project were required to explain upfront how it is distinct from other related projects and what makes its work unique. Even better would be if a BETO representative at future peer review meetings could address the project's uniqueness and why it was initially awarded funding as part of its normal introduction of each project presentation.

#### FOCUS

All of the projects in the WtE session involve appropriate and representative technologies for this topic. As pointed out earlier, however, the projects in this session deal with a more specific subset of WtE (i.e., wet wastes) than the session heading name implies. This review panel recommends that BETO do one of the following to correct this mismatch: (1) change the name of this session from "Waste-to-Energy" to "Wet-Waste-to-Energy" to more accurately reflect the intended focus, or (2) expand the number of projects in this session to include a greater diversity of waste feed types (the latter being the option preferred by this review panel). Several projects have already stated an intent under future work to explore the use of waste plastics or the organic fraction of MSW as a feedstock, which should be encouraged by BETO. It is also encouraging (and timely) to see BETO specifically call out the topic of "Renewable Energy from Urban and Suburban Wastes" in its most recently announced Fiscal Year (FY) 2019 Bioenergy Technologies Office Multitopic Funding Opportunity Announcement (FOA) (DE-FOA-0002029) in May 2019. This is clearly a step in the right direction to better utilize a greater quantity and variety of waste resources.

In the process of increasing the diversity of waste types as feedstock, BETO should, at the same time, narrow its definition of acceptable wastes for this session to be those materials having a negative or near-neutral feed cost. This is a simpler yet accurate definition of a waste in the specific context of BETO's objectives. Waste feedstocks that meet this definition will have an overall reduced process cost for conversion to fuels or chemicals relative to feedstocks that must be grown, harvested, and/or purchased. As a result, these materials allow the best chance that the product(s) can meet BETO's target fuel production cost, and thereby maximize the potential return on limited research dollars.

Back on the topic of wet wastes, one area in the WtE portfolio that could benefit from additional emphasis is additional hydrothermal conversion technologies. As has been pointed out earlier, HTL has a number of advantages for processing wet wastes. HTL also generates a liquid fuel product, which is consistent with BETO's preferences and justifies the funding provided to date for the development of this technology. However, there are other forms of hydrothermal processing that may be worth supporting, either in addition to or in parallel with HTL, depending on the specific application. These other types of hydrothermal conversion technologies have similar advantages to HTL but differ in the particular process conditions and therefore the spectrum of products generated. Baseline technical and economic evaluations of expanded hydrothermal technologies could include supercritical water gasification and hydrothermal carbonization (HTC).

Supercritical water gasification generates hydrogen gas as its major product, but with an appropriate catalyst, the major product can be changed to methane under either supercritical or subcritical conditions. HTC produces solid char (or biochar) as the major product, which has many potential uses such as fuel, soil enhancer, etc. BETO support for further development of these related hydrothermal technologies should be considered for inclusion in the WtE portfolio along with HTL to provide for a more diverse set of fuel and chemical products. The best hydrothermal technology or technologies to use in any situation ideally could then be chosen based on the specific needs, constraints, and economics associated with each potential application.

#### TECHNOLOGY DEVELOPMENT PIPELINE

Taking an innovative concept and proving that it can succeed at the bench scale is of course a necessary and important step in the process of new technology research and development (R&D). Funding these types of projects is something that BETO has and continues to do very well. However, funding up to the proof-of-concept point is not enough for most technologies to attract sufficient private funding in their commercial development. There are usually significant unknowns associated with scale-up that keep investors wary. Abandoned by government funding but not yet able to secure private funding, this is the infamous "valley of death" referred to earlier which many otherwise promising technologies have not succeeded in passing. BETO can and should play a role in helping good technologies bridge this economic chasm by funding more pilot-scale projects. While not taking away from funding traditional R&D, BETO should also consider funding projects that demonstrate operation of continuous, integrated, pilot-scale systems of conversion technologies to generate the long-term operating and maintenance data that private industry and investors need to see before their inherent skepticism and risk aversion may be overcome.

It is encouraging to see that several projects in the WtE session are already moving in this direction. PNNL has built and operated its own pilot-scale HTL system and is participating in another BETO-funded team project that will be testing a commercially designed HTL pilot system at a wastewater treatment plant (though this latter project is part of the Advanced Development and Optimization session). The ANL arrested AD project intends to test a 200-gallon-sized version of its anaerobic membrane bioreactor (AnMBR) for VFA production in the coming year as part of its project. The NREL project on biogas upgrading not only has operated at large scale (700 L) but also plans to build a 30-L-capacity mobile version of their technology in their project. Where appropriate, mobile versions of conversion technology systems are another good way to demonstrate operation at scales of commercial interest and to bring the technology directly to an industrial site or feedstock location for further visibility. While none of the above is new or in disagreement with BETO's past funding philosophy, recent actions by DOE at the direction of the current administration suggest a retreat to focusing solely on research-scale projects, and this is of concern. This review panel therefore feels it necessary to emphasize the continued importance of funding pilot-scale projects to help new technologies fully complete their successful transition to qualifying for commercial lending and funding.

Of the existing projects in this session, some aspects of the biomethanation and arrested AD projects may require additional attention. For biomethanation, more focus on how to recover the dissolved methane from these aqueous systems is needed, because this is not trivial or easy. In arrested AD, focus is needed on demonstrating long-term operation of these systems regardless of the type of reactor chosen. This will be challenging because of the unknown behavior of the genetically modified microbial consortia over time, the use of a heterogeneous carbon and energy source, and the possibility of end-product inhibition. A more complete fundamental understanding of the microbial consortia and the impact of arresting the methanogenesis reaction is needed, along with a better understanding of feedstock and metabolite composition changes during the process.

Most of the projects in the WtE session discussed the inclusion of one or more collaborators, partners, or advisors from private industry that are on the project team. This is a smart strategy with respect to technology development for several reasons. Having industrial input to a project helps provide guidance and a sanity check for the direction of research so that the technology is developed in a way that will be most useful to the potential end users. It also allows the research team to tap into valuable knowledge and resources in the industrial community for more efficient use of time and funding. The flow of information, however, is not just one way. Having industry personnel as team members also helps keep industry apprised of research results and engaged in the research process, thereby generating awareness and hopefully interest in future development as the technology matures. This policy is a win-win for everyone and is therefore an essential aspect of BETO's project management that should be encouraged in all current and future projects.

#### RECOMMENDATIONS

The recommendations for further improvement of this WtE session as submitted by this review panel are as follows:

- Expand the WtE session to include more diverse waste feedstocks, including MSW. Alternatively, if BETO specifically wants to focus only on wet wastes or their derivatives, as is the case now, this session should be renamed to "Wet-Waste-to-Energy" to reflect the intended feedstock more accurately.
- Encourage the use of neutral or negative cost waste feedstocks in current and future projects in this session. Along with matching the feedstock to the appropriate conversion technology (e.g., water-based technology for wet wastes), this will provide the best opportunity to minimize unnecessary fuel (or chemical) production costs, optimize process economic viability, and meet the target BETO fuel selling price of \$3/GGE.
- Increase funding for pilot-scale development of sufficiently promising conversion technologies to help bridge the "valley of death" with respect to commercial maturity. The continued support beyond bench scale is important to demonstrate acceptable performance, provide critical operating data, and reduce technical risk at a scale where private industry and lending institutions are more likely to be willing to take over with further commercial development of the process. This additional investment by BETO also increases the chance that the total investment made by BETO in a technology from the start is not ultimately wasted.

Though not specifically related to the WtE program, the following recommendations for both BETO and researchers are also offered to improve the presentation format and associated review:

- BETO staff should provide a brief introduction prior to each presentation that includes the original rationale for the project choice for funding and what makes each project unique from or related to others in the session on the same general topic.
- Both the baseline status of the technology being investigated at the start of the project and the impact of the project results presented on the overall commercialization timeline should be stated in each presentation (i.e., describe where you started and where you are now with respect to commercialization). This information will help reviewers gauge both the degree of progress made and how far away the technology is from being market ready.
- Repetitive (i.e., the same in every project) and less-useful information with respect to technical evaluation (e.g., management approach) should be eliminated from the presentations to allow more time and space for technical content. This is not to say that this information is not important for BETO to gather, only that it does not need to be included in the technical presentations given the constraint of limited time and space.
- Statistics quantifying the stability and variance associated with key results (e.g., error bars) should be included wherever and whenever available.
- A list of acronyms used in each presentation should be required.

• For TEA, resource, and other modeling-based projects, a list of critical assumptions that underlie the results presented should be stated.

## WTE PROGRAMMATIC RESPONSE

#### INTRODUCTION/OVERVIEW

The Conversion R&D Program Area would like to take the opportunity to thank the four WtE reviewers for their time and careful review of the portfolio.

The review panel noted that the title of the session led to confusion with regards to the feedstocks being investigated across this session and elsewhere in the BETO portfolio. While this session was entitled "waste-to-energy," it focused on wet-waste streams (municipal wastewater sludge, manure, food waste, fats, oils, and greases, and biogas derived from these streams). In future peer reviews, BETO will more explicitly explain which waste streams are/are not included in respective sessions given that the definition of waste can be very broad.

Related to this, the review panel discussed that technologies and projects related to the conversion of municipal solid waste were not represented in this session. Working on MSW is an emerging area of interest for BETO given that it is a highly heterogeneous stream and presents unique compositional and resource challenges. The program has already begun resource assessment to focus on nonrecyclable fractions of MSW, including plastics, paper, and construction and demolition wastes. BETO recently identified seven areas of particular interest in a report on ways to improve the economics of municipal solid WtE.<sup>1</sup> BETO has also issued several funding opportunity announcement topics directed specifically toward MSW and has issued a request for information on strategies for the utilization of food waste.

As the panel has identified, BETO concurs that technologies for converting MSW may be considerably different than those being explored within the wet WtE space. For example, HTL may be amenable to the food waste fractions of MSW but less well suited for other fractions therein. As with the Conversion R&D Program Area's first forays into wet wastes, the program intends to guide the development of conversion technologies with resource assessment and TEA.

The following sections specifically address the top recommendations from the review panel:

#### Recommendation 1: Expand WtE to include MSW.

As discussed above, the program acknowledges that the title of this session was misleading because the projects presenting only covered a subset of wastes. In some cases, other waste streams (e.g. carbon dioxide [CO<sub>2</sub>]) were explicitly covered in separate and parallel review sessions, and there are fractions of waste (e.g., food waste) that have not been explored to a considerable extent within the portfolio. The program has already begun to increase its activity with regards to strategy and utilization around MSW and would expect to have a number of projects that are targeting those streams. As discussed above, BETO will ensure that definitions of waste are clear to avoid this confusion.

<sup>&</sup>lt;sup>1</sup> Bioenergy Technologies Office. 2019. Waste-to-Energy from Municipal Solid Wastes. Washington, D.C.: U.S. Department of Energy. DOE/EERE-1796. https://www.energy.gov/sites/prod/files/2019/08/f66/BETO--Waste-to-Energy-Report-August--2019.pdf.

#### Recommendation 2: Encourage the use of neutral or negative-cost feedstocks.

The program concurs that the utilization of zero- or negative-cost feedstocks presents a unique set of opportunities for moving technologies from bench and pilot scale into the market and simultaneously meeting office cost target objectives. In many cases, these feedstocks represent an environmental and cost liability to the producer or company managing, which presents a unique and attractive value proposition. To this end, analysis efforts in the WtE portfolio of projects have begun conducting "hot-spot" analyses to identify these opportunity areas and which might represent opportunities for first-of-kind facilities. While not presented in detail during these sessions, these areas tend to have shared attributes such as dense populations, organics diversion regulations, and/or limited landfill capacity, amongst others. The program will continue to encourage that these analyses be published and shared with both municipalities and with technology providers.

The program also appreciates the comment to appropriately match the feedstock to the conversion technology. To this end, HTL has been a technology of particular interest given that it is amenable to high-moisture feedstocks and can convert a diverse composition into a more homogenous TRL, and the program has sought to explore multiple solutions in parallel as a risk-mitigation strategy. For example, this has been the strategy with the arrested AD projects. As resources allow, the program continues to explore additional technological solutions for these wet wastes that are guided by TEA and move towards clear technical targets such as waste conversion efficiency.

#### Recommendation 3: Increase funding for pilot-scale development and continue benchscale development.

BETO fully concurs that it is critical to support technological development beyond the bench scale and into pilot scale. There are many technological R&D barriers that cannot be solved, and in some cases identified, until a technology has been scaled up or integrated with other upstream and downstream unit operations. Overcoming these integration and scaling challenges is a key objective of the Advanced Development and Optimization (ADO) Program Area. As resources allow, BETO is committed to funding projects beyond the bench scale to ensure that technologies are at a risk level that enables them to move into the market.

To date, the program feels that HTL is the only wet WtE technology within its portfolio that achieved a sufficiently high TRL to scale up. As such, the ADO Program funds pilot-scale research on HTL to address scaling and integration barriers. Simultaneously, the program has continued to support the bench-scale R&D work on this technology to respond to barriers identified at a larger scale and to continue to optimize process parameters in a cost-effective way.

The program recognizes that there are ways to improve the collaborations between the bench-scale and pilotscale researchers and improve the coordination within BETO. For technologies that achieve the requisite technological maturity, the program is working to formalize the interface between the Conversion R&D Program, ADO Program, and other BETO programs as appropriate. These could include joint project milestones, coordinated technical targets, harmonization of TEA and life cycle assessment (LCA) assumptions, and most importantly to identify which barriers and technical problems are being addressed at which scale.

# THERMOCHEMICAL INTERFACE

#### **Pacific Northwest National Laboratory**

#### **PROJECT DESCRIPTION**

Most studies on microalgae HTL are currently conducted in small laboratory batch reactors with a few research teams reporting on continuous systems. Scalable designs and strategies for optimal algal HTL configurations require data for nutrient recovery, water treatment and recycling, enthalpies of HTL reactions, residence times and space velocities, heat recovery, corrosion, separations, and removal of heteroatoms (i.e., upgrading to hydrocarbons). In addition, variations in seasonal algal cultivation require approaches to capital asset utilization and balancing of energetic tradeoffs associated with feedstock management and storage. Benchmarking how these technical issues impact the costs of algal HTL conversion and tracking how

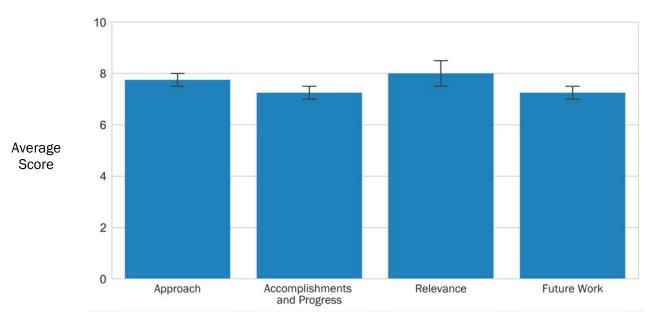
| WBS:                      | 1.3.4.101          |
|---------------------------|--------------------|
| CID:                      | NL0026324          |
| Principal Investigator:   | Mr. Dan Anderson   |
| Period of<br>Performance: | 4/1/2014-9/30/2019 |
| Total DOE Funding:        | \$4,860,000        |
| DOE Funding FY16:         | \$1,520,000        |
| DOE Funding FY17:         | \$1,200,000        |
| DOE Funding FY18:         | \$1,390,000        |
| DOE Funding FY19:         | \$750,000          |
| Project Status:           | Ongoing            |
|                           |                    |

improvements reduce capital and operating costs are a responsibility of BETO.

The project team at PNNL has more than five years of experience with continuous algal HTL systems and is developing advanced HTL processing methods to improve process efficiency and reduce capital and operating costs for the production of drop-in biofuel blendstocks from microalgae. One strategy for achieving full utilization of capital assets (and minimizing operational costs) is to blend algal feedstocks with woody materials during lean algal seasons. The project is developing methods for coprocessing algal/woody feedstock blends and has identified synergistic effects beyond what was expected.

#### Weighted Project Score: 7.6

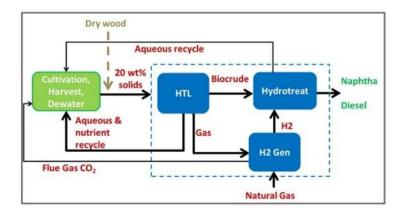
Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

Upgrading technology for the production of finished fuels blendstocks is a critical subtask of the project, as are studies of nutrient recycle from HTL waste streams for algal cultivation. A major accomplishment so far includes demonstration of recycling HTL byproduct streams to supply 100% of the nutrients required for algal cultivation, with 89 culture cycles completed by Q4 of FY 2018.

In recent years, the project supported the acquisition and testing of an engineering-scale HTL process development unit at PNNL with three skids for (1) feedstocks prep, (2) HTL processing, and (3) product separations. All data from bench- and engineering-scale HTL efforts feed directly into algal HTL process models for examining TEA and LCA impacts of different system configurations. The process models inform BETO's annual SOT evaluation and are also used to determine the most useful R&D targets for driving down fuel costs.



#### **Current Algae HTL Conversion Process**



Photo courtesy of Pacific Northwest National Laboratory

#### **OVERALL IMPRESSIONS**

- This project demonstrates further progress in optimizing HTL process technology with the goal of meeting BETO's liquid biofuel cost target. Results achieved over this review period have shown how increases in feed solids loading for biocrude production and pretreatment and an improved catalyst for upgrading are helping to drive down the overall cost towards the BETO goal. PNNL staff have continued to investigate methods of improvement to the HTL process from many angles, as shown by the results of blending tests and nutrient recycle tests. While it is understood that the HTL algal work has laid the groundwork for subsequent tests with real wet wastes (e.g., sludge), the algae used in these tests are not waste and therefore this project may not really belong in this group (although this is a BETO decision). However, eutrophic algae would qualify as a waste and its negative feedstock cost would further help meet the BETO biofuel cost target, so it should be considered as a future feedstock. The only major concern with the work shown is the apparent disconnect in the modeling cost results between that shown in this project and in the formal TEA modeling project (2.1.0.301), also performed by PNNL staff. Future modeling work in any of the PNNL HTL projects should all be performed on the same basis with the same cost categories to avoid confusion.
- This is a relevant project and HTL has tremendous potential given the wide applicability to feedstocks that are not easily or economically amenable to other treatments. I would like to see a bit more detail on the choice of feedstock and feedstock blends. The focus on the recycling of water and recovery of nutrients is very good. This being said, the technical and economic feasibility of upgrading by hydroprocessing remains a critical unknown and the weakest link in the TEA, even accounting for the future work. HTL may be the only practical thermochemical technology working with wet streams.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments. This project is part of the Advanced Algal Systems Program at BETO, specifically focused to develop an HTL conversion pathway for algal biomass to produce biofuels. We do agree that the placement of this project in the WtE Program Review and not in Advanced Algal Systems Program Review may have resulted in some confusion for WtE reviewers. On the positive side, we were able to show the reviewers how this algal HTL project had laid the technical groundwork for establishing the HTL conversion and modeling projects focused on wet wastes. However, there was a disconnect with the algae project and its relationship to the wet-waste process/TEA because the associated algal HTL process model project was reviewed in the Advanced Algal Systems Program Session. This project has a direct connection with HTL algal model/TEA project from the very beginning, but it was not presented to the reviewers. So, there is direct connection between the algal HTL conversion project and the algal HTL modeling effort as the reviewers suggest. We do agree that focusing on eutrophic algae as a potential negative-cost feedstock makes sense and we are pursuing project opportunities in that area.
- Input from the NREL/PNNL resource assessments and the algal TEA/modeling team have driven the selection of the feed blendstocks we are testing (i.e., loblolly pine residuals and algae). Some pine plantations are located in the southern United States, close to the candidate locations for algal farms (e.g., Florida, Texas). Also, pine residuals have a relatively low moisture content and can be beneficially combined with more dilute algae, eliminating some of the dewatering requirement.

# WTE SYSTEM SIMULATION MODEL

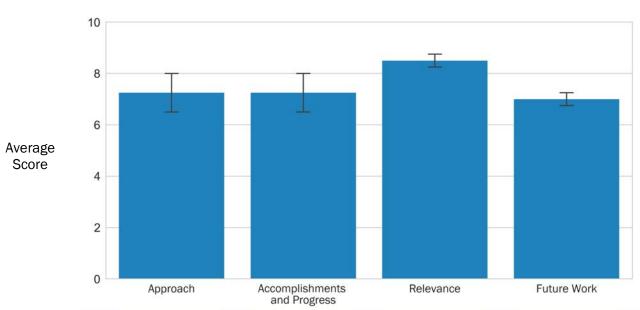
### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

Leveraging existing waste from landfills, confined animal feeding operations, and publicly owned treatment works for energy and chemical production could add revenue to existing waste disposal treatment operations and contribute to high-level sustainability goals. Although these waste streams are readily available throughout the country, most of the current WtE projects only utilize biogas to produce electricity. Transitioning from the current status of disparate projects producing low-value energy to a cohesive industry optimized around producing fuels and chemicals from waste will require a systems approach to understand the impacts of external factors, internal feedbacks, and key levers and to maximize the impact of

| WBS:                      | 2.1.0.104           |
|---------------------------|---------------------|
| CID:                      | NL0029525           |
| Principal Investigator:   | Dr. Danny Inman     |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$1,440,000         |
| DOE Funding FY16:         | \$400,000           |
| DOE Funding FY17:         | \$390,000           |
| DOE Funding FY18:         | \$350,000           |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | Ongoing             |
|                           |                     |

DOE efforts. The objective of this project is to perform systems analyses to elucidate the impact of policy, R&D, and techno-economics on the WtE system as a whole, as well as at specific points in the supply chain and for individual sectors (e.g., landfills, confined animal feeding operations, publicly owned treatment works). This project will leverage existing DOE models (e.g., the Waste-to-Energy System Simulation Model), along with current DOE techno-economic data, resource assessment data, and stakeholder input to perform analyses that are directly tied into BETO goals.



#### Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

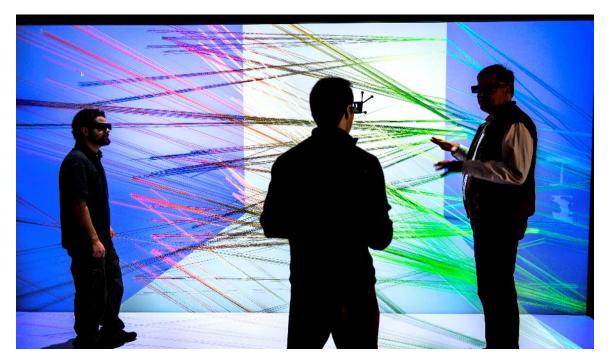


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project represents another important modeling effort to benefit the efficient development of wasteconversion technologies to energy, with this model aiding in predicting WtE industry performance and behavior over long-term periods. The systems dynamics approach is innovative and can provide interesting and valuable information on energy trends and nonintuitive results. Of course, one reason a result may appear nonintuitive is that it is incorrect. There is some concern as to how well the model predictions are able to be and have been independently validated, especially in trying to predict trends up to 20 years in the future. Explaining some of the operating philosophy of the model as well as key inputs and assumptions used would help better understand the basis for results presented and increase confidence in how these results are generated. The project would also benefit from a clear list of detailed tasks and a schedule to track progress.
- This presentation outlines a good project that tackles a challenging topic and attempts to gain insight by building a model sophisticated enough to capture all the key factors, yet simple enough to be manageable. The discussion about strengths and weakness is particularly difficult as one may be easily assumed or request exceedingly high standards or expect unrealistic accuracy. What may be seen as weaknesses for a predictive model used in the design become a natural feature in a model designed or used to support decision making and high-level analysis. With this in mind and realizing that this project mostly delivers the latter and not the former, I found this project of great interest and I would encourage the development to be continued in such a way to provide the most value to those engaged in that effort. I appreciate the PIs showing regional application as it also shows that it can likely be scaled further down the geographical scale. More precise quantification of intuitive insight is valuable, yet the model has not—at least in my view—delivered any significant counterintuitive insight as is often the case in systems dynamics.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their helpful and supportive feedback. We will incorporate these suggestions into our future workplans.

# ANALYSIS IN SUPPORT OF BIOFUELS AND BIOPRODUCTS FROM ORGANIC WET-WASTE FEEDSTOCKS

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

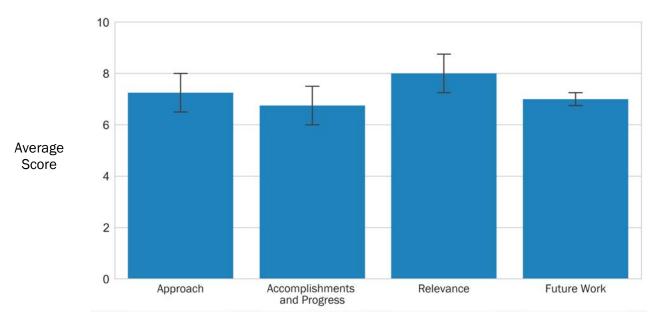
Total wet-waste feedstocks present an annual energy resource of 11.3 billion GGE, including wastewater residuals, animal waste, food waste, fats, oils, and greases. Conversion of wet-waste feedstocks into transportation fuels and chemicals not only represents a significant opportunity for additional expansion of transforming underutilized resources into a variety of value-added fuels and chemicals, but also reduces landfills. TEA is critical for guiding WtE pathways from R&D to widespread deployment. Thus, the goal of this project is to develop conversion-process design concepts and perform cost analyses to evaluate WtE opportunities to identify R&D needs and prioritization by BETO and industry. From FY 2018 to FY 2020, this project performs TEA to support

| WBS:                      | 2.1.0.111           |
|---------------------------|---------------------|
| CID:                      | NL0033389           |
| Principal Investigator:   | Dr. Ling Tao        |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$400,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$200,000           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

three ongoing projects on biological conversion (arrested AD). The arrested AD produces higher-value fuel, chemicals, or their precursors by arresting methanogenesis while utilizing all organic substrates (carbohydrates, lipids, fats, proteins) in the waste feedstocks. At the end of the project, we will report identified key performance targets and understanding on potential economic viability to assist R&D prioritization decisions. We should also have a broad range of wet-waste conversion technologies investigated

#### Weighted Project Score: 7.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${f I}$  One standard deviation of reviewers' scores

for their economic and environmental sustainability potentials, offering opportunities to reduce biofuel and bioproduct production costs by converting cheap, readily available waste streams.

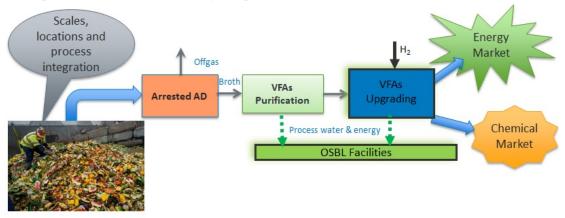


Photo courtesy of National Renewable Energy Laboratory Note: OSBL = outside battery limits facilities

#### OVERALL IMPRESSIONS

- This project provides critical TEA modeling support to the three research projects devoted to developing the arrested AD process. By working closely with these experimental groups and with industry partners, this project will help assess whether the arrested AD process can be economically viable and what particular variables to focus on to achieve viability. Though it is not clear if the model has begun working with experimental data from the research projects yet, there has been an analysis of the base case of biogas production from conventional AD, which is a good comparison to have, as well as a theoretical assessment of performance metrics and energy yields for VFA product generation versus biogas. While the general direction of this project is sound and clear, how the project intends to implement its many activities is a bit vague. There needs to be a specific task list and schedule developed, along with prioritization of these tasks to ensure that as much of the intended work can be performed in the remaining time available and that efforts will be efficiently coordinated with the tasks and schedule of the research teams.
- I like the overall current and future framework. The critical support to the relevant projects—some of those in their review may have been judged as lacking in the TEA—makes this project very useful. The results thus far are not yet providing substantive novel insight, but I expect that to change. Product economics are weak; what are the commercial assumptions for the organic acids? Biogas economics seems skewed towards high prices, which need to be understood lest we provide a biased assessment of the alternatives.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their helpful insights and feedback. Our work is highly integrated with ongoing R&D efforts and with the overall BETO portfolio. Although we have not yet vetted experimental data into the TEA models, we have worked with R&D teams on developing the conceptual process design with all major unit operations, key process parameters for each operation, as well as process integration strategies. To improve input data quality for credible TEA results, we will solicitate feedback from expert stakeholders to seek assistance and industry-relevant input for validating the models, major assumptions, and relevant analysis data. In line with our project goals and approach, we will also perform sensitivity analyses and uncertainty evaluations on key cost drivers based on inputs from subject-matter experts from both industry and R&D teams. Although the focus of the current funding phase is to support and guide arrested AD R&D, the overall goal of this project is to develop defensible studies in support of the WtE platform by identifying R&D opportunities and economic and sustainability targets. By FY 2020, we will report key cost drivers, cost breakdowns, a value proposition over the current approach of disposing wet wastes, and a project path forward to achieve BETO's cost targets for fuels and chemicals. We will also report SOTs for all three projects with vetted research data.

# WTE: FEEDSTOCK EVALUATION AND BIOFUELS PRODUCTION POTENTIAL – NREL

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

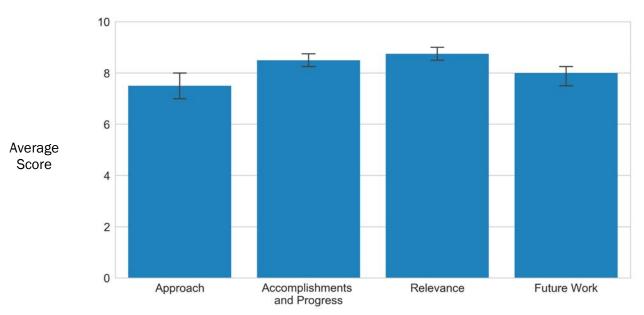
The goal of this project is to provide foundational data, strategic analyses, and modeling critical to the economic and environmental viability of the emerging WtE industry. The project began in the last quarter of FY 2015 to support BETO's objectives in accelerating development of WtE technologies. These technologies offer alternative and sustainable solutions to waste disposal, a growing concern across the nation as the population grows, and could present a niche opportunity for the bioeconomy of the future. Our approach is rigorous economic and geospatial modeling with input from key stakeholders. Accomplishments to date include: (1) a comprehensive estimate of wet WtE resource prices at the county level and

| WBS:                      | 2.1.0.112            |
|---------------------------|----------------------|
| CID:                      | NL0029526            |
| Principal Investigator:   | Ms. Anelia Milbrandt |
| Period of<br>Performance: | 10/1/2017-9/30/2019  |
| Total DOE Funding:        | \$814,000            |
| DOE Funding FY16:         | \$0                  |
| DOE Funding FY17:         | \$0                  |
| DOE Funding FY18:         | \$514,000            |
| DOE Funding FY19:         | \$300,000            |
| Project Status:           | Ongoing              |
|                           |                      |

national state supply curves; (2) preliminary results of a wet WtE resources "hot-spot" analysis; and (3) baseline, AD, and composting pathway models for cost-benefit analysis of food waste (preliminary results have been provided to BETO). Our estimate of wet WtE resource prices indicate that some portion of the feedstock exists at a negative price. If a resource has been commoditized (e.g. fuels, oils, greases [FOG]), its price is determined by market demand. If a resource is regarded as waste, its price is driven by the cost of its disposal. This analysis provides the first estimate of wet WtE resource prices. Our resource opportunity or

#### Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

"hot-spot" analysis indicates that high and very high potential is present in many states and follows population dynamics where fuel consumption is also high. Preliminary results for the cost-benefit analysis of food waste indicate that for a pathway to break even, it requires: (1) a tipping fee, (2) a facility of particular scale (larger facilities are able to offset their costs easier), and to a lesser extent depends on the value of products. Geographic variances in pathways stem from differences in tipping fees, fuel energy prices, and local wages. Project challenges include data availability and quality, which were mitigated by ongoing industry input.

#### **OVERALL IMPRESSIONS**

- As with the corresponding PNNL-based project (2.1.0.113), this project is performing an exhaustive yet essential task in collecting and organizing wet-waste feedstock quantity, location, and cost data down to a regional level. These data are critical in the development of corresponding waste-conversion technologies and the ability to determine where and how the overall cost of biofuel can be minimized by taking advantage of available low-cost wet wastes as feedstocks. The work in this project complements the work being done on the analogous PNNL-based project. The development of resource supply curves and cost-benefit analyses for various wet-waste feedstocks and conversion technologies is informative and the hot-spot analysis maps are particularly innovative. Starting a resource assessment study on MSW components is particularly encouraging in that it would represent a first attempt to characterize this large but underutilized feedstock. It would be helpful to see a specific list of tasks, milestones, and schedule for this project, which would allow one to get a better feel for whether the team has achieved its initial goals and whether there is sufficient time to complete the remaining work. Based on what information is provided, there does not appear to be sufficient time to complete the remaining work before the end of this project at the end of FY 2019. If this is the case, this project should be extended to at least complete the MSW component resource assessment.
- I do strongly believe that this type of project can provide the most significant contributions for the industry. These type of data sets are often inexistent or not widely available. The benefit provided to the industry by this analysis to the industry—an investigation that is difficult to carry out inside a private organization—cannot be overstated. The challenges that WtE has always had is competing with landfilling. Landfill margins are in general quite high, and when presented with the diversion to WtE, landfill operators have often been able to recapture those streams by undercutting the WtE solution to a point where WtE is no longer competitive. While landfill capacity remains high west of the Mississippi River, it is increasingly constrained east of it. Furthermore, changing dynamics in transportation costs are further limiting haulage of waste to distant landfills. It would be useful to overlay these maps to regional landfill locations, capacities, and trends and provide at least a qualitative direction on landfill disposition.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their comments and positive evaluation. Apologies for not including more information on milestones and schedule. The project is scheduled to continue through year 2020, which will allow us to complete all planned work.
- We thank the reviewers for their comments and positive evaluation. We certainly agree with the stated challenges that the WtE industry is facing and we will continue to work towards providing information in support of the industry's further development and decision making. We also agree with the reviewers' recommendation to analyze landfill locations, capacities, and trends; it is currently ongoing under the cost-benefit analysis task.

# WTE: FEEDSTOCK EVALUATION AND BIOFUELS PRODUCTION POTENTIAL – PNNL

#### **Pacific Northwest National Laboratory**

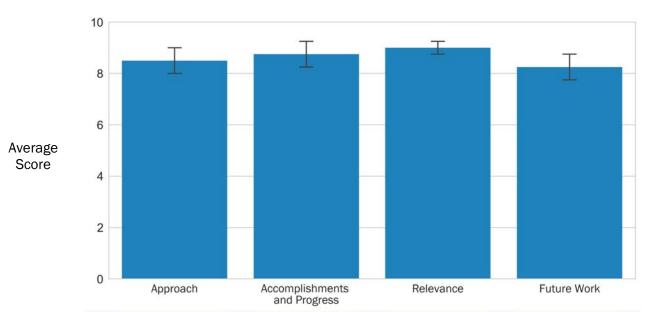
#### **PROJECT DESCRIPTION**

Waste is a liability, but it is also an underutilized source of carbon that could be diverted to renewable fuels and products. Which wastes offer the best value propositions (e.g., availability, existing collection infrastructure, ease of conversion, result in high-quality fuels)? What are the tradeoffs inherent to WtE enterprises? This project provides foundational data, modeling, and analyses to enable a nascent WtE industry to capitalize on the national, renewable stockpile of underutilized organic wet wastes.

The Biomass Assessment Tool (BAT), a high-resolution modeling platform developed with BETO support, was used to import site-specific waste resource data and pose

| WBS:                      | 2.1.0.113           |
|---------------------------|---------------------|
| CID:                      | NL0029527           |
| Principal Investigator:   | Dr. Timothy Seiple  |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$692,051           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$392,051           |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | Ongoing             |
|                           |                     |

WtE enterprise questions. Recent outcomes include assessment of wet WtE resources, estimated at approximately 76 million dry tons per year (MDT/yr), of wastewater sludge, animal manure, FOG, and food waste distributed among 56,000 sites. Using HTL as a proxy for thermochemical wet feedstock conversion, these wet wastes have annual average production potential of 5.6 billion diesel gallons equivalent.

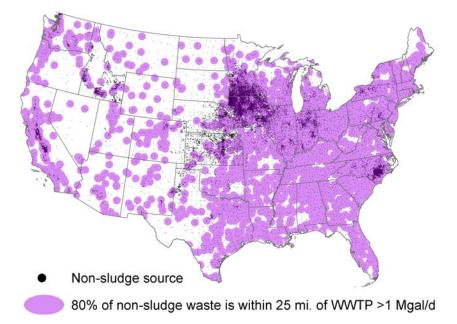


#### Weighted Project Score: 8.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

Current efforts include development of cost-benefit and feedstock blending analysis tools to (1) compare alternative wastewater solids treatment options to maximize energy recovery, minimize waste and disposal costs, and quantify cost-effective feedstocks; and (2) assess impacts of feedstock aggregation and blending on HTL biocrude yield, to provide "optimal" blending strategies based on biochemical composition for a given regional feedstock inventory. An illustrative finding from this work is that using 2017 solids treatment costs and 10-year average biofuel revenue conditions, HTL could economically utilize 11 MDT/yr of sludge, produce 1 billion diesel gallons equivalent, and reduce solids treatment and disposal costs by \$1.5 billion per year from current practice.



## Wet wastes are highly co-located

Photo courtesy of Pacific Northwest National Laboratory Note: WWTP = waste water treatment plant, Mgal/d = million gallons per day

#### **OVERALL IMPRESSIONS**

• Because of the importance in understanding feedstock distribution and availability and because of the impact feedstocks have on the overall biofuel cost, the resource assessment work described in this project is critical to developing cost-effective biofuels. There is a tremendous amount of regional data that have to be uncovered, sorted, and processed in a project like this, so it is impressive to see what has been accomplished so far for wastewater solids as a feedstock. The insight gained on HTL economic feasibility and the economic comparison of HTL to AD are very valuable and show the considerable advantages that HTL has for handling sludge and for the wastewater utility industry, also justifying further development to commercial scale. Blending study results are consistent with those obtained by the HTL experimental and TEA teams but provide additional insight into what feedstocks are available and how blending might be accomplished on a regional level. It would be helpful to see a specific list of tasks and milestones for the remaining duration of this project so that it will be clear exactly what activities will be performed under the given broad topics (e.g., characterizing manure feedstock) and when they will be finished. There are so many directions in which one can go with the feedstock data developed in this project that there needs to be a clear, agreed-upon path forward.

• The systemic modeling exercise has intrinsic value, as they provide unique insight into a problem even when the final and actual solution may differ than what the model predicted. The comparison between HTL and AD is particularly insightful as it identifies a strong justification for the continued development of the technology. Internal economics (e.g., transportation) are not fully developed or at least explained in the presentation. Lastly, I would desire to see an effort in identifying possible externalities that may impact the system. For instance, an AD system in confined animal feeding operations provides a variety of ecological or environmental services, which are the main reason for their deployment. Examples of ecological or environmental services include odor control, nutrient management, water management, and solid recycling, with energy recovery being a desirable cost offset but not in most cases the primary driver. It essential that a way to assess these values and to ensure that they are maintained is considered in future work within this project or any possible follow up. The project is nonetheless a valuable contribution as it highlights and justifies, as already mentioned, continued work into the emerging HTL technology.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their time and critical review.
- To summarize the overall project, and context for current work, we previously focused on assessing feedstock quality and quantity for priority wet-waste sources, including sludge, manure, food waste, and FOG. Next, we assessed economically sustainable sludge feedstocks, blending potential and blend optimization. We are now quantifying economically sustainable manure feedstock sources and magnitudes and estimating the minimum feasible deployment scale of standalone on-farm HTL, with comparison to AD. These activities are all a precursor for a comprehensive economic, optimized blending and biorefinery integration assessment. The following milestones are defined for the remainder of the project:
  - o Characterize manure systems for manure source terms (March 31, 2019; complete)
  - Develop a national-scale cost model (June 30, 2019)
  - Quantify sustainable manure sources, magnitudes, and scale (September 30, 2019)
  - Assess feasible waste aggregation, blending, and biorefinery integration (September 30, 2020).
- We agree that many internal economic assumptions are encapsulated in the data and models. A lot of work went into retaining spatial, temporal, and operational realism at the site, regional, and national scales. Our complete methodology and results will be in a peer-reviewed journal publication with downloadable detailed supplemental material.
- We will consider different strategies for waste aggregation for blending, by transporting either raw material, bio-oil, or a mix of both, depending on scale. We will model transportation logistics in the next phase to develop more realistic service areas.
- We agree with the reviewers that the externalities associated with WtE projects should be considered. As a follow-on, we have submitted a multi-lab proposal to develop a triple bottom line accounting framework to capture the value of ecosystem services provided by WtE technologies such as HTL.

# ANALYSIS AND SUSTAINABILITY INTERFACE

#### Pacific Northwest National Laboratory

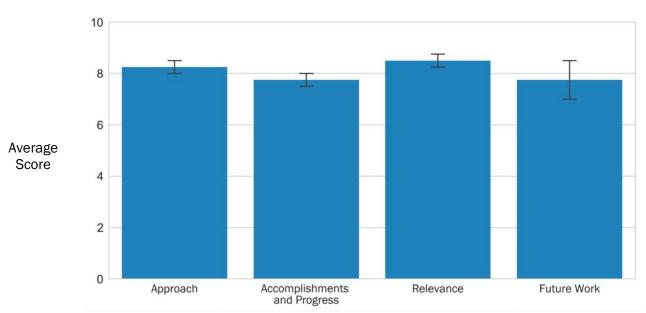
#### **PROJECT DESCRIPTION**

This project provides TEA and LCA for biomass conversion routes to hydrocarbon fuels and chemicals in order to direct research towards high-impact results. Targeted conceptual biorefinery models are developed with researcher input and compared against benchmark models that incorporate currently achieved research results. This (1) identifies barriers, cost-reduction strategies, and sustainability impacts; (2) helps set technical and costs targets; and (3) tracks research progress.

While this project provides analysis support in several biomass conversion research areas, the focus of this

| WBS:                      | 2.1.0.301           |
|---------------------------|---------------------|
| CID:                      | NL0019451           |
| Principal Investigator:   | Ms. Sue Jones       |
| Period of<br>Performance: | 10/1/2016-10/1/2019 |
| Total DOE Funding:        | \$3,052,813         |
| DOE Funding FY16:         | \$875,000           |
| DOE Funding FY17:         | \$925,000           |
| DOE Funding FY18:         | \$727,813           |
| DOE Funding FY19:         | \$525,000           |
| Project Status:           | Ongoing             |
|                           |                     |

presentation is on TEA support for the wet-waste HTL and biocrude upgrading pathway. Building on extensive work with wood and algal feedstocks, HTL testing of municipal wastewater treatment plant sludges shows promising results in terms of fuel yields and quality. An added advantage is that this waste stream is a zero-cost, reactor-ready feedstock that is currently available and requires little preprocessing. The technology has garnered much interest from industry as an attractive future solution to current sludge management and disposal challenges.



#### Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

A goal case design projecting research targets achievable by 2022 for the HTL and biocrude upgrading pathway was published in 2017, and the first SOT assessment was developed in FY 2018 to baseline progress to date and guide research and track advancement toward the goal. A key aspect to success is the continual integration of the experimental and analysis team's effort to define and target the research that will most significantly reduce cost while meeting sustainability goals. Research areas identified from this effort that are needed to achieve the target minimum fuel selling price include improved upgrading throughput rates and catalyst life, improved efficiency (reduced capital) for the HTL heat exchangers, and increased sludge feed solids content and biocrude yields.

In addition to the wet-waste HTL task, another specific key outcome of this project was the support for meeting the 2017 BETO goal, "by 2017, validate an n<sup>th</sup> plant modeled minimum fuel selling price of \$3/GGE (2014\$) through a conversion pathway to hydrocarbon biofuel with greenhouse gas emissions reduction of 50% or more compared to petroleum-derived fuel." This was met by working closely with LanzaTech and the PNNL team, who developed and demonstrated the technology to convert syngas to fuels and chemicals. Idaho National Laboratory (INL) provided feedstock costs and a life cycle inventory was provided to ANL for the greenhouse gas emissions calculations. In a similar way, the wet-waste HTL analysis task is directed towards meeting BETO's 2022 cost-reduction goals for fuel production.

Data availability is a common challenge for all analysis projects. This is mitigated by frequent, close interactions with researchers to exchange information and review sustainable cost-reduction strategies. Collaboration with analysts at ANL, INL, NREL, and Oak Ridge National Laboratory (ORNL) enhance project effectiveness. Frequent communication with BETO technology leads ensures impactful outcomes. Disseminating results for use by stakeholders is achieved through publications and presentations.

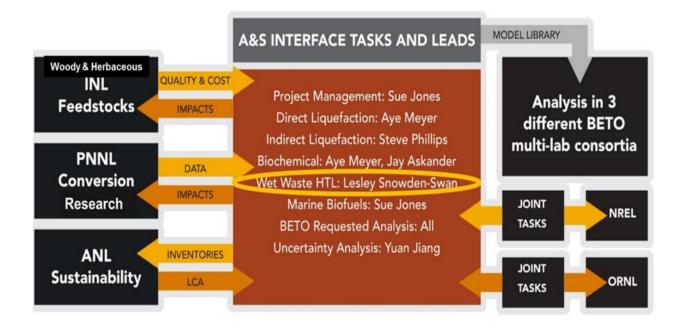


Photo courtesy of Pacific Northwest National Laboratory

#### OVERALL IMPRESSIONS

- This project demonstrates the value and importance of incorporating TEA modeling with experimental research work. The work in this project complements the PNNL HTL experimental work on wet wastes nicely and provides a pathway to identify the parameters that may have the biggest impact on overall biofuel cost and therefore justify further research attention. While predicted results do not always match reality, the approach described and being implemented in this project to verify and inform research is likely the most efficient way to converge on the BETO overall biofuel cost target of \$3/GGE. The preparation of yearly SOTs starting in 2018 will provide a yearly benchmark to assess how close the team is to achieving the BETO target. This project, which is scheduled to end at the end of FY 2019, has clearly demonstrated its value and deserves to be continued.
- Overall, I like the project and the modeling framework presented is undoubtedly of value and worth further development. However, it may be overambitious for the time left, and while the important insight on cost reduction of hydrotreating is very valuable, it should be further developed in detail.
- Overall a really good project, providing insight into the economic trajectory necessary for HTL of wet waste to be an economically successful fuel.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We very much appreciate the reviewers' time and efforts in providing critical evaluation and valuable feedback for this project.
- We may have inadvertently communicated in the "Future Work" slide that the wet-waste HTL task within the project is ending this year along with other parts of the project. However, the intent is to propose that this work continue in a new three-year project to focus on this pathway through FY 2022, when the technical and cost goals for the pathway are expected to be met.
- While it was difficult with the time allotted to present the details of the models, a table of primary inputs and assumptions could have been presented to provide the reviewers more background. In addition, the design case and other publications will be referenced for providing the details of the model.
- The lifecycle carbon intensity is evaluated for each pathway and integrated into the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model. Revenue streams from renewable fuel program credits are not included in BETO pathway TEAs in order to avoid overestimating the future economic potential when such programs may not exist. However, the need to include biofuel credits in the economics was echoed by several in the audience who feel it is unfair to ignore this potential revenue stream, and somewhat counterproductive because these programs are specifically intended to help foster new technology commercialization.
- The missing feedstock cost category has been brought up by our industry partners and perhaps deserves revisiting based on the reviewer's comment. A possible way to manage this in future work is to present an additional graph of feedstock cost versus minimum fuel selling price in the BETO Multi-Year Plan, to represent the avoided cost that would be incurred by a wastewater treatment plant today, as well as the variability that exists.
- We are currently investigating methods and associated costs for removal and recovery of nutrients from the waste streams, including ammonia nitrogen from the HTL aqueous phase and phosphorus from the HTL ash/solids.

# **BENCH-SCALE HTL OF WET-WASTE FEEDSTOCKS**

#### **Pacific Northwest National Laboratory**

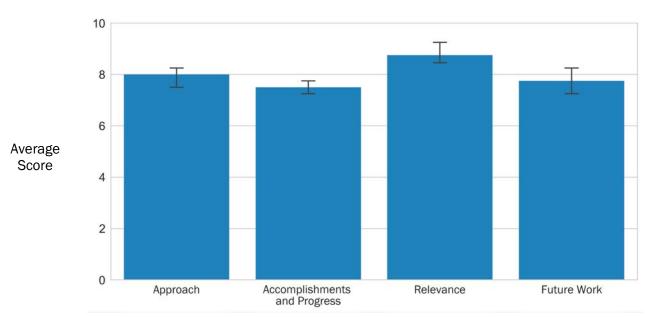
#### PROJECT DESCRIPTION

Waste is a liability, but it is also an underutilized source of carbon that could be diverted to renewable fuels and products. Sewage sludges and manures are high-moisture, high-ash feedstocks that benefit from robust wetprocessing technologies such as HTL. Early-stage R&D is essential for understanding wet feedstock performance and blended feedstock behavior, as well as options for aqueous-phase treatment and/or recycling.

PNNL has adapted HTL operations and cultivated relationships with industrial partners needed to advance the HTL pathway for wet-waste feedstocks, resulting in reduced overall conversion cost, improved sustainability,

| WBS:                      | 2.2.2.302           |
|---------------------------|---------------------|
| CID:                      | NL0034882           |
| Principal Investigator:   | Mr. Justin Billing  |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$360,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$O                 |
| DOE Funding FY19:         | \$360,000           |
| Project Status:           | Ongoing             |
|                           |                     |

and decreased technological risks for industrial partners in support of BETO's mission to reduce technological costs and risks. Experiments are designed to develop foundational understanding of HTL conversion to biocrude, catalytic biocrude upgrading, and aqueous-phase treatment technologies, and to generate data packages for the Analysis and Sustainability project, which reports the annual SOT for the HTL of the sewage sludge pathway. In turn, future research is identified and prioritized from SOT modeling and TEA such that areas of greatest impact and highest technical risk are addressed first.



#### Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

Feedstock selection is guided by the WtE resource assessment project, a PNNL and NREL collaboration. Geospatial representation of feedstock availability highlights sites and regions where resources may support the scale of operations required for commercialization. Testing selected feedstocks at the bench scale provides valuable feedback on the biofuel production potential of a given resource and refines the assumptions of the resource assessment. Bench-scale testing also helps screen and qualify feedstocks for the Hydrothermal Process Development Units project.

Recent findings indicate that yields up to 45% of energy-dense biocrude can be produced from sewage sludge with significant ash content (up to 30%). Streams of underutilized FOG such as wastewater scum can be blended into sewage sludge to boost yields even more. Much of the technology development on algal feedstocks has been found to apply to wet-waste feedstocks, including strategies for catalytic upgrading of the biocrude. If low-cost wet-waste feedstocks perform as well on the HTL platform, there is a real opportunity for scale-up and deployment.

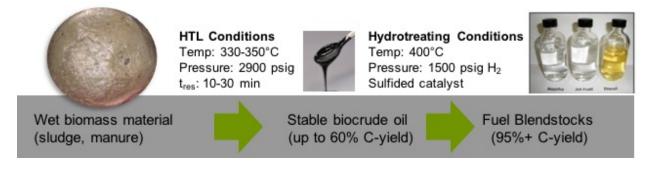


Photo courtesy of Pacific Northwest National Laboratory

#### **OVERALL IMPRESSIONS**

- This project, which utilizes a wet-waste feedstock for conversion to liquid biofuels through HTL, represents an ideal pathway for meeting many of BETO's most significant goals. In trying to achieve the elusive \$3/GGE biofuel cost target, the use of waste feedstocks eliminates the feed cost (or creates an even better situation with a negative cost) from the overall fuel cost. The use of HTL technology eliminates the relatively expensive costs to dry and extract particular components from the feed. The close coupling of experimental and modeling work as demonstrated in this project is critical to helping target research on parameters and threshold values most critical to the overall cost. As a whole, this project represents a methodical, efficient approach to reducing the remaining production costs as they strive to reach the BETO target. The fact that there are plans for the construction and demonstration of two HTL pilot-scale systems outside of this project further demonstrates the level of maturity and interest by external customers. While there were relatively limited test data reported at the current time, the project as currently defined has only been in existence for about five months and has a total duration of only one year. Because the mechanism and management appear to be set in place for significant advancements in HTL technology, the project duration should be extended to allow several research/modeling cycles to occur to see if the results live up to the potential.
- HTL has several exciting characteristics, as it can handle wet or watery streams and provide a liquid feedstock suitable for direct hydrotreating into fuel or a fuel blendstock. While the integration of all the various components is not trivial, HTL is undoubtedly better suited to WtE than fast pyrolysis. While still in its infancy compared to AD, HTL has potential benefits that justify this effort. Work at the bench scale with a variety of feedstocks is critical. Experimentally, this work appears to be quite good. I see several weaknesses in the analysis part, especially as it pertains to the impact to the TEA and the boundary interaction with other technologies, such as hydrotreating, which could be used to directly treat

some of the feedstocks (e.g., FOG) identified as a blendstock. Some of the numbers are a bit overoptimistic in real life, while technically correct (e.g., carbon fuel yield). Is the use of HTL bio-oils directly as fuel for combined heat and power feasible?

• As a non-engineer or chemist, I appreciate the introduction to HTL.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for a thorough evaluation of the HTL technology as applied to wet-waste feedstocks and plan to propose continuing research in accordance with the recommendation to extend the project duration.
- The HTL team thanks the reviewer for recognition of the importance of continued bench-scale research and for correctly assessing the opportunity available for the conversion of wet waste. Using wastewater treatment plant scum (FOG) as a feedstock blend is one option to increase yield but scum addition is not integral to the process and will be responsive to the site-specific market conditions. HTL biocrude could likely be combusted or co-combusted for combined heat and power but our project focus is aligned with the BETO goal of advanced liquid transportation fuels from wet-waste feedstocks.
- We are thankful for the question about combined heat and power, as this question comes up frequently in discussion with wastewater treatment plant operators whose primary interest is sludge disposal and secondary interest is heat, electricity, or natural gas for reuse onsite, or renewable natural gas credits in the case of natural gas. The small and distributed nature of wet-waste resources might drive pioneering projects to consider routes besides catalytic upgrading because downscaling a standalone hydrotreater is not economical and the path to refinery coprocessing may not be established. In time, increasing regional production of HTL biocrude may support a standalone hydrotreating unit and/or the path to coprocessing will be better defined.
- We appreciate the time and effort required of the reviewer to learn and evaluate WtE technologies such as HTL.

# ARRESTED METHANOGENESIS FOR VOLATILE FATTY ACID PRODUCTION

#### **Argonne National Laboratory**

#### **PROJECT DESCRIPTION**

This project supports BETO's mission to develop new technologies that produce biofuels and products from nonfood U.S. feedstock resources such as agricultural residues and wet waste (e.g., food waste). We rewire the dark fermentation process to produce short-chain organic acids through arrested methanogenesis. The proposed technology has the potential to make a substantial contribution to BETO's advanced biofuel pathway portfolio.

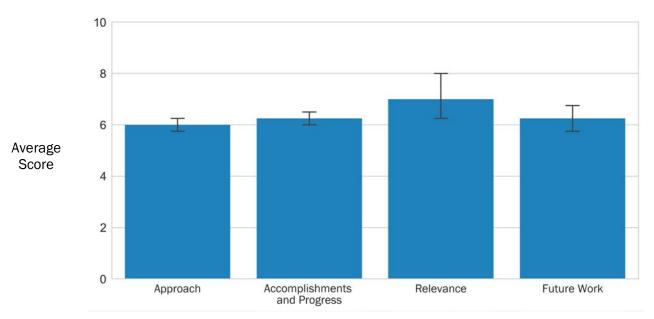
The project objectives are to (1) define concepts and develop tools to transform low-value or negative-value high-strength organic waste streams into high-value short-chain organic acids (C2–C6); (2) rewire the dark

| WBS:                      | 2.2.4.100                     |
|---------------------------|-------------------------------|
| CID:                      | NL0026648                     |
| Principal Investigator:   | Dr. Meltem Urgun-<br>Demirtas |
| Period of<br>Performance: | 10/1/2015-9/30/2020           |
| Total DOE Funding:        | \$2,300,000                   |
| DOE Funding FY16:         | \$750,000                     |
| DOE Funding FY17:         | \$550,000                     |
| DOE Funding FY18:         | \$500,000                     |
| DOE Funding FY19:         | \$500,000                     |
| Project Status:           | Ongoing                       |
|                           |                               |

fermentation process to produce organic acids via arrested methanogenesis sustainably; (3) regulate acidogenic metabolism toward enhanced organic acid production; (4) establish highly efficient, robust, and productive community structures for organic acid production; and (5) develop new arrested AD technologies (a.k.a. the carboxylate platform). Our ultimate goal is to develop new AD technologies from a proof of concept, TRL 2 to TRL 4 at the end of three years of project duration to produce organic acids continuously at a titer of 12.5 g/L

#### Weighted Project Score: 6.4

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

in 200-gallon digesters. We have been developing a new high-rate arrested AD process for transforming organic waste by supplanting starch, sucrose, or glucose currently used as feedstock into organic acids. We design and construct an anaerobic membrane bioreactor technology to produce and separate organic acids from the fermenters to facilitate high product yield, minimize the toxicity of organic acids, reduce mass transfer limitations, and ensure the health, stability, and productivity of AD communities.

This research specifically determines the links between organic wastewater characteristics, microbe community structure, and the design and operation of high-rate arrested AD system at the bench scale. Specific research targets include the isolation and integration of highly diverse microbial functionalities within high-rate arrested AD fermenters for high-strength organic wastewater treatment coupled to renewable chemical production. We started with wastewater streams generated at dairies and breweries as initial carbon sources because of their high carbon content and biodegradability.

The outcome of this project is a new cost-effective AD technology at TRL 4 at the end of the project. Additionally, this technology is appealing because it has the potential to produce high-value chemicals without competing either directly or indirectly with food or animal feed production.

#### OVERALL IMPRESSIONS

- This project is one of several looking at arrested AD in which the conventional AD process mechanism is stopped at the VFA production step rather than going on to produce methane. Thus, the focus is on producing intermediate chemical products rather than biogas, which generally results in a product of greater value. The concept is a good one and this project has generated quite a bit of good data on microbial consortia that will deliver the VFA concentrations near target levels under a variety of operating conditions and feedstocks at the bench-scale level, even though it is not entirely clear how the methanogenesis step is being shut down. As a result, the project has proven the arrested AD concept for generating VFAs, at least during short-term operation. Data on separation of VFA products are not as encouraging at the present time, and it is not clear what methods will be further investigated and/or used in larger-scale systems. Without knowing what the actual market value of the low-carbon VFA species being generated is (relative to the base case of biogas generation), difficulty in isolating the desired product(s) may result in a process that is not economically viable. An additional concern with this project is that two scale-ups will need to be performed and demonstrated in the remaining year and a half of the project duration, which may be difficult to achieve even with an industrial partner on board.
- This is one of several projects looking at arrested AD to produce higher-value products. I think the choice of reactor configuration may limit its relevance if scaled up to low dissolved solids streams, a relatively smaller subset of wet wastes. Furthermore, ion exchange resin for organic acid separation is an expensive approach for a mixed stream of chemical commodities. The economic value is only in a small subset of organic acids, and the lack of TEA makes it difficult to evaluate its relevance.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Methanogenesis was inhibited by following different methods: acid and heat treatment of inoculum, increasing organic loading rate and reducing hydraulic and sludge retention times, as well as running the digesters at pH ≤ 6.0 instead of an optimum pH range of 6.5–7.5. Increasing the loading rate and reducing the retention time was done to washout any slow-growing, methane-producing bacteria and archaea. Additionally, high concentrations of organic acids and salts inhibit the growth of methanogens in the digester environment. Please see the presentation for more information.
- For the separation of acids from the fermenter broth, ion exchange resins and membranes are currently being used at industrial-scale applications. Resins and membranes were purchased from the manufacturers (e.g., Dow and GE). The scalability of the tested separation technologies is not an issue because they're currently at the field scale. For example, reverse-osmosis membranes are used for recovery of acetic acid from the petrochemical plants and food production plants.

- Our project is guided by the outcomes of TEA conducted by NREL (PI: Tao; 2.1.0.111) The TEA is used to synergize research from waste collection and handling to VFA production, purification, and utilization (e.g., platform chemicals). The project team will provide results of the detailed process modeling and simulation efforts to NREL. NREL's integrated approach will project cost potentials and research targets from an overall economic point of view. This is to determine titer, yield, productivity, and recovery targets necessary to produce an economically viable organic acid production for various applications and uses. In order to answer critical questions such as "At what R&D level would the proposed technology make economic sense?" we will perform sensitivity analyses and provide contour plots of economics for key matrices or cost drivers. We will outline barriers, highlight R&D needs for conversion and separation strategies, and provide critical inputs to successfully approach \$2/GGE. These key findings will then be informed to the R&D team and BETO.
- AD and membrane-based technologies are very well known and can be easily scaled up from bench to pilot scale. The project team believes that three years of project duration would be sufficient to scale up the modular AD technology.
- As described in the presentation, two different reactor configurations specifically sequencing batch anaerobic reactor and anaerobic membrane reactor have been developed. This was done due to wastestream characteristics and application points and sizes of the new AD at the utilities and facilities.
- We partially agreed with the reviewer's comment. Ion exchange resins were purchased from commercial resin manufacturers. These resins have been used for organic acid separation at field scale. TEA of organic acids is also a part of NREL's project (2.1.0.111).

# BIOGAS-TO-LIQUID FUELS AND CHEMICALS USING A METHANOTROPHIC MICROORGANISM

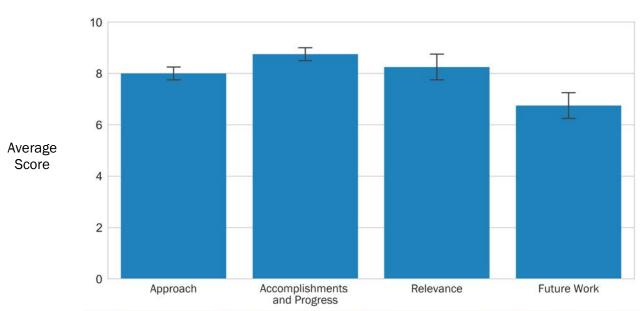
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

Biogas derived from anaerobic digestion of waste streams such as biorefinery wastewater, animal, agricultural, and MSW offers a versatile renewable energy source. Total domestic methane potential from landfill material, animal manure, wastewater, and organic waste is estimated to be greater than 4 quadrillion British thermal units (Btu). Additionally, biogas generated from AD of lignocellulosic biomass resources is estimated to offer 4 quadrillion Btu potential energy. This energy potential could displace nearly half of current domestic natural gas consumption in the electric power sector and all current natural gas consumption in the transportation sector. However, despite the promise of biogas as a high-volume, renewable energy

| WBS:                      | 2.3.2.102           |
|---------------------------|---------------------|
| CID:                      | NL0026680           |
| Principal Investigator:   | Dr. Mike Guarnieri  |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$1,515,008         |
| DOE Funding FY16:         | \$250,000           |
| DOE Funding FY17:         | \$400,000           |
| DOE Funding FY18:         | \$465,008           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

source and natural gas replacement, its gaseous state prevents facile integration with extant transportation and industrial infrastructure. At present, biogas is primarily flared or used to produce combined heat and power. Alternatively, AD biogas can be scrubbed for conversion to biomethane that can, in turn, be utilized as a renewable option in natural gas applications.



#### Weighted Project Score: 7.9

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

Microbial conversion of biogas to liquid fuel and chemical intermediates using natural methane-consuming bacteria (methanotrophs) offers valorization potential. However, biogas biocatalysis is currently limited by low conversion efficiencies and incomplete biogas utilization. The development of a biocatalyst capable of high-efficiency co-utilization and conversion of methane (CH<sub>4</sub>) and CO<sub>2</sub> would allow for complete utilization of biogas streams, significantly improving process economics and enhancing carbon conversion efficiency to target products. Additionally, development of a CH<sub>4</sub>/CO<sub>2</sub> co-utilizing biocatalyst would dramatically shift the landscape of carbon capture and conversion pursuits, providing a novel, photosynthesis-independent  $CO_2$  biocatalyst.

The Biogas Biocatalysis annual operating plan aims to develop a carbon- and energy-efficient biogas bioconversion process via rational, techno-economic-informed strain and fermentation engineering strategies. Specifically, we will evaluate mechanisms of  $CH_4$  and  $CO_2$  utilization in phylogenetically diverse methanotrophs and leverage those learnings to develop an industrially relevant biocatalyst capable of  $CH_4$  and  $CO_2$  co-utilization. Concurrently, this project targets the development of methanotrophic biocatalysts with broad product suite capacity through rational metabolic engineering and adaptive laboratory evolution strategies. The resultant methanotrophic biocatalysts will provide a direct path to improve process economics and efficiency of lignocellulosic biorefineries and standalone AD infrastructure.

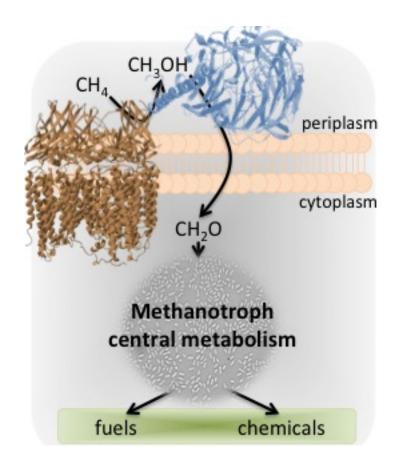


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• This project looks to improve on conventional AD in two ways: (1) by converting relatively low-value biogas to higher-value liquid chemical products (e.g., organic acids) and (2) co-utilizing CH<sub>4</sub> and CO<sub>2</sub> in

the biogas conversion to liquid products, thereby increasing the carbon efficiency. These improvements all revolve around genetic engineering of methanotrophs, guided by TEA modeling, to achieve the target goals. The results so far have been impressive, with significant achievements made in organic acid product titer, rate, and yield and in modified microbes with enhanced CO<sub>2</sub> uptake capabilities. The collaboration among academia and industry stakeholders is also encouraging. Although future work has not been as clearly articulated as it could be, continued research on improving methanotroph strains to produce higher chemical product yields while utilizing more of the total carbon in the biogas, along with continued informed guidance from TEA modeling and sensitivity analysis, will help further enhance the viability of this work.

• In the last several years, we have seen increased interest in the development of processes based on methanotrophic organisms given the abundance of inexpensive natural gas as a carbon source. Adding to that the ability to directly use CO<sub>2</sub> makes the work on methanotrophs of even higher relevance for biogas, as it both increases the carbon efficiency of the waste feedstock transformation and has other process benefits such as reducing the need for expensive biogas treatment or accepting a diluent in the feedstock stream. Gas fermentation remains intrinsically challenging and much work remains to be done before a viable pathway to commercialization can be demonstrated. Nonetheless this is work of great value as it tackles and provides insights on the fundamental issue of general industrial value.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their positive and encouraging feedback. As noted by the review panel, we feel the development and deployment of methanotrophic biocatalysts with complete biogas substrate utilization and broad biosynthetic capacity will have a significant impact upon the burgeoning methane bioconversion space, as well as a substantial impact on the BETO WtE platform.
- We agree with the reviewers' assertion that gas fermentation remains intrinsically challenging. Though gas fermentation reactor development is outside the scope of this project, it is our hope that the development of robust methanotrophic biocatalysts with maximal C1 carbon conversion capacity will minimize the technical barriers associated with the microbial component of gas fermentation. To this end, our metabolic engineering efforts have generated the most carbon-efficient methanotrophic biocatalyst reported to date, possessing CH<sub>4</sub>/CO<sub>2</sub> co-utilization capacity.
- The development of enhanced methane biocatalysis strategies offers a means to expand BETO's feedstock portfolio and represents a significant commercial opportunity to deploy WtE technologies. Additionally, the methanotrophic bioconversion strategies under evaluation have the potential to enhance the economics and sustainability of lignocellulosic refining as a bolt-on technology. To this end, future efforts will explicitly target cost reductions and yield enhancements to lignocellulosic refining via coproduction of high-value coproducts derived from wastewater AD biogas. Continued metabolic engineering and TEA efforts to identify the performance metrics required to incur a net economic and life cycle benefit will be pursued. Additionally, fundamental research targeting enhanced CH<sub>4</sub>/CO<sub>2</sub> co-utilization will continue to be a core focus of our work. Our team is excited to continue these efforts and looks forward to continued progress in the development of a viable biological biogas conversion platform.

# SEPARATIONS IN SUPPORT OF ARRESTING ANAEROBIC DIGESTION

#### National Renewable Energy Laboratory

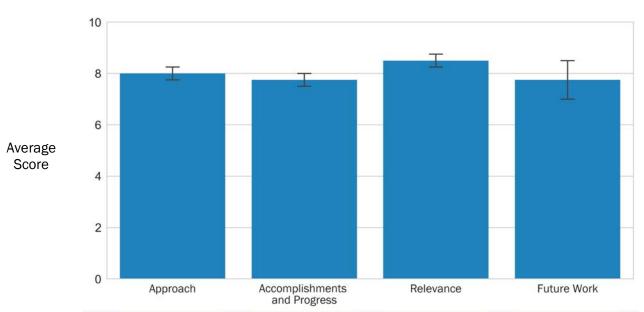
#### PROJECT DESCRIPTION

In support of BETO's interest in converting waste feedstocks to fuels and chemicals, this project aims to develop and demonstrate a system for the production of platform carboxylic acids by arresting AD of wet-waste feedstocks. The project addresses three key technology barriers in developing the bioeconomy, specifically (1) feedstock availability and cost, (2) selective separation of organic species, and (3) first-of-a-kind technology development. The project has been operational for 1.5 years of its planned 3-year timeline and is currently on track.

| WBS:                      | 2.3.2.107           |
|---------------------------|---------------------|
| CID:                      | NL0033407           |
| Principal Investigator:   | Dr. Eric Karp       |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$500,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$250,000           |
| DOE Funding FY19:         | \$250,000           |
| Project Status:           | Ongoing             |
|                           |                     |

In the existing lignocellulosic biorefinery model,

feedstocks typically account for 60%–70% of the produced biofuel cost. This feedstock cost can be overcome through the use of waste feedstocks that are cost advantaged or often cost negative (e.g., MSW, food waste). However, only recently have chemical products other than methane been the subject of R&D from the AD of waste. In an anaerobic digestor, a nonsterile microbial consortium converts waste through a series of four steps: (1) hydrolysis, (2) acidogenesis, (3) acetogenesis, and (4) methanogenesis. Each step occurs sequentially and is thermodynamically downhill in energy from the previous step. Accordingly, the process is driven continuously because the final methane product leaves the system as a gas.



#### Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb I}$  One standard deviation of reviewers' scores

This project aims to produce platform carboxylic acid chemicals by the *in situ* product recovery (ISPR) of VFAs that are produced during anaerobic digestion in step 2 above. To achieve this, work within this project is designing and building a first-of-a-kind ISPR system to recover neat VFAs as they are produced, and work focusing on the biological aspects of the AD unit are also undertaken to identify feedstocks, conditions, and cultures that are most appropriate to facilitate VFA production.

Key results from the project are that in order for the ISPR system to work, the AD unit must operate at a pH less than 5 and reach steady-state titers greater than 17 g/L. This places pressure on the culture to operate in low-pH environments. Results from serum bottle experiments and semicontinuous cultures have shown that a nonsterile culture can achieve these operational targets provided a readily digestible feedstock is used, as the hydrolysis step is the rate-limiting step in AD. Work is continuing to identify ideal feedstocks and cultures for these operational parameters and to integrate the ISPR system with a VFA-producing AD unit. Currently, the ISPR system has been demonstrated with mock cultures matching the VFA profiles measured from the semicontinuous culture and the AD unit has met the required operational targets. In the following 1.5 years of the project, the ISPR system is being adapted to handle higher solids content usually found in AD units and the AD unit will be integrated for a demonstration of *in situ* production purified VFAs.

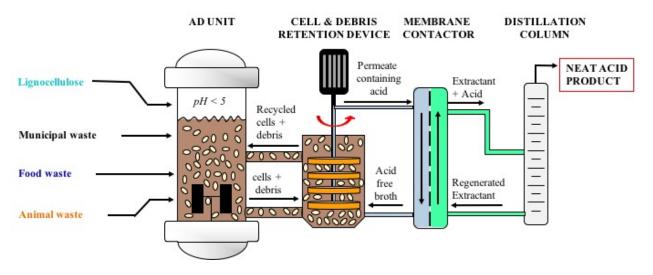


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

• This is one of several projects focusing on the development of arrested AD for bioproduct generation instead of biogas. Splitting the project up into two parts (biology and separations technology) under separate control makes sense because these are the two areas where work is needed for this technology development. It appears that notable progress has been made so far on this project in terms of microbe culture choice for verifying the concept of VFA product generation, demonstrating 90% recovery of VFA products in a model of the proposed separations system and verification of flash drum behavior. The remaining work of completion of assembly of an integrated, functioning system that can meet predetermined VFA targets is reasonable and logical for assessing the full viability of the arrested AD concept. A critical demonstration will be to show long-term stable operation and a stable microbe community while being able to continuously remove VFAs before they can be transformed to methane. A discussion on the actual current market value of the low-carbon VFA species being targeted relative to the base case of biogas generation in conventional AD is not provided, but should be because it is important in assessing whether the cost of the arrested AD process being developed has a chance at being economically viable.

• Overall one of the more game-changing projects I saw in the review, due to the ISPR technology.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The information on the TEA of this and other projects was presented separately in an analysis presentation following this presentation. That task is WBS 2.1.0.111.

# REVERSING ENGINEERING ANAEROBIC DIGESTION OF WET WASTE FOR BIOFUELS INTERMEDIATES AND BIOPRODUCTS

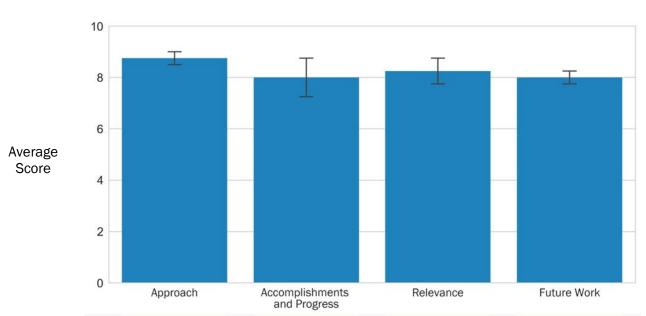
#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

The project addresses BETO's increasing interest in conversion of wet waste to fuels and chemicals through anaerobic digestion by targeting increased hydrolysis of lignocellulosic wet wastes. Typical mass conversion in anaerobic digesters is on the order of 40%–60%, leaving a significant fraction of the feedstock underutilized. With the primary exception of FOGs, many wastes contain significant fractions of lignocellulosics, which are disproportionately under-converted in standard AD processes, as other carbohydrates, lipids, and proteins are much more readily digested. Cellulose contents range from 13%–37% for manures, 20%–35% in sewage, and 40%–60% for MSW. Food service waste ranges from 2%–17%

| WBS:                      | 2.3.2.108           |
|---------------------------|---------------------|
| CID:                      | NL0033408           |
| Principal Investigator:   | Dr. Steve Decker    |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,000,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$500,000           |
| DOE Funding FY19:         | \$500,000           |
| Project Status:           | Ongoing             |
|                           |                     |

cellulose, with food processing wastes running much higher: approximately 35% cellulose in cattle rumen fiber and approximately 25%–35% in citrus waste. Depending on the digester and feedstock, 50%–70% of the cellulose may remain unconverted, representing a significant fraction of lost yield and potentially high-value cellulosic biofuel (D3) renewable identification number (RIN) credits.



#### Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

Advances in hydrolysis of lignocellulosics in wet waste provides significant potential enhancements that will provide social and economic drivers for wet-waste conversion, including:

- Faster conversion rates for reduced footprint and capital costs
- Greater extent of hydrolysis for reduced waste volume, higher yield and titers of product, and increased D3 RIN credit potential
- Expanded feedstock range, reducing landfill volume and increased flexibility
- Applicability in many cases to both methanogenic and acidogenic anaerobic digestion.

This project is approximately 50% through its planned three-year timeline. During this time, we have developed collaborations with multiple industrial partners in the brewing, food processing, and water treatment industries. We have focused our efforts on digesting cattle rumen fiber (i.e., "paunch") more effectively while focusing on reducing methane production and increasing VFA product titers. Rumen fiber is highly lignocellulosic and difficult to digest, so improvements will be applicable to other wet wastes containing lignocellulosics.

Technically, we have developed stable mixed consortia derived from multiple seed inocula that converts 50%–60% of the rumen fiber at 8% solids and producing 60%–65% methane. Cellulase augmentation enhances VFA production under low pH arrested methanogenesis conditions, while hemicellulase and laccase have mixed impacts. Thermomechanical pretreatment enhances VFA production fourfold when combined with enzyme augmentation. Elevated temperature or low pH leads to low VFA titers, as VFA inhibition of hydrolysis VFA production is a limiting factor when methanogenesis is arrested. Removal of VFAs during digestion results in approximately four times higher VFA production.

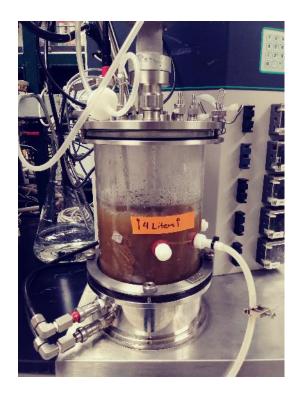


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This is one of several projects focusing on the development of arrested AD for bioproduct generation instead of biogas. This project focuses specifically on improving cellulose conversion during the arrested AD process, with the hope of generating a higher yield of the desired VFA product at a higher rate. This work intends to use the separations technique being developed by a related NREL project (2.3.2.107), so the research being performed is consistent with the constraints required by this separation's technology (e.g., working at low pH). This project appears to have achieved considerable success in its research so far, achieving relatively high VFA titers as a result of a combination of several modifications made to the AD process (e.g., enzyme use, pretreatment, and removal of VFAs as they are formed). The remaining work on this project is all viable, yet ambitious in scope, and should be prioritized to ensure that the most promising tests are performed first with the remaining time available on this project. There also appears to be some overlap in the microbe consortium screening work with the other NREL team (2.3.2.107). While it is recognized that the two teams have performed their microbe research using different feedstocks, it is recommended that one team be responsible for future research in this area so as not to duplicate efforts and use time and monetary resources most efficiently if the intent is to find the most promising culture for the proposed arrested AD system. Because this project team (2.3.2.108) is looking at the most advanced conditions by incorporating cellulose hydrolysis, it is probably the one to lead the microbe consortium development work. A discussion on the actual current market value of the lowcarbon VFA species being targeted relative to the base case of biogas generation in conventional AD is not provided, but should be because it is important in assessing whether the cost of the arrested AD process being developed has a chance at being economically viable.
- Good project with the potential to improve understanding of basic AD mechanisms. While the results may be considered obvious (e.g., hydrolysis as a rate-limiting step), attempts to quantify and correct AD digestion limiting factors have never been carried out systemically. It is not the first time that the potential benefit of pretreatment and enzyme addition has been discussed, yet this is probably a more fundamental and systemic approach to the analysis than most and uniquely couples the consideration of the role of microbial consortia. The main weakness of the project is still a relatively undeveloped TEA component—although mitigated by another project explicitly focusing on this—and the lack of distinct pathways to industrial implementation. Given the generality of the problem and the rather fundamental level at which the PIs are operating at this time, I do not consider this a significant problem and I think it can be addressed in due course at a more appropriate time.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the comments. We have been working with the separations task and have realized the overlap in certain areas. We are considering merging these efforts into a consolidated task, with resources from 2.3.2.108 being used to screen different feedstocks and consortia for increased VFAs/decreased methane. This will allow the 2.3.2.107 project resources to be focused on testing and enhancing the separations methodology and equipment. The combined tasks will be more efficient, and this will allow some resources to focus on improved analytical methods for characterizing the feedstock and residuals in order to gain a better understanding of the TEA.
- Thank you for pointing out the lack of understanding regarding the nature of the limiting factors in AD. Clearly, developing this knowledge will allow a more directed focus on the areas that are most impactful to the overall economics. Gaining a better, more expanded TEA analysis is a major need here and fundamental knowledge on AD limitations will enable improved and more relevant TEA.

# BIOGAS VALORIZATION: DEVELOPMENT OF A BIOGAS-TO-MUCONIC-ACID BIOPROCESS

#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

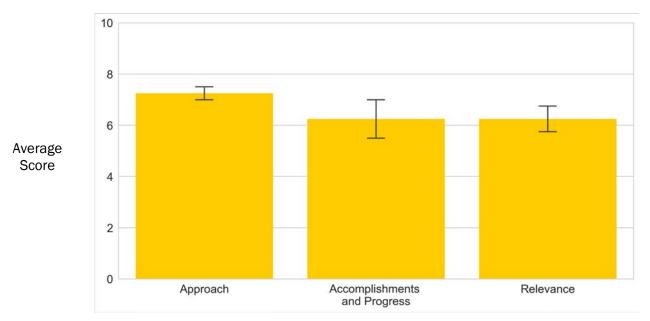
Biological methane conversion offers a scalable, modular, and selective approach to biogas upgrading. However, gas fermentation process intensification remains a primary hurdle in methane biocatalysis. To this end, the Biogas Valorization task targets the development of an integrated bioprocess to produce platform chemical intermediates from biogas. The project will integrate core competencies from government, industrial, and academic partners,

| WBS:                      | 2.3.2.201          |
|---------------------------|--------------------|
| CID:                      | EE0006877          |
| Principal Investigator:   | Dr. Mike Guarnieri |
| Period of<br>Performance: | 6/1/2015-9/30/2018 |
| Total DOE Funding:        | \$2,241,411        |
| Project Status:           | Sunsetting         |
|                           |                    |

including metabolic strain engineering, metabolic flux analysis, low power input bioreactor design, AD, and TEA in order to develop a conversion process demonstrating the production of organic acids from a renewable biogas feedstock stream. The project encompasses the development a novel methanotrophic biocatalyst and a high-efficiency, low-power fermentation configuration. Successful implementation of this target scope will enable facile integration with AD infrastructure and offer substantial biogas valorization potential. Importantly, developments here will also be applicable to an array of substrates, including syngas, natural gas, and CO<sub>2</sub>. This work is relevant to BETO's Multi-Year Plan (MYP) for developing cost-effective, integrated WtE processes to produce bioproducts, and it explicitly targets BETO MYP barriers, including catalyst development, biochemical conversion process integration, WtE roadmap hurdles, and process intensification.

#### Weighted Project Score: 6.5

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 ${f I}$  One standard deviation of reviewers' scores

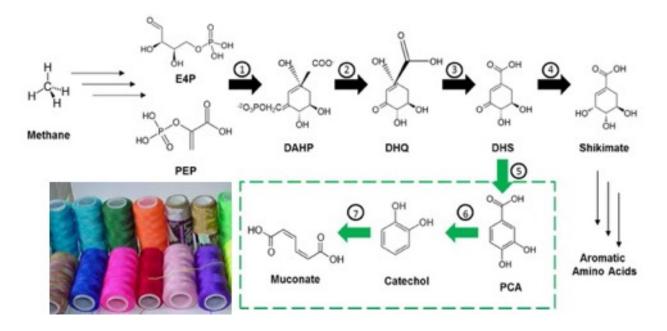


Photo courtesy of National Renewable Energy Laboratory

#### **OVERALL IMPRESSIONS**

- The intent of this project was to improve on conventional AD by converting the relatively low-value biogas produced by AD to a more high-value chemical intermediate product—muconic acid. Although the target yield of muconic acid ultimately could not be met due to constraints in the genetic structure of the methanotrophs used, there were several very valuable results that came out of the work in this project. First, the concept of muconic acid production from methanotrophs via genetic engineering was proven (just not at concentrations sufficient for scale-up). Second, reactor design advances led to a system that exhibited enhanced methane uptake and significantly improved mass transfer. Finally, although muconic acid could not be generated at acceptable concentrations, the project showed that succinic acid was produced at concentrations that may be high enough to be of commercial interest. Because succinic acid is a chemical that, like muconic acid, has broad applications in the chemical industry (e.g., as a precursor to many products and as a supplement in the food industry, to name a few), it would have been worthwhile to consider changing the focus on this project to generate succinic acid rather than termination. This is still something to consider for future work, if this potential is confirmed by an initial market study and/or TEA evaluation. Regardless, the information gained and lessons learned from this project in terms of genetic engineering of methanotrophs and associated reactor design should be able to be utilized and extended in future work, thereby making the current project successful from this perspective.
- The project was carried out in exemplary fashion with rigor, and while it did not achieve some of the original targets, the author pivoted and demonstrated feasible pathways with a new product and new reactor technology. Scalability issues remain to be addressed with the new immobilization concept presented.
- Although terminated, this project made significant technical advances in the configuration of bioreactors feeding on gas substrates. This technology will be picked up by other researchers and commercial companies for biological gas-to-liquid projects.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their complimentary and constructive commentary. We are pleased that, despite failing to meet productivity target metrics, efforts on this project achieved critical enhancements to gas mass transfer and process intensification for biogas fermentation processes. Thus, we agree that this project led to numerous valuable lessons learned and has laid the foundation for follow-on studies targeting alternative end products with more favorable biological compatibility. The resultant data have enabled important insights into methanotrophic metabolism and biogas cultivation capacity and led to the evaluation of three novel gas fermentation reactor configurations, each with unique characteristics that may be suitable for scalable deployment. Future efforts may entail piloting of reactor(s) at larger scales to determine scalability and lifetime, as well as comparative technical and techno-economic analyses to identify the most suitable reactor configuration as a function of target product and scalability. Importantly, the data generated from these efforts will provide critical inputs to complementary biogas biocatalysis projects focused upon microbial development and will inform pertinent metabolic engineering strategies. We also note the potential applicability of the design principles established here to conversion of an array of gaseous substrates, including CO<sub>2</sub>, carbon monoxide (CO), and hydrogen  $(H_2)$ . Thus, we believe this project's efforts offer significant synergistic potential with other conversion platforms, importantly informing gas fermentation design principles and strain-engineering strategies related thereto. We look forward to alternative opportunities to continue pursuit of this work.

# BIOMETHANATION TO UPGRADE BIOGAS TO PIPELINE GRADE METHANE

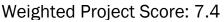
#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

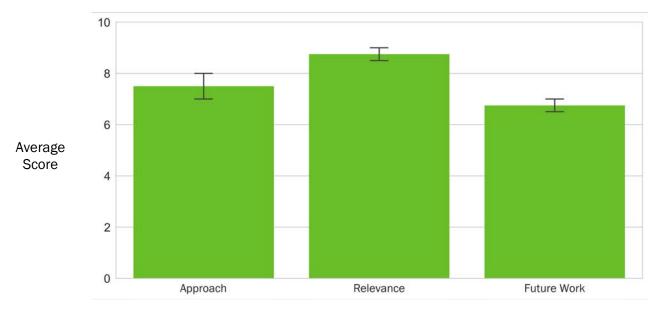
The move to renewable electricity sources is happening on a global scale to decarbonize the electricity sector. The biomethanation technology, being developed under this biopower project, intersects and can help solve many challenges we face by enabling higher penetrations of solar- and wind-generated electricity sources and leverages the DOE's fossil, nuclear, and renewable energy program initiatives like H2@Scale. This biomethanation process advances the concept of electrons to molecules by recycling and utilizing carbon and storing the renewable natural gas (RNG) in the existing natural gas network. Step one in the process requires low-cost, low-carbon, and otherwise curtailed electricity sources to produce low-cost

| WBS:                      | 5.1.3.102          |
|---------------------------|--------------------|
| CID:                      | NL0034005          |
| Principal Investigator:   | Dr. Kevin Harrison |
| Period of<br>Performance: | 6/1/2018-5/31/2021 |
| Total DOE Funding:        | \$1,500,000        |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$0                |
| DOE Funding FY18:         | \$1,500,000        |
| DOE Funding FY19:         | \$0                |
| Project Status:           | New                |
|                           |                    |

hydrogen (H<sub>2</sub>) from a water electrolysis system. Step two, the biomethanation process combines H<sub>2</sub> with a biogas source, containing CO<sub>2</sub>, with single-celled biocatalysts to produce methane, water, and heat. The RNG requires very little cleanup to achieve pipeline-quality natural gas, which is then a direct "drop-in" replacement fuel injected alongside fossil-based natural gas. The RNG acts as a long-duration energy storage solution for renewable electricity sources and can help decarbonize the transportation sector at over 2,000 compressed and liquid natural gas stations across the United States.



Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${\mathbb I}$  One standard deviation of reviewers' scores

This project advances the science of scaling the biomethanation process from 700 L down to 30 L, enabling increased process development and progressing scientifically based scaling functions that will inform nextgeneration megawatt-scale bioreactor design and operation. The scaling functions will be applied to the utilization of biogas CO<sub>2</sub> from different sources with nutrient and controls optimization to accommodate varying biogas feedstock. Varying feedstocks will be investigated to understand the time and spatial composition differences of biogas sources from field sites across the country. Partnering with Southern California Gas (SoCalGas) provides guidance to map the technology for early-market opportunities at the megawatt scale. Electrochaea GmbH is supporting this project by providing in-depth process control, nutrient management, and a license to use the methanogen Methanothermobacter thermautotrophicus. Electrochaea is also supporting the development of advanced analytical methods for mass balances (e.g., carbon, nitrogen, sulfur, hydrogen, phosphorus), nutrient optimization, and the identification of potential coproducts produced by the methanogens under varying biogas conditions. The design and build of the pressurized 30-L scaleddown bioreactor will be based on the 700-L system provided by SoCalGas. This mobile 18-bar bioreactor system will overcome a significant challenge in developing this technology by traveling to actual biogas sites to perform research versus obtaining sufficient gas samples and transporting them back to NREL. Optimization and control of the gas feedstocks, nutrients, liquid levels, pressure, pH, and temperature will provide scientifically based scaling functions between the two systems. The project aims to demonstrate continuous operation of both bioreactors at pressures up to 18 bar using biogas feedstock (actual and synthetic) to produce a product gas composition capable of direct injection into the natural-gas network. In the end, this project will inform, guide, and enable megawatt-scale biogas upgrading through systems integration, reduced capital cost, and improved biocatalyst performance to accelerate the deployment and economics of WtE technologies using biogas sources.

#### OVERALL IMPRESSIONS

- This project aims to upgrade biogas (i.e., convert CO<sub>2</sub> in biogas to CH<sub>4</sub>) using H<sub>2</sub> derived via electrolysis of water with renewable electricity from wind or solar power. On paper, this project has many significant benefits and great potential, including generation of a gaseous product equivalent to renewable natural gas, removal of CO<sub>2</sub> from the environment, and providing a market and use for excess wind and solar power. The design and operation of a mobile system is also an innovative approach that could be used to move the conversion technology to point sources of biogas for operation. The system, if successful, could be readily included as an "add-on" technology to existing waste conversion systems that generate biogas. However, there are some concerns with the project as described. Electrolysis is a very expensive way to make H<sub>2</sub> and the economics will heavily depend on the price of electricity. It is not clear how the project will ensure that the electricity it uses comes from renewable sources (emissions associated with electricity generated from fossil fuel would eliminate any benefit of CO<sub>2</sub> conversion in the process) at an acceptable price. Also, no information has been provided on how the H<sub>2</sub> will effectively be transported to the microbes, whether the microbes will be able to generate  $CH_4$  to the concentrations desired (>97%), and how the product CH<sub>4</sub> will be fully recovered from the aqueous matrix. In addition, the need to perform more than one scale-up along with design, fabrication, and operation of the corresponding system during the three-year period of this project will be challenging.
- This is an excellent project showing good progress in the bioprocessing area with a good plan for field tests. This is highly relevant. I believe the project would benefit from deemphasizing the characterization of very different biogas streams and instead focus on establishing a realistic baseline to be achieved by using commercial off-the-shelf desulfurization technologies when necessary. The integration with the power network for efficient use of renewable energy resources needs more development. The TEA is, in general, wanting, as the potential for high capital cost is a significant risk for future deployment.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipients choose not to respond to the reviewers' overall impressions of their project.

# MODULAR MICROBIAL ELECTROMETHANOGENESIS FLOW REACTOR FOR BIOGAS UPGRADING

#### Lawrence Livermore National Laboratory

#### **PROJECT DESCRIPTION**

The majority of the cost of biogas production is the removal of inerts (such as  $CO_2$ ) and contaminants (H<sub>2</sub>S, siloxanes). This cost is particularly prohibitive for smallscale biogas producers (e.g., dairy farms and feedlots), which collectively make up the majority of biogas potential. Technologies that remove  $CO_2$  either vent it, contributing to greenhouse gas emissions, or must find an economical use for the gas, which is particularly difficult for small-scale producers. A more carbon-efficient approach is to convert the  $CO_2$  to  $CH_4$  in order to upgrade the gas to pipeline quality, rather than simply removing the  $CO_2$ . Methanation has the potential to be significantly more energy efficient and less capital intensive than  $CO_2$ -

| WBS:                      | 5.1.3.104          |
|---------------------------|--------------------|
| CID:                      | NL0034001          |
| Principal Investigator:   | Dr. Sarah Baker    |
| Period of<br>Performance: | 6/1/2018-5/31/2020 |
| Total DOE Funding:        | \$800,000          |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$0                |
| DOE Funding FY18:         | \$800,000          |
| DOE Funding FY19:         | \$0                |
| Project Status:           | New                |
|                           |                    |

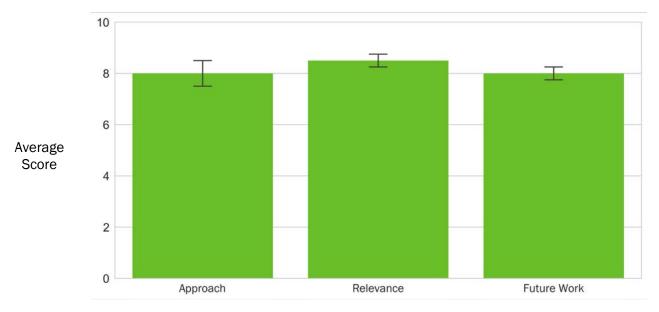
CH<sub>4</sub> separation, while virtually eliminating CO<sub>2</sub> emissions. Methanogenic microbes can utilize electrical energy to methanate CO<sub>2</sub> with high energy efficiency and selectivity. Additionally, this

"electromethanogenesis" provides a pathway for storing electrical energy in chemical bonds for long-term storage of renewable electricity.

To unlock the potential of microbial electromethanogenesis for biogas upgrading and energy storage, Lawrence Livermore National Laboratory has partnered with Stanford University and SoCalGas, a major

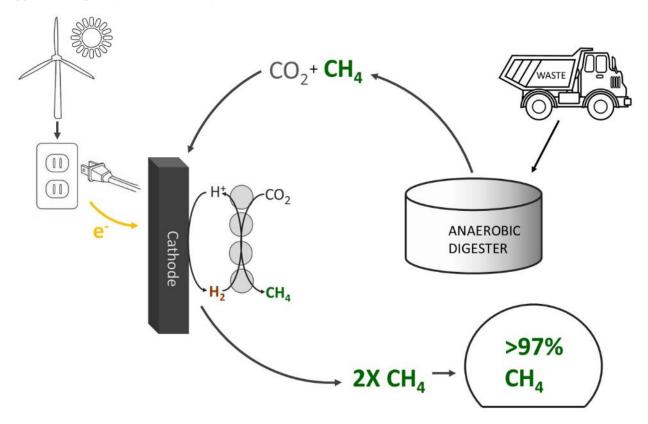
#### Weighted Project Score: 8.1

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

natural gas distributor, to develop a proof-of-concept reactor that upgrades biogas to pipeline-quality biomethane. To increase the maturity of the technology, the team will measure the effects of biogas composition and electrochemical reactor conditions on the productivity of electromethanogenic consortia, isolating strains that have high cell density under operation. Additionally, the team will use advanced manufacturing to generate high surface area electrode materials that reduce energy consumption, increase volumetric productivity, and have scalable surface area. The team targets a process energy efficiency of 0.03 g/Wh, based upon a TEA performed by SoCalGas, while producing pure biomethane. The team will also determine the overall process parameters necessary to generate biomethane at this target energy efficiency, including contaminant tolerances, biogas purity, and associated pre- and post-treatment requirements. These parameters will be used to conduct a TEA of the technology for biogas upgrading and power-to-gas applications, paving the way for larger-scale demonstrations.





#### OVERALL IMPRESSIONS

• This project utilizes a combination of methanogenic microbes in an electrochemical cell to upgrade biogas to pipeline-quality natural gas. If successful, the benefits would include not only generation of fossil-quality gaseous fuel (of which it would help displace) but also a means to sequester CO<sub>2</sub>. Though at an early stage, the project shows great potential in solving H<sub>2</sub> generation and transport issues by use of the reactor also functioning as an electrochemical cell, and through the use of innovative electrode materials (aerogels), which combine high surface area and porosity to bring the microbes and H<sub>2</sub> gas in close contact. However, as clearly shown in the presentation, there are a significant number of constraints in the system as designed and tradeoffs that will need to be considered in choosing the best microbe strains and material choices to withstand these constraints. The collective challenges make the

success of this project anything but certain, but worth the investigation. Having SoCalGas as a partner is a good move for obtaining input with respect to end-user needs and other commercialization issues as the technical development of components occurs. This project lacks a discussion of costs, which is important to assess how economically viable this will be even if the technical challenges are overcome. In particular, it is expected that electricity costs will play a crucial role in this determination. To reap the full environmental benefits of this project, electricity will need to be obtained from renewable sources and not fossil-fuel-burning power plants, but there is no discussion on how this can be guaranteed. Also, there is very little discussion on how the TEA will be constructed and used with respect to the experimental data that will be generated. This presentation is also missing a schedule that shows how all of the described activities fit together relative to each other and with respect to project milestones.

• A good project that touches a very relevant biogas upgrading topic. Early to define in rigor scalability and economics, but more details—especially on what could be the capital cost of this type of reactor at scale—would be beneficial.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their time and constructive feedback. We agree that *in situ* production of hydrogen to generate reducing equivalents for methanogenesis may reduce energy and capital costs relative to systems that deliver gas-phase hydrogen to stirred-tank reactors. While the project is very early stage, based upon the reviewer comments we have initiated a TEA, which will help us make more informed decisions as the project progresses. The TEA will include a sensitivity analysis of the effects of electricity costs on operating expenses. We agree with the reviewers that if this project reaches pilot stage or higher TRL it needs to be proven with intermittent renewable energy to demonstrate maximum benefit. California curtailed 450,000 MWh in 2018, and renewable curtailments are projected to rise. Availability of renewable electricity and biogas will play a major role in choosing a pilot site. A project schedule was included in the peer-review slide deck; we apologize that we did not formally present it to the committee.

# PRODUCTION OF METHANE FROM ORGANIC WASTE STREAMS WITH NOVEL BIOFILM-ENHANCED ANAEROBIC MEMBRANE BIOREACTORS

#### **Argonne National Laboratory**

#### **PROJECT DESCRIPTION**

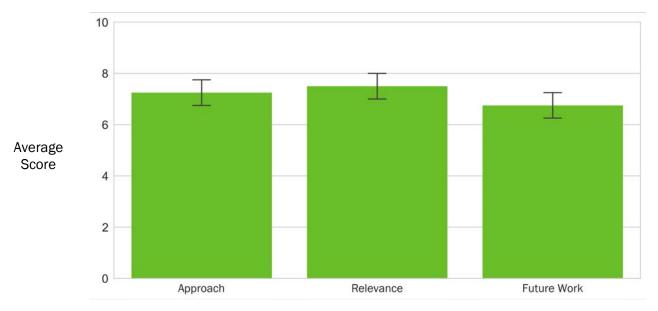
We have been developing an innovative, scalable anaerobic membrane biotechnology that converts organic waste streams into renewable methane using a two-stage novel anaerobic membrane bioreactor (AnMBR) system. The proposed research is motivated by the high volume of wet organic waste streams generated in the United States and has the potential to harness the associated energy. For example, estimates of yearly MSW generation in the United States vary from 254 to 347 million tonnes, of which 55% consists of food, paper, and yard waste. As AD converts organics into renewable methane, it is an ideal option for small

| WBS:                    | 5.1.3.105                 |
|-------------------------|---------------------------|
| CID:                    | NL0034002                 |
| Principal Investigator: | Dr. Meltem Urgun-Demirtas |
| Period of Performance:  | 5/1/2018-4/30/2021        |
| Total DOE Funding:      | \$1,275,000               |
| DOE Funding FY16:       | \$0                       |
| DOE Funding FY17:       | \$0                       |
| DOE Funding FY18:       | \$1,275,000               |
| DOE Funding FY19:       | \$0                       |
| Project Status:         | New                       |
|                         |                           |

decentralized communities or industries to locally treat their wastes and produce biopower. The AD capacity will likely increase in coming years. However, due to the economy of scale, biopower production for scales smaller than one ton/day currently is not economically feasible in the United States. Our ultimate aim is to develop a sustainable process that diverts an organic fraction of MSW (OFMSW) from landfills and incineration while generating renewable energy and capturing nutrients to meet the demands of organic waste generators and hauling companies.

#### Weighted Project Score: 7.1

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

The project goals and targets are to improve the techno-economic viability of biopower production by developing a sustainable two-phase AnMBR system that diverts OFMSW from landfills and incineration while generating methane and renewable bioproducts. To achieve this goal, the proposed project entails five tasks:

- Develop a flexible feedstock-blending plan for the urban organic waste streams produced by a typical U.S. city that meets treatment requirements and maximizes energy recovery while considering seasonal waste fluctuations
- 2. Develop a first-phase AnMBR inspired by the stomach physiology of ruminants that enhances hydrolysis and acidogenesis to maximize VFA production
- 3. Develop a second-phase AnMBR that exploits biofilm growth to enhance methanogenesis and optimize the conversion of VFAs to methane
- 4. Perform process simulation and analysis to model full-scale performance of the proposed technology.
- 5. Conduct TEA and LCA using the newly developed performance model to assess economic and environmental viability of our novel technology and further facilitate its implementation at full scale.

This project addresses BETO goals of developing economical and sustainable bioenergy systems by advancing efficient strategies for biofuels generation. We will develop and demonstrate proof of concept for a new methane production technology using organic waste streams generated in a typical U.S. city. Two novel biofilm-enhanced AnMBRs at TRL 4 will be developed and integrated as a two-phase system to facilitate high methane yields and low carbon footprints. The outcomes of this project are:

- A scalable, high performance, low-cost, two-phase modular AnMBR technology at TRL 4 that has the potential to extend the economic viability of AD to smaller scales
- Linkage between waste characteristics, microbial community structure, methane yield and recovery, and design and operation of the AnMBRs
- Updated GREET LCA model addressing energy and environmental benefits of new technologies from organic waste streams
- Development of new process modeling tools for AD of OFMSW.

#### **OVERALL IMPRESSIONS**

• This project proposes several modifications to the conventional AD process in order to improve the yield and methane production rates. Splitting the AD process so that it takes place over two reactors instead of one appears to be a good idea in that each reactor can be run at separate conditions more conducive to the steps in the AD mechanism that will occur in them (hydrolysis, acidogenesis, and acetogenesis steps in the first reactor, and the methanation step in the second reactor). The downside is that it increases the process cost and complexity, so that the improved performance will need to offset this increase in order to justify the project's value. The nature of the proposed changes to the AD process make it likely that the proposed improvements, if successful, could not be easily "bolted on" to existing AD systems. The design of the first reactor based on the bovine rumen and the intent to focus on underutilized food waste and the organic portion of MSW as a feedstock are also very good aspects of this project. More details on the two reactor system scale-ups that are proposed over the course of this project are needed to assess whether there will be sufficient time for this ambitious plan. While improvements in efficiency to any bioenergy process are valuable, the focus on AD does not appear to be one of the high priority stated goals of BETO.

- I struggled with this project as I am not quite sure what the overarching goal was. Develop a new (cheaper, better-performing, more compact, etc.) reactor? Develop arrested digestion? Increased gas production? Maximize feedstock flexibility? Make AD feasible at lower scale than conventional approaches? These are all valuable points but somewhat confusing in the way it is presented today. While it may be too early for detailed TEA, if the PIs do not know their possible economics, then they should at least know the targets they aim to beat.
- I would recommend an outreach strategy to report the successful outcome of this project to associations of sanitation agencies, landfill operators, and food processing plant owners in a case study description of an emerging technology.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Our initial results showed that the first-stage anaerobic digester has achieved very good performance with a hydraulic retention time (HRT) of only 12 hours instead of days (usually 3–10 days). Therefore, capital cost will not be as high as conventional two-stage systems. While we partially agree that the operation of two-phase systems can be little bit more complex than conventional one-phase systems, the two-stage configuration has been considered as a viable approach to improve the overall AD performance in terms of biodegradation, rates, process stability, biogas yield, and energy recovery. Because of the short HRT, the new one-phase system developed in this project can be a 2-20-times smaller footprint than a conventional one-phase system. Also, both the first-phase and second-phase system developed in this project are anaerobic bioreactors that rely on dynamic membranes operated at lower transmembrane pressure and are made of cheaper materials than that of micro- and ultrafiltrationbased membrane reactors. Hence, new technology will exhibit lower operational costs and less complexity compared to conventional AnMBRs. AD and membrane-based technologies are very well known and can be easily scaled up from bench to pilot scale. The project team believes that a three-year project duration would be sufficient to scale up the modular AD technology. This project, selected from BETO Funding Opportunity Announcement (DE-FOA-0001085) entitled "Lab Call for Biopower R&D (DE-LC-000L045)." In this call, "Topic 4: Alternative Approaches to Anaerobic Digestion" was specifically related with improvement of the techno-economic viability of AD at scales of one dry ton/day. The lab call also required the development of new technologies to overcome current challenges to efficient AD operation, including the energy requirements of minimizing membrane fouling and recovery of dissolved methane in the effluent at scales that match feedstock availability. Therefore, our first aim is to develop a techno-economically viable process at small scale, then consider the application of this process into existing AD systems, which usually consist of multiple ADs.
- The goal of this project is to make AD economically feasible for small-scale operation by addressing the challenges that prevent the application of this technology at scales of one dry ton/day. In order to do this, challenges related to the slow rate of the anaerobic degradation of waste, low methane yield and methane loss in the effluent, and the demand for processes handling of a diverse feedstock need to be addressed. The novel design of the two-stage bioreactors has focused on addressing challenges with (1) the rate of hydrolysis by using rumen microbial cultures and mimicking rumen operations, (2) low methane yield by long sludge (cell) retention time and separation of hydrolysis/acidogenesis from methanogenesis, and (3) sustainable feedstock supply requirement by developing a feedstock blending plan. Regarding the economics, conventional digesters operate at HRTs of 20–40 days. Our system will operate at a total (first and second phase combined) HRT of 4–5 days, which means that capital costs have the potential to be reduced by 2–10 times. Operational costs are also expected to be lower than conventional AnMBRs, but not conventional AD systems, due to the simplicity of operating a dynamic membrane compared to microfiltration membranes. Conventional AD systems without membranes are simpler than our system.
- As mentioned throughout the presentation, the targets are the production of VFAs at a yield of 0.35 g/volatile solids in phase 1 AnMBR and methane with a yield of 0.4 liter/g volatile solids fed on a

sustainable basis in two-phase ANMBR system. These targeted values were taken from the literature reported for the cost-effective production of methane from organic waste streams.

• Our business project partners are Metropolitan Water Reclamation District of Greater Chicago, which operates seven wastewater treatment plants in the Chicago area; Gray Brothers LLC, which is a waste hauler and a landfill operator in Pennsylvania; and Roeslein Alternative Energy, which produces and injects renewable methane produced from manure and agricultural waste streams. We also plan to publish our results in technical papers and present them at the conferences to disseminate the results as a part of our outreach efforts. With respect to the suggested outreach strategy in the comments, we plan to identify additional waste generators, landfill operators, facilities, and AD users where this technology can be applicable to meet stakeholder needs moving forward.

# ANALYSIS AND SUSTAINABILITY

# **PROGRAM AREA**

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## INTRODUCTION

The Analysis and Sustainability (A&S) program is one of 14 related technology areas reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 26 projects were reviewed in the A&S session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$41,868,415 (fiscal year [FY] 2016–2019 obligations), which represents approximately 4.9% of the BETO portfolio reviewed during the 2019 Project Peer Review. During the Project Peer Review meeting, the principal investigator (PI) for each project was given 30–45 minutes (depending on the funding level) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the Project Peer Review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the A&S Program, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Alicia Lindauer as the A&S technology area review lead, with contractor support from Diana Raggio (Allegheny Science & Technology). In this capacity, Ms. Lindauer was responsible for all aspects of review planning and implementation.

## ANALYSIS AND SUSTAINABILITY OVERVIEW

BETO is committed to growing a bioenergy industry that enhances energy security, promotes environmental benefits, and creates economic opportunities. To that end, the A&S Program addresses the challenges related to sustainable bioenergy production and use by supporting research, analysis, and tool development to better understand the economic, environmental, and social dimensions of advanced bioenergy and bioproducts. The program works with BETO's research and development (R&D) programs to conduct integrative analyses that facilitate insights across the bioenergy supply chain. These include analyses that integrate economic and environmental dimensions to understand trends, synergies, and tradeoffs. The A&S Program operates through two integrated subprograms: Strategic Analysis and Crosscutting Sustainability.

#### ANALYSIS AND SUSTAINABILITY SUPPORT OF OFFICE STRATEGIC GOALS

The A&S Program works to develop science-based strategies to understand and enhance the environmental, economic, and social benefits of advanced bioenergy and bioproducts relative to conventional energy systems.

The Crosscutting Sustainability strategic goal is to understand and promote the positive environmental, economic, and social effects and reduce the potential negative impacts of bioenergy production activities.

The Strategic Analysis strategic goal is to provide context and justification for decisions at all levels by establishing the basis of quantitative metrics, tracking progress toward goals, and informing portfolio planning and management.

#### ANALYSIS AND SUSTAINABILITY SUPPORT OF OFFICE PERFORMANCE GOALS

The Strategic Analysis subprogram works to identify overall BETO goals and priorities and covers issues that cut across all program areas. System-level analyses inform strategic direction and planning efforts; they also help BETO focus technology development priorities and identify key drivers and hurdles for maximum

national impact. Technology-specific analyses explore sensitivities and identify areas where BETO investment could lead to the greatest impacts as well as outline R&D needed to further develop emerging ideas.

The Crosscutting Sustainability subprogram area supports BETO's strategic goals by providing crosscutting, science-based quantification of the sustainability of advanced bioenergy to support an industry that delivers improved environmental performance and other benefits relative to conventional energy systems. The Crosscutting Sustainability subprogram area interfaces with and impacts all elements of the biomass-to-bioenergy supply chain and each stage of technology development. Considering sustainability early in technology development—rather than after systems are finalized and replicated—enhances the future economic and technical viability of those technologies. The Crosscutting Sustainability subprogram generates scientific knowledge that proactively addresses issues affecting the scale-up potential, public acceptance, and long-term viability of advanced bioenergy systems.

#### ANALYSIS AND SUSTAINABILITY APPROACH TO OVERCOMING CHALLENGES

BETO has identified the following key barriers and challenges in which improvements are crucial to achieving the goals of the A&S Program:

- Analysis to inform strategic direction
- Analytic tools and capabilities for systems-level analysis
- Data availability across the supply chain
- Identifying new market opportunities for bioenergy and bioproducts
- Quantification of economic, environmental, and other benefits and costs
- Science-based methods for improving sustainability
- Social acceptance and stakeholder involvement
- Consensus, data, and proactive strategies for improving land-use management.

The A&S Program works to overcome these challenges by developing and disseminating knowledge, tools, and mechanisms for more informed decision making and better resource management. Key partners include national laboratories—primarily Argonne National Laboratory (ANL), Idaho National Laboratory (INL), National Renewable Energy Laboratory (NREL), Oak Ridge National Laboratory (ORNL), and Pacific Northwest National Laboratory (PNNL)—academia, nongovernmental organizations, industry, and international organizations. This technology area coordinates internally and externally, working closely with other BETO technology areas, DOE offices, and federal agencies such as the U.S. Department of Agriculture (USDA), U.S. Environmental Protection Agency (EPA), U.S. Department of Defense (DOD), and U.S. Department of Transportation. Robust stakeholder engagement—through workshops, roundtables, and other means—helps advance crosscutting objectives.

The scope of A&S Program projects includes:

- Resource and technical assessments that provide the analytic basis for program planning and assessment of progress
- Advancement of scientific methods and models for measuring and understanding bioenergy sustainability across the full supply chain
- Dissemination of practical tools for analyses, decision making, and technology development that enhance sustainable bioenergy outcomes

- Data compilation to develop and maintain models, tools, and data sets to assist in collecting, compiling, and analyzing data
- Quantification of environmental performance and potential benefits and costs of bioenergy and bioproducts relative to conventional energy systems
- Development of sustainable system design approaches that increase bioenergy and bioproduct production while enhancing economic, social, and environmental outcomes.

# ANALYSIS AND SUSTAINABILITY REVIEW PANEL

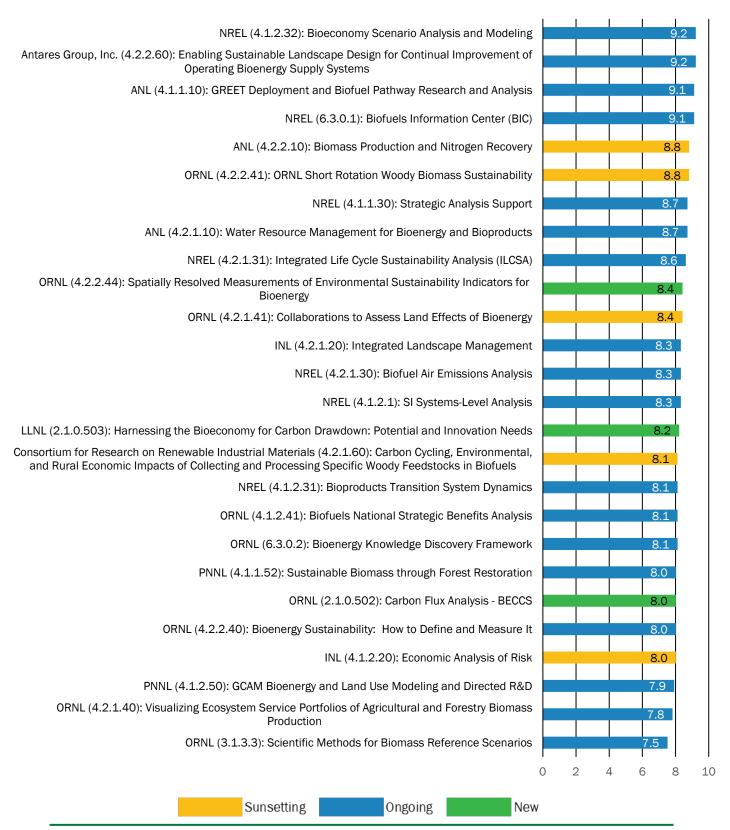
The following external experts served as reviewers for the A&S Program during the 2019 Project Peer Review.

| Name              | Affiliation                                      |
|-------------------|--|
| Kristin Lewis*    | U.S. Department of Transportation – Volpe Center |
| Christopher Clark | U.S. Environmental Protection Agency             |
| Kevin Fingerman   | Humboldt State University                        |
| Harry Baumes      | Independent Consultant                           |
| Bret Strogen      | U.S. Secretary of the Army                       |
| * Lood reviewer   |  |

\* Lead reviewer

# **TECHNOLOGY AREA SCORE RESULTS**

#### Average Weighted Scores by Project



## ANALYSIS AND SUSTAINABILITY REVIEW PANEL SUMMARY REPORT

#### Prepared by the Analysis and Sustainability Review Panel

The A&S program is a comprehensive and extremely valuable program within BETO. It is successful at identifying key emerging issues and developing the capacity to address those issues. The portfolio has produced crosscutting and integrative approaches to addressing important bioeconomy-related challenges.

The five-person peer-review panel reviewed a total of 26 projects during three days, covering a broad range of strategic, modeling, analytic, and field-based projects. The peer-review panel was very impressed with the diversity and strength of the program overall and the value of the individual projects. The review panel thanks the PIs for their innovative approaches, valuable contributions, and presentations.

The management of the projects, as well as the portfolio overall, are thoughtful and effective. The review panel observed substantive effort to communicate among project teams and integrate activities. In the following summary, the peer-review panel addresses the impact, innovation, and synergies among projects, addresses the current and future focus of the portfolio, and offers recommendations to continue strengthening the value and reach of the portfolio.

#### IMPACT

The role of the A&S program portfolio is to provide tools and methodologies to support a variety of bioeconomy-related analyses and then to execute those analyses. The A&S portfolio has significant impact within BETO as well as across the bioeconomy sector. This project portfolio has produced key widely used tools and models that are of high value and utility and enable responsiveness to emerging issues. The analyses exemplify the integration of those tools and models as well as innovative approaches to landscape management, environmental measurements, valuation of ecosystem services, and sustainable biomass production. The strategic mapping of linkages among modeling tools, as well as the use of the map across projects in the portfolio during presentations, helped the panel see the strength of interlinkages among tools and the effort to avoid duplication.

Although most projects scored high in the reviewers' assessments, some projects received particularly high marks and/or very strong positive comments from reviewers:

- The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model is a landmark tool. The model is widely used inside BETO and around the world, including in some highly impactful policy applications, such as California's Low-Carbon Fuel Standard Program. The team continues to put forward necessary and valuable improvements. The review panel had some concerns that broadening GREET's scope to include environmental impacts such as water scarcity might be better addressed by leveraging other teams' work (e.g., the Water Analysis Tool for Energy Resources [WATER] model or components thereof) and should be evaluated carefully to ensure that further developments are in the strategic best interest of the GREET model itself, the BETO A&S Program portfolio, and the broader bioeconomy analysis community.
- The Biomass Scenario Model (BSM) is another extremely strong program. The researchers pursued a key goal of identifying specific factors that contribute to the cost effectiveness of subsidies so that they can be better structured and applied. The model is unique in that it addresses feedstock use, alternative conversion technologies, adoption of technology, and end-use fuels. The BSM model has been used in several high-profile analyses, including the modeling of scenarios to expand the use of bio-based jet fuel. A high-profile research award and uptake in academic research and teaching imply methodological rigor as well as potential for future influence. Strategic planning for increased exposure beyond the research sphere is warranted to ensure impact for this modeling platform. The effort to make analysis and the model available to the public is a positive outreach activity.

- The Biofuels Information Center (BIC) is highly effective; has well-defined activities and regular, consistent products; and is a worthwhile use of BETO funds. The value of this program is evidenced by the fact that BIC's website has received more than 800,000 page views.
- Analyses using the Global Change Assessment Model (GCAM) provide a broader economy-wide perspective, and because this model is also widely used, it links BETO analyses to the broader research community.
- Analyses using the U.S. Environmentally Extended Input-Output (USEEIO) model (Work Breakdown Structure [WBS] 4.2.1.31 Integrated Life Cycle Sustainability Analysis) is also especially pertinent to many federal and state decision makers because very few studies to date have examined the life-cycle effects of biofuels beyond greenhouse gases.
- Two field-related studies that stood out for the panel were the Integrated Landscape Management (ILM) project (Antares) and the short-rotation woody crops (SRWC) analyses. The panel found the Antares project to be quite comprehensive as well as practical, generating specific key technological (equipment), modeling, and biomass production advancements. The panel sees value in expanding this approach to multiple locations across the national level using the best practices and tools developed with the current Antares project, with consideration given to potential economic viability. The SRWC analysis stood out as a very comprehensive empirical assessment of the production potential, value proposition, and viability of SRWC.

#### INNOVATION

Many models and programs within the A&S program portfolio have provided innovative advances in analytic options and methodologies, as evidenced by their broad adoption and use. Many of these innovative tools and models have become long-term investments for BETO, leading to ongoing expansion and improvement over time, which enhances the value of the originally innovative tools.

The new project on Spatially Resolved Measurements of Environmental Sustainability Indicators for Bioenergy using drones to collect water-quality data could eventually yield large rewards because current information relies on grab samples that are few in number and labor intensive (e.g., the U.S. Geological Survey National Water-Quality Assessment Project, the EPA National Aquatic Resource Surveys).

Understanding the potential for the bioeconomy to contribute to carbon drawdown, as well as emissions mitigation, will become more important in the future. The two new complementary projects focused on carbon management (Harnessing the Bioeconomy for Carbon Drawdown: Potential and Innovation Needs and Carbon Flux Analysis - Bioenergy with Carbon Capture and Storage [BECCS]) are moving BETO toward a more comprehensive, systemic approach to assessing opportunities to reduce climate-change impacts and address the value proposition of the bioeconomy. The review panel recommends that BETO identify this emerging need and take steps to begin addressing it, although some reviewers expressed caution regarding the centrality of these topics to the BETO mission.

#### SYNERGIES

The A&S portfolio is diverse, and evident effort has been made to coordinate it thoughtfully. The panel suggests that deepening those efforts to leverage synergies and avoid duplication is key for this diverse portfolio. Some projects are well connected and take advantage of synergies for both project execution (e.g., overlapping field case studies) and tool complementarity, but it was not always easy for the panel to tell whether this was happening, and to what extent. It also appeared to the review panel that many project teams attempt to incorporate multiple sustainability elements in a cursory manner into their models to show breadth of coverage even when the main contribution of the project was its depth of insight into a particular aspect of sustainability. Although there is good communication among teams, many teams seem to feel the need to generate their own approach and data for the same areas (e.g., sustainability indicators), whereas the panel

would have liked to see groups leverage the approaches of teams that specialized in other particular areas of interest. Researchers who are more proficient in a field can take those roles under a bigger umbrella, rather than having many separate groups researching and coming up with cursory proxies for sustainability elements in which they are not experts. The review panel suggests there might be value in convening researchers in a workshop to develop a larger synthesis project or approach.

The panel also saw a lot of effort to develop and release decision-support tools. Some of these could be very useful, and the panel thought that by integrating these into one or a few models, rather than having many separate models, they might increase their value and be more useful for a broader audience, though the panel recognizes that the integration and maintenance of more comprehensive models can be challenging because of compatibility issues among models and the level of coordination required.

The panel found the Systems-Level Analysis group's model mapping effort helpful as an internal management tool to see how different models link together but found that it does not sufficiently distinguish uniqueness among models as a communications tool. It did not help reviewers to determine where there is duplication, which seems to be a key potential use case for such a tool; rather, because of the selected categories used, the chart suggests there is duplication among models. The reviewers felt it needed more differentiation and/or elimination of defunct models to use it effectively as a communications tool.

The panel discussed the value of field studies. Large umbrella projects such as the Antares Landscape Management project are invaluable because they provide venues for data collection, ground-truthing of models, real-world implementation of strategies, and validation of best practices. For modeling, ground truthing is important until data are sufficiently understood to separate the modeling effort from the field. When evaluating land management approaches, field work is inherently necessary. The panel felt that it might be helpful to expand the number of complementary studies done on the same case study field sites to provide more in-depth analysis for a given location. There is value in expanding the landscape-level projects to more and larger locations nationally when substantive additional insights can be gained by applying such an approach to a different region or context.

The review panel believes these opportunities will help align efforts further to minimize duplication and develop comparable results across multiple case studies and locations.

#### FOCUS

The A&S program portfolio covers a broad range of topics to continue filling sustainability data gaps across the bioeconomy supply chain, a key role.

In addition to the model mapping, which focused on mapping across the supply chain, the review panel suggests that BETO map how the projects address the domains of sustainability (e.g., environmental, economic, social) and the elements within those domains (e.g., within the environmental domain, air and water quality). In doing so, the BETO A&S management team would be able to identify where there is heavy emphasis within the portfolio and where there is less (e.g., social and economic factors, or specific areas such as biodiversity), enabling BETO to identify gaps and evaluate whether the current emphasis areas are appropriate.

The panel appreciated the case studies presented; however, it was not always made clear how the locations and/or details for the case studies (e.g., the species selected for a biodiversity case study) were selected. To most cost-effectively facilitate the development and deployment of the bioeconomy, the panel thinks it is critical that the case studies executed under the A&S portfolio focus on identifying, prioritizing, and/or overcoming key barriers to developing, growing, or manufacturing more bioproducts in an environmentally sound manner.

The panel suggested that the A&S portfolio should continue to include analyses of induced impacts (e.g., interaction between the bioeconomy and food prices). The proper degree of attribution of effects (e.g., indirect socioeconomic impacts such as food price impacts, land use change) to biofuels generally, and the Renewable Fuel Standard program specifically, remain significant unresolved concerns associated with the net effects of biofuels and bioproducts.

One gap the panel discussed is the need for external coordination and verification and validation of models. For example, GREET is a key successful model that needs to be maintained. Because it is such a flagship model that is so widely accepted and used, errors or issues internal to the tool are likely to be perpetuated in many other models and outside analyses; therefore, the panel felt that there would be value in BETO funding external researchers to execute verification and validation on the model as a quality control and assurance effort. The panel identified the parallel analyses the GREET team has already undertaken with other modelers (e.g., Joint Research Centre) as very valuable for verification and validation as well. External verification and validation would be valuable for many of the public models presented.

## TECHNOLOGY DEVELOPMENT PIPELINE

The A&S program portfolio is meant to provide tools and resources to address barriers to technology development and deployment. The tools and resources being developed under the A&S portfolio are in many cases already widely adopted by researchers and industry or have the potential to be widely adopted once made public.

The models that are being developed and publicly released must be maintained and updated on some reasonably regular basis. The review panel felt that there could be opportunities to expand coordination—including potential long-term sharing of resources to support the development and maintenance of models—with other organizations.

#### RECOMMENDATIONS

The review panel recommends the following three key areas of portfolio enhancement in the near to medium term:

- 1. Portfolio coordination: The top recommendation of the A&S review panel is to enhance portfolio coordination using the following elements:
  - A. Enhance depth of expertise where it resides and leverage that depth for crosscutting analyses (sustainability, life cycle assessment [LCA], carbon management)
  - B. Align indicators, model use, and field studies as appropriate
  - C. Provide more opportunities for BETO researchers to thoughtfully collaborate
  - D. Focus case studies on key barriers to deployment (e.g., monetizing ecosystem services and/or other externalities, concerns related to endangered species)
  - E. Create a "project map" to help identify synergies and links among the projects and coverage of sustainability areas and indicators, which would enable the BETO team to more easily identify underrepresented areas in the portfolio
  - F. Expand coordination and cost share with other agencies (e.g., USDA) to develop and maintain model resources
  - G. Coordinate with international research efforts.

- 2. Field studies: The review panel recommends continuing to support field studies, which are important as the basis for modeling efforts and are necessary to establish and test land management practices. The review panel felt that there is value in executing multiple complementary studies within the same geographic location.
- 3. External verification and validation of GREET (in depth) and scope assessment: The review panel suggests that the flagship GREET model undergo a detailed peer review to further enhance its credibility and identify errors or gaps.

Overall, the A&S Program portfolio is extremely successful and could continue to offer valuable insights to BETO program managers and bioeconomy stakeholders through enhancing and expanding upon the program's ongoing efforts.

# ANALYSIS AND SUSTAINABILITY PROGRAMMATIC RESPONSE

# INTRODUCTION/OVERVIEW

We thank the peer-review panel for their time, active engagement, and constructive review of the A&S Project portfolio. We appreciate the reviewers' recognition that the portfolio is designed to have significant impact and the tools and methodologies developed by A&S are used to inform decision making at strategic and project levels. The peer-review panel recommendations will be used to further enhance the effectiveness of the program's activities and contribution to BETO's goals.

The 2017 peer review panel provided several recommendations for the A&S technology area to act on, and the 2019 peer review panel recognized the progress made on those recommendations. This year's reviewers specifically acknowledged efforts to communicate among projects, integrate activities, expand and improve tools and models over time, and take steps to address emerging needs such as carbon management. We are pleased that we have been able to continue to build an effective portfolio and that our efforts to implement feedback have been fruitful.

Reviewers provided feedback on each project within the A&S portfolio, and in response the PIs are working to address this project-specific feedback to strengthen their future work plans. The reviewers also provided feedback to the overall A&S technology area, which was organized into three general recommendations. BETO technology managers for A&S greatly appreciate these recommendations and are already incorporating these suggestions into priorities for FY 2020 and beyond.

#### **Recommendation 1: Enhance portfolio coordination.**

The reviewers called on the A&S Program to enhance the coordination efforts among projects within the portfolio as well as with other agencies and international research efforts. Elements of coordination identified by our reviewers include the alignment of indicators, model use, field studies, and the creation of a project map to better visualize linkages. We greatly appreciate this feedback, and the team will explore ways to better communicate linkages across the projects in the portfolio. It will be useful for the PIs to be able to show how their project relates to the bigger picture and their unique capabilities in addressing research questions as well as how they interface with other modeling and analysis efforts. To support this, A&S will continue to use and improve upon the model mapping tool to identify synergies and gaps in the portfolio.

The A&S Program will continue to focus on creating and promoting platforms for the PIs to interact and discuss their work. The program will continue to hold monthly calls with the PIs to facilitate collaboration and will host biannual modeling workshops to increase coordination of bioenergy modeling efforts. Mechanisms

for interagency coordination will be explored through the Sustainable Bioeconomy and Analysis interagency working groups under the Biomass R&D Board.

#### Recommendation 2: Increased support of field studies.

The reviewers recommended further support of field studies, recognizing their importance as the basis for model development and validation. The panel applauded the Antares Landscape Management project for providing a valuable resource to other projects in the portfolio to collect data, see strategies implemented in the real world, and validate best practices. The A&S team is excited for Antares to continue working with the national laboratories to increase collaboration on field studies. Also, starting this year, three new projects from the Affordable and Sustainable Energy Crops (ASEC) funding opportunity announcement will join the A&S portfolio. These projects will add to our arsenal of field studies and provide further depth of analysis for other projects to learn from and expand on, and we have plans for the ASEC PIs to hold regular calls to align data collection and enable cross-pollination. The A&S Program will continue to explore opportunities to fund additional field studies in the future.

#### **Recommendation 3: Gather external feedback on GREET.**

Reviewers emphasized the need to update publicly available models on a reasonably regular basis. Recognizing the importance and widespread use of the model, the review panel recommended that the GREET model undergo a detailed peer review to further enhance its credibility and identify potential gaps. The A&S team appreciates the panel's recognition of the value of one of our most widely used and trusted models and have begun talks with ANL to identify opportunities for an external review of the model.

# CARBON FLUX ANALYSIS – BECCS

# **Oak Ridge National Laboratory**

## **PROJECT DESCRIPTION**

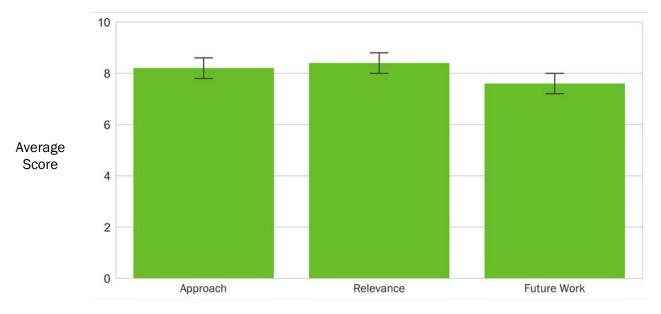
The objective of this project is to assess the potential quantity and economic accessibility of carbon dioxide (CO<sub>2</sub>) management of the U.S. bioeconomy through BECCS. BECCS combines bioenergy with geologic carbon capture and storage to produce negative CO<sub>2</sub> emissions. Carbon-negative technologies such as BECCS might be an important component of overall strategies to reduce atmospheric CO<sub>2</sub> concentrations. If demand for carbon mitigation and associated offsets increases, BECCS could become a major strategy to achieve carbon management, which could provide additional revenue streams and value propositions for the emerging bioeconomy. To better understand the national potential

| WBS:                      | 2.1.0.502           |
|---------------------------|---------------------|
| CID:                      | NL0034938           |
| Principal Investigator:   | Dr. Mark Langholtz  |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$667,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$667,000           |
| Project Status:           | New                 |
|                           |                     |

for BECCS in the United States, the cost of BECCS as a function of both biomass feedstock and its proximity to geologic formations suitable for BECCS needs to be quantified. The costs of BECCS on a per-ton  $CO_2$  basis are influenced by logistic configurations, feedstock availability, proximity to suitable geologic sequestration basins, and techno-economic assumptions. Thus, it is critical to identify how a nationwide infrastructure for biomass processing, logistics, conversion, and sequestration could provide the capacity to meet increasing demand for carbon offsets. An economic assessment of BECCS requires capabilities in biomass supply and yield analysis (feedstock carbon flux), biomass logistics, and supply-chain modeling. Biomass supply analytics capabilities at ORNL are well suited to these analyses of BECCS. Online interactive visualization of the *2016* 



Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f ar I}$  One standard deviation of reviewers' scores

*Billion-Ton Report* demonstrates both the analysis capabilities at ORNL and the reach and accessibility of online resources that can be leveraged from the Bioenergy Knowledge Discovery Framework (KDF). The Biomass Infrastructure Logistics and Transportation model developed at ORNL with DOE support is applicable to analysis of the spatial allocation of feedstocks and CO<sub>2</sub>. The Center for Transportation Analysis at the National Transportation Research Center provides resources for spatial modeling of national infrastructure. External resources relevant to this project include National Energy Technology Laboratory's Carbon Capture and Storage Database and the National Carbon Sequestration Database and Geographic Information System.

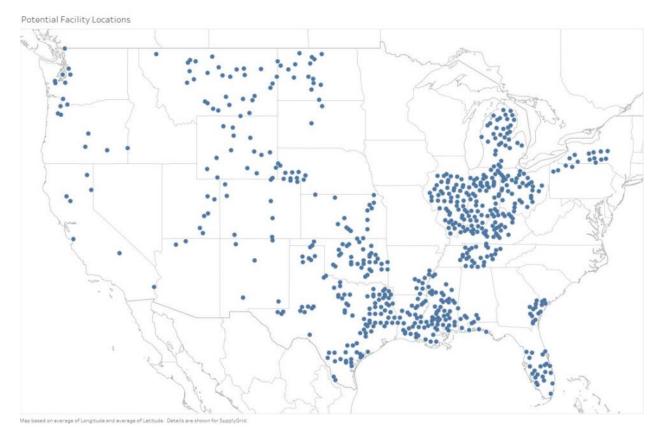


Photo courtesy of Oak Ridge National Laboratory

# **OVERALL IMPRESSIONS**

- This new project is addressing an area not yet fully explored by BETO as a potential ancillary revenue stream for the bioeconomy industry, with the appropriate goal to quantify and estimate costs associated with managing CO<sub>2</sub> through BECCS.
- This project will be a valuable component of BETO's increasing focus on carbon management, and it will help us understand the potential contribution of BECCS to overall national carbon management. A peer-reviewed publication or report would be a helpful final deliverable as well as the KDF landing page. If this approach is likely to have significant potential for carbon sequestration and carbon management in the economy, other avenues of results dissemination (e.g., stakeholder meetings) should also be considered. It should also be explicit that this project will complement the broader BETO carbon management analyses/programs.
- This project will assess the potential quantity and economic feasibility of CO<sub>2</sub> management in the U.S. bioeconomy through BECCS.

- This research focuses on BECCs, which is a key rising issue/concept in bioeconomy. Supply curve development is an interesting/useful approach—it is based on actual geospatial data on feedstock as well as facility siting. It would be useful to broaden the concept of BECCS for this research by evaluating pathways other than injection as well as considering CO<sub>2</sub> stream sources other than bioethanol.
- As mentioned elsewhere, it would be worth considering a merger or at least direct coordination between this effort with other BECCS project in the BETO portfolio. The two would dovetail nicely, with this project bringing geospatial rigor while the other could contribute its broader scope.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for this feedback.
- We agree that results in accessible literature will be valuable products from this project.
- We agree that coordination with other projects involved in carbon management is valuable.

# HARNESSING THE BIOECONOMY FOR CARBON DRAWDOWN: POTENTIAL AND INNOVATION NEEDS

# Lawrence Livermore National Laboratory

# **PROJECT DESCRIPTION**

| Integrated assessment modeling has identified the                    |  |  |
|--|--|--|
| importance of establishing robust and large-scale CO <sub>2</sub>    |  |  |
| removal technologies to reduce atmospheric CO <sub>2</sub>           |  |  |
| concentrations. CO <sub>2</sub> removal technologies include both    |  |  |
| physical (so-called "direct air capture") and biological             |  |  |
| strategies. This project focuses on bioeconomy pathways, a           |  |  |
| subset of biological CO <sub>2</sub> removal technologies, which are |  |  |
| specified combinations of biological feedstocks,                     |  |  |
| conversion processes, and products. The goal of this                 |  |  |
| project is to compare the techno-economic analysis (TEA)             |  |  |
| potential of multiple, diverse bioeconomy pathways to                |  |  |
| draw down CO <sub>2</sub> from the atmosphere. Potential pathways    |  |  |
| include biopower with CO <sub>2</sub> capture and sequestration,     |  |  |
|  |  |  |

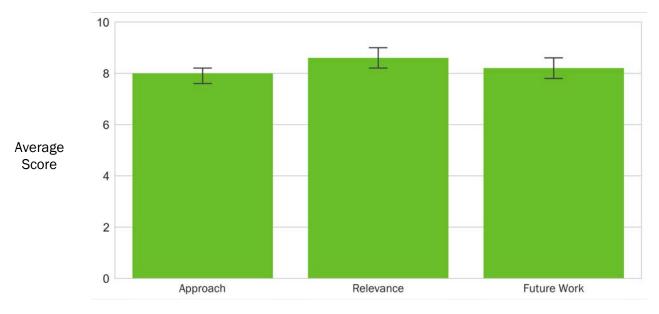
| 2.1.0.503           |
|---------------------|
| NL0034850           |
| Dr. A.J. Simon      |
| 10/1/2018-9/30/2019 |
| \$167,915           |
| \$0                 |
| \$0                 |
| \$167,915           |
| \$0                 |
| New                 |
|                     |

biofuels with process CO<sub>2</sub> capture, bioplastics and other chemical products, and biochar applied to augment soil carbon storage.

Each molecule of biogenic  $CO_2$  (from, for example, the use of a biogenic energy carrier) has the same radiative forcing as any other molecule of  $CO_2$ , and the avoidance of its emission has the same value as avoiding fossil emissions. The traditional assumption of excluding biogenic  $CO_2$  from emissions accounting is insufficient to capture the value of bioeconomy pathways. This project advances methods for carbon accounting in scenarios

# Weighted Project Score: 8.2

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

that include negative emissions. To date, we have enumerated myriad bioproduct pathways and qualitatively rated them on both technological and market readiness. We have also developed an LCA framework that leverages existing LCA tools and extends their carbon accounting to the feedstock production, conversion, use, and disposition life-cycle stages of bioeconomy pathways designed for carbon drawdown.

## **OVERALL IMPRESSIONS**

- This meta-analysis of proposed carbon drawdown and management approaches will be an important baseline study for BETO's expanding focus on carbon management in the bioeconomy. It is important that we understand the option space for reducing atmospheric greenhouse gases (GHG), and this study will provide a consistent framework for comparing those options. This initial qualitative analysis should eventually transition to more quantitative approaches (similar to the BECCS study) to help understand the relative importance of these potential technologies/approaches within the bioeconomy for reducing/managing atmospheric CO<sub>2</sub>.
- This project pursues important questions surrounding the economics of BECCS systems integrated with agro-industrial systems generating a suite of products and ecosystem services. The researchers have carried out a strong meta-analysis evaluation of technology readiness, market readiness, and other technical factors. This project pursues a strategic direction and is well integrated with BETO goals.
- It would be worth considering a merger or at least direct coordination between this effort with other BECCS project in the BETO portfolio. The two would dovetail nicely, with the other project bringing geospatial rigor while this one would bring expanded scope.
- This project will use TEA to evaluate and rank various bioeconomy pathways to draw down CO<sub>2</sub> from the atmosphere, which is a valuable (albeit unconventional) space for BETO to fund.
- Because atmospheric CO<sub>2</sub> reduction is one of the main (even if only implied) justifications behind favorable bioenergy policies and research programs around the world, this project should help research portfolio managers better understand the GHG significance of a variety of projects (from sequestration to fuels and bioproduct development).
- Carbon drawdown is an important issue. The goal is to compare the technical and economic potential of the bioeconomy pathways to draw down CO<sub>2</sub> from the atmosphere. This is a preliminary analysis project qualitative mete-analysis and quantitative analysis of four to five selected pathways based on CO<sub>2</sub> drawdown. Carbon management informs the R&D community and longer-run decision makers. This is a new project.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# SCIENTIFIC METHODS FOR BIOMASS REFERENCE SCENARIOS

# **Oak Ridge National Laboratory**

## PROJECT DESCRIPTION

The goal of this project is to engage stakeholders in a process to develop and test a protocol for reference scenarios involving bio-based systems. The protocol will provide a set of rules and procedures for selecting reference scenario input parameters and documenting the choices used to characterize the reference scenario. This is important because under the current state of the art, variable and inconsistent assessment results have been attributed to different reference scenario assumptions. The lack of standard procedures constrains fair and comparable analysis, confuses decision makers, and undermines clear communications and trust among stakeholders. The project invited interested experts from diverse backgrounds to

| WBS:                      | 3.1.3.3             |
|---------------------------|---------------------|
| CID:                      | NL0033318           |
| Principal Investigator:   | Mr. Keith Kline     |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$250,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$250,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Ongoing             |
|                           |                     |

develop consensus around what an appropriate reference scenario should contain when assessing the effects of biomass-based products. The project addresses a fundamental issue, relevant to most BETO A&S activities and other DOE Office of Energy Efficiency and Renewable Energy (EERE) projects. A literature review, conducted at the project's start, verified the need for better guidance to support transparent and reasonable reference scenario assumptions.

# Average Score 4 2 0 Approach Accomplishments & Progress

# Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

op One standard deviation of reviewers' scores

Project status (40% complete):

- More than 60 participants from civil society, industry, universities, government agencies, private research centers, standards-setting bodies, 11 international organizations, and industrial interests contributed to the literature review as well as drafting and discussions to develop a first draft
- The draft protocol was distributed to more than 100 stakeholders for further review and comment
- An action plan to address comments received was developed and reviewed by the drafting team.

The draft protocol provides key definitions that occupy four pages of single-space text. Definitions include:

- Reference scenario: characterization of conditions that would occur in the absence of the bio-based option (the test case being studied)
- Test scenario: characterization of conditions that occur under the test case that are relevant to the assessment goal.

The team defined the scope as:

- Analyses, evaluations, and comparisons of options to supply energy, chemicals, and other products and coproducts when one option involves biomass as a feedstock. These analyses include but are not limited to LCA, sustainability analyses, and TEA.
- Reviews and evaluations of the suitability of the reference scenario selected for an existing study or comparison.
- All bio-based production systems and materials, including forestry, agriculture, residues, coproducts, and wastes.

The action plan lays out steps for future work:

- Changes recommended by stakeholders will be incorporated into three documents: a literature review and rationale manuscript, an ASTM International standard (initiated December 2018, based on the initial draft protocol), and a paper recommending best practices for reference scenario development and documentation.
- The draft protocol will be tested in partnership with other BETO projects, and these trial applications will both help address specific project needs and provide additional feedback to improve the final protocol.

The expected outcomes of this project are:

- Net effects of an expanding bioeconomy are more clearly and consistently documented
- Best practices for a science-based approach to justify parameters used in reference scenarios will be published
- An international standard will provide guidance to increase the comparability and transparency of input values and assumptions when assessing the relative sustainability of bio-based products
- Two manuscripts will be prepared for peer-reviewed publication
- The application of the protocol generates more consistent quantification of tradeoffs and opportunities to guide decision making.

Figure: What would happen in absence of a bioenergy option? There are many potential answers to such questions. This project provides guidelines for identifying an appropriate reference scenario.



Photo courtesy of Oak Ridge National Laboratory

#### OVERALL IMPRESSIONS

- This project seeks to develop and test a protocol for reference scenarios involving bio-based systems. The PI has astutely identified the challenge posed by the subjectivity inherent in many LCA studies and seeks to address this through a novel protocol that would enable comparability and transparency across analyses as well as robust meta-analysis. This is a worthwhile agenda, but it poses two key challenges:
  - There might not be a definitive reference case, and if there is, BETO is not positioned to be the final arbiter on what it should look like
  - No civil society involvement means missing a key constituency for this research and a risk in failing to establish consensus.
- This project aims to address a long-term, crosscutting gap in bioenergy research: to establish and articulate reference scenarios.
- Although the team has clearly done an extensive literature review and stakeholder engagement, some audience members had trouble understanding and/or imagining tangible outcomes of this work.
- This is a new project, begun last year (funded under the Advanced Development and Optimization [ADO] platform).
- Better guidance is needed to support more transparent and reasonable reference scenario assumptions. The objective of this is to engage with a broad group of stakeholders in a process to develop and test a protocol for reference scenarios involving bio-based systems. The protocol will provide a defined set of rules and procedures for selecting reference scenario input parameters and documenting the choices used to characterize the reference scenario.
- This project addresses the following barriers: At-E: Quantification of Economic, Environmental, and Other Benefits and Costs; and ADO-C: Codes, Standards, and Approval for Use.
- A reference scenario is an essential starting point from which to measure impacts and inform how synergies can be enhanced and tradeoffs minimized.

• Every study needs a reference scenario, and it is valuable to have a well-defined approach to generating reference scenarios. The challenge will be in creating a scalable approach that fits multiple analysis types as well as dissemination for practical use. Although all can agree that in general it is important to build an appropriate reference scenario, there are valid reasons for people to differ in their assumptions and interpretations when developing a reference scenario that such a protocol cannot address. It will be interesting to see this overall protocol once finalized.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you. Two points of clarification: Civil society was invited and has participated in many forms. One of our constructive contributors, for example, works for the Union of Concerned Scientists. Regarding the observation that there "might not be a definitive reference case," we agree. Indeed, the draft protocol noted that there is an infinite number of potential reference scenarios, and the best choice might be to use more than one to frame the results within a reasonable range.
- Thank you. Tangible results include: (1) consensus-based journal publications with definitions of key terms and best practices, (2) an ASTM International standard balloted and published, and (3) clear guidance to improve comparability and transparency of input values and assumptions used in assessments of effects of bio-based products. We are also applying the protocol in two case studies.
- Thank you. We agreed that challenges are many; yet, thus far, we appear to have a "scalable approach." We welcome contributions to help address challenges constructively. The differing perspectives might represent challenges, but they also make the process enlightening and interesting for participants.

# GREET DEPLOYMENT AND BIOFUEL PATHWAY RESEARCH AND ANALYSIS

# **Argonne National Laboratory**

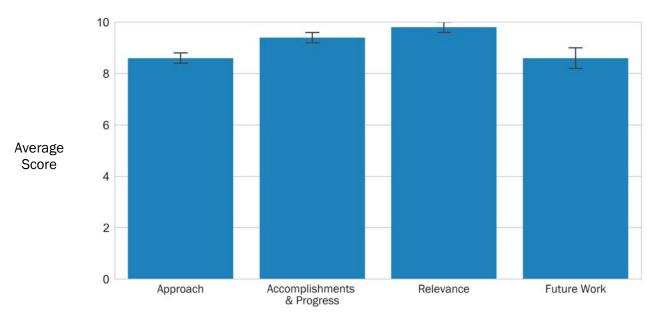
# **PROJECT DESCRIPTION**

With BETO support, ANL has been developing the GREET model to conduct LCA of biofuel bioproduct pathways to holistically quantify energy and environmental effects of production and use of biofuels and bioproducts. The model and its results have been used by BETO and other agencies and organizations to provide information about the system-wide energy and environmental implications of biofuel bioproduct systems to help R&D and other policy decisions. With this project, ANL has been able to develop the GREET model with modeling consistency and transparency and to provide BETO and the bioenergy community with rigorous, reliable, and timely results in responding to key questions regarding biofuel bioproduct energy and environmental sustainability.

| WBS:                      | 4.1.1.10            |
|---------------------------|---------------------|
| CID:                      | NL0026651           |
| Principal Investigator:   | Dr. Michael Wang    |
| Period of<br>Performance: | 10/1/2014-9/30/2020 |
| Total DOE Funding:        | \$4,327,077         |
| DOE Funding FY16:         | \$1,462,000         |
| DOE Funding FY17:         | \$262,000           |
| DOE Funding FY18:         | \$1,343,077         |
| DOE Funding FY19:         | \$1,260,000         |
| Project Status:           | Ongoing             |
|                           |                     |

# Weighted Project Score: 9.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

ANL's key accomplishments since March 2017 include:

- Adding new biofuel and bioproduct pathways and updating baseline pathways—for example, by conducting LCA of jet-fuel pathways for BETO and the International Civil Aviation Organization
- Organization of United Nations assessing water stress from GREET-simulated water consumption results and conducting supply-chain sustainability analysis
- Addressing emerging LCA issues, such as how to assign metrics to coproducts from integrated biorefineries with a large amount of bioproduct output and tracking the carbon flows, carbon sources, and sinks of bioplastics versus fossil plastics
- Quantifying the carbon balances for woody feedstock systems, including land-use change (LUC), soil organic carbon flux, and woody feedstock carbon flows throughout time
- Providing in-depth environmental systems analysis of new conversion technologies, including waste-toenergy pathways, industrial waste CO<sub>2</sub> to bioenergy, and advanced algal systems.

GREET has been an integral part of BETO analysis to address bioenergy sustainability with consistent, complete modeling of the bioenergy supply chain with close interactions with other national laboratories, agencies, and key stakeholders. ANL has published extensively to document data, methods, and results of GREET model development and applications. At present, there are more than 35,000 registered GREET users globally, with key users including governmental agencies, conventional and new energy companies, universities, and research institutions.

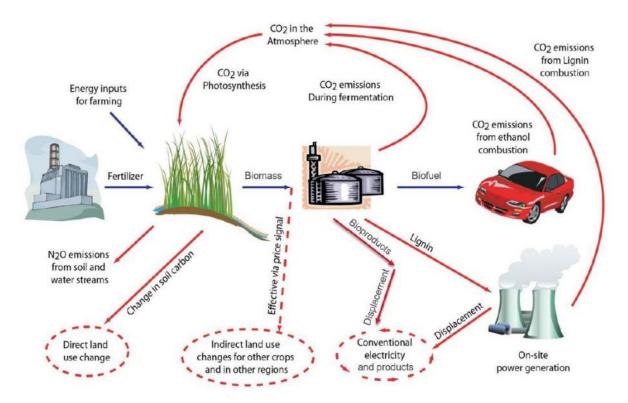


Photo courtesy of Argonne National Laboratory

### OVERALL IMPRESSIONS

- GREET is a longstanding (since 1994) DOE-sponsored tool that is respected and used to shed insight on direct and indirect environmental impacts (and tradeoffs) from transportation fuel production and supply systems.
- GREET was a useful resource during my Ph.D. a decade ago, and it is great to see that the tool and team have evolved to help answer emerging questions relevant to the large community of policy-focused and academic research-oriented users.
- GREET is a widely used and trusted model, and the recent advances have made it even more comprehensive. To continue to bolster the already high credibility of the model, the GREET team should continue to work with other teams on parallel LCA or external reviews to continue to enhance verification and validation of the model, and the team should work with other teams from national laboratories when incorporating additional sustainability aspects.
- I have some concern about the scope of GREET and whether Available Remaining Water for the United States is at the same level of quality and validation as GREET's core strengths. I would like to see the GREET team leverage the depth of expertise in other team's modeling water availability and water footprinting (e.g., the WATER modeling group) and maintain the overall quality and trust in GREET by putting equal care into the water scarcity analysis/tool as is used for the core GHG LCA modeling and data quality. GREET could represent an opportunity to integrate several additional tools, resources, and analytic approaches in the long term, and it is important that it be as strong in these additional areas (e.g., water scarcity) as it is on the GHG LCA side. Leveraging strengths from other teams will ensure that the quality remains even across different modules if GREET is expanded further to incorporate other sustainability considerations besides GHG emissions.
- The overall objective to identify and quantify the life-cycle energy and environmental impacts of biofuels with analytic tools is supportive of the EERE BETO mission. The analytic capabilities of the GREET model and the ANL team support the BETO mission to enable sustainable, nationwide production of biofuels that are compatible with today's transportation infrastructure and can reduce GHG emissions relative to petroleum-derived fuels.
- GREET is the giant in the biofuel LCA space. This brings many opportunities and strengths, but there are also some potential liabilities. This is perhaps the A&S portfolio's most impactful effort because it has influenced analysis and policy broadly, and it should be supported and expanded.
- GREET risks becoming an industry unto itself as it continues to grow. Any error or debatable assumption is amplified as other researchers and policies use the tool. BETO should consider funding a critical analysis of GREET to evaluate sensitivities, the impact of key assumptions, etc. Also, is expanding GREET's scope to cover further-flung feedstocks (e.g., waste CO<sub>2</sub>, woody feedstock carbon dynamics throughout time) and alternative end products (e.g., bioplastics) limiting development of targeted LCAs in these spaces and weakening GREET's role as it becomes a jack-of-all-trades?

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The GREET team thanks the reviewers for their encouraging comments and constructive suggestions. We work hard to meet the needs of our stakeholders with rigorous analyses; holistic and peer-reviewed approaches; and up-to-date, high-quality, transparent, and complete data in GREET. The GREET project is focused on BETO's priorities, and we keep a close eye on emerging issues to inform BETO.
- The expansion of GREET's scope responds to the need for more inclusive analysis capabilities to support the development of a prosperous bioeconomy. As R&D progresses, designs incorporate additional feedstock options, carbon sources, and bioproduct outputs to address economic and

sustainability goals. Wastes and forest residues are included as attractive feedstocks because they do not put pressure on agriculture land or product markets, while offering a means to use waste materials in a cost-effective and environmentally beneficial manner. Meanwhile, bioenergy pathways producing multiple value-added coproducts, such as biochemicals and bioplastics, improve market scalability and environmental profiles.

- We would welcome the opportunity to perform a critical analysis of GREET to identify areas where GREET's capabilities should be expanded to meet stakeholder needs moving forward.
- We recognize that LCA is inherently integrative and interdisciplinary. We work closely with collaborators to coordinate and streamline efforts across BETO projects. There appears to be confusion regarding GREET LCA, WATER, and the available water remaining in the United States (AWARE-US). All are part of the ANL biofuel analysis team. GREET LCA tracks water consumption across the life cycles of fuels, vehicles, and products. WATER estimates the water available in a region for new feedstock growth. AWARE-US estimates regional water stress, considering hydrologic factors as well as existing anthropogenic demand. These three efforts use common inputs and shared outputs to address different aspects of bioenergy water sustainability. We will continue to work closely with the other BETO projects and external collaborators to improve and integrate these efforts.
- Moving forward, we will remain focused on quantifying the life-cycle energy and environmental impacts of bioenergy and bioproducts to inform R&D and business decisions related to the developing bioeconomy.

# STRATEGIC ANALYSIS SUPPORT

# National Renewable Energy Laboratory

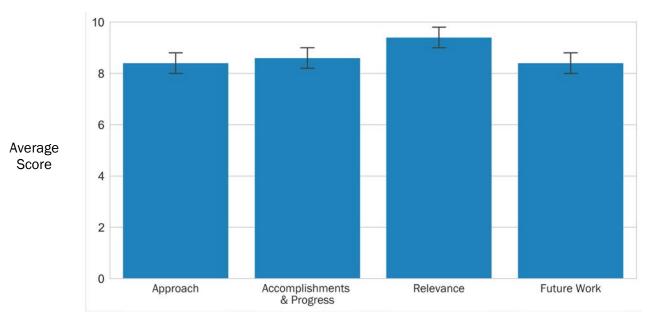
## **PROJECT DESCRIPTION**

The objective of the NREL strategic support project is to provide sound, unbiased, and consistent analyses to inform the strategic direction of the DOE BETO office. This project addresses key technological questions; provides critical data needed to inform strategy; and highlights barriers, gaps, and data needs in support of the DOE BETO mission to improve the affordability of bio-based fuels and products.

This task employs various quantitative (TEA) and qualitative (gap analysis) approaches to allow for direct comparisons of biomass conversion technologies across a wide slate of processing platforms and products. Further,

| WBS:                      | 4.1.1.30            |
|---------------------------|---------------------|
| CID:                      | NL0027592           |
| Principal Investigator:   | Dr. Mary Biddy      |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$2,532,325         |
| DOE Funding FY16:         | \$650,000           |
| DOE Funding FY17:         | \$500,000           |
| DOE Funding FY18:         | \$932,325           |
| DOE Funding FY19:         | \$450,000           |
| Project Status:           | Ongoing             |
|                           |                     |

this project develops and uses novel analyses beyond traditional biorefinery-focused TEA LCA to identify both technical (e.g., in sustainable design) and nontechnical (e.g., in value proposition) barriers as well as to outline mitigation strategies and R&D needs for emerging technologies. Additionally, the project is tasked with evaluating drivers that support the growing bioeconomy, which is achieved by the development and public release of tools to advance the understanding and facilitate comparisons of socioeconomic impacts along the supply chain.



# Weighted Project Score: 8.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

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 and reviewing the results of these analyses to overcome this challenge. Any remaining uncertainties associated with the analysis efforts are clearly defined and quantified.

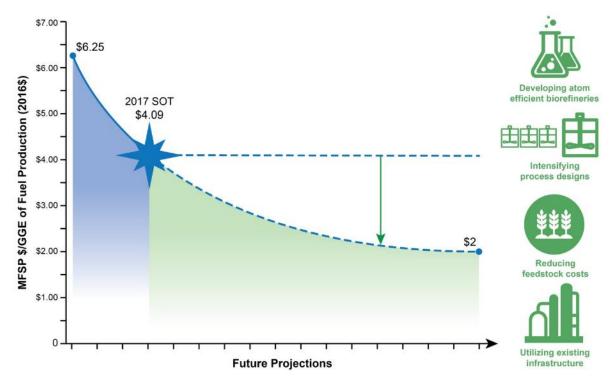


Photo courtesy of National Renewable Energy Laboratory

# **OVERALL IMPRESSIONS**

- This multifaceted program, started in 2010, has played an important role in shaping BETO's strategic shifts (e.g., ethanol to drop-ins and bioproducts), and the team continues to stay relevant by developing tools to address technical and financial barriers to the deployment and adoption of bioenergy and bioproducts.
- The strategic analysis support team provides a key function for the A&S portfolio by integrating data from many BETO studies into publicly accessible databases and by executing strategic analyses that the project teams should focus on more deeply, such as the analysis to identify key cost drivers for biofuels. This is a broad suite of analyses that effectively contribute to the strategic integration and communication of the BETO portfolio. The intentions to develop a common approach of transparent/rigorous models with consistent assumptions, detailed vetting by stakeholders, and communications are great. Following are a few specific comments on individual pieces of this portfolio:
  - It's not clear from the summary of the TEA database whether the authors include a sensitivity/range of TEA parameters (or some sort of guidance for stochastic TEA) in the database itself for a given element or if there is a function for crowdsourcing data (e.g., enabling outside researchers to submit data for review/inclusion).

- It would be helpful to know if the cost-reduction levers from the aviation fuel \$2.50/gal analysis are the same or different from the \$2/gasoline gallon equivalent (GGE) gap analysis.
- The strategic goal to identify job creation and the economic benefit of the bioeconomy seems to have significant opportunities to connect with the integrated LCA project and should clearly indicate if results are an input to the latter.
- The use of the EPA's GREENSCOPE tool requires a lot of data for a variety of different sustainability performance indicators and perhaps should be a joint effort among multiple teams to leverage the depth of knowledge on the different performance criteria.
- This project develops tools and performs analyses to address key questions and provide key data needs in support of the strategic direction of the DOE BETO. The objective of the NREL strategic support project is to provide sound, unbiased, and consistent analyses to inform the strategic direction of the DOE BETO office.
- This project addresses the following barriers: At-A: Analysis to Inform Strategic Direction; At-D: Identifying New Market Opportunities for Bioenergy and Bioproducts; and At-E: Quantification of Economic, Environmental, and Other Benefits and Costs.
- The Jobs and Economic Development Impact (JEDI) model and the TEA database seem strong, but GREENSCOPE seems to be biting off too much to do it rigorously.
- This it generally true, but especially for the emerging technologies, that this project group rightly identifies as warranting detailed evaluation. It is not clear how to achieve this detailed level of evaluation on emerging technologies for which there might not be much data. Does this project have necessary buy-in across the BETO portfolio? Its efficacy depends on other research teams feeding data into this analysis. It is not this team's fault, but too many such projects could risk engagement fatigue across research teams.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their helpful insights and feedback. Our team works to be highly integrated within the A&S platform portfolio and the overall BETO portfolio. For example, the job analysis work is highly integrated with the A&S-supported integrated LCA project as well as with the Co-Optimization of Fuels and Engine analysis efforts, among others. For the TEA and the GREENSCOPE tasks, our team works closely with researchers within the other BETO-supported platforms and with external collaborators to ensure we use the best information available as well as the most appropriate methodologies for our analyses. As we continue to apply the GREENSCOPE methodologies to emerging technologies, we will work closely with the researchers and analysts developing these ideas to ensure we have the most up-to-date and best information. We will continue to perform sensitivity analysis and uncertainty evaluations to understand the impact that assumptions have on the underlying output of these studies. The goal for all our analyses is to develop defensible studies and tools in support of the strategic direction of the DOE BETO.
- We have been using the JEDI outputs to inform the integrated LCA project with respect to job growth opportunities and economic impacts along the entire supply chain. Because most biofuel pathways have not been commercialized and are not represented in the USEEIO model, the method to disaggregate the industrial sectors in the JEDI model for these pathways is also used to inform the disaggregation of the USEEIO model for the integrated LCA.

# SUSTAINABLE BIOMASS THROUGH FOREST RESTORATION

# **Pacific Northwest National Laboratory**

## PROJECT DESCRIPTION

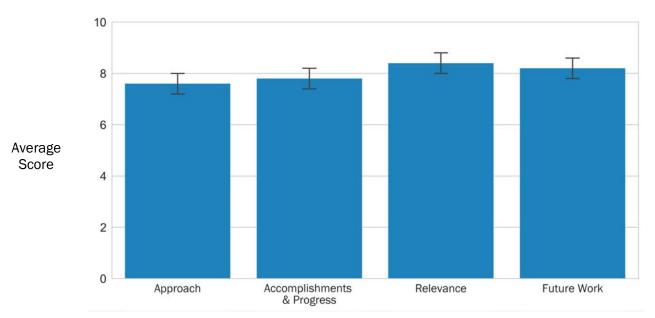
Forest restoration has the potential to reduce high fuel loads and fire risk; provide a significant source of bioenergy; and provide increased ecosystem services, such as improved flow regimes for aquatic habitat. However, additional planning and decision-support tools are needed to ensure economic and environmental sustainability. A multiagency collaboration between DOE and the U.S. Forest Service (USFS) is using high-resolution, 30-m by 30-m topographic, soils, and vegetation data along with detailed road network data to develop accurate estimates of sustainable forest biomass along with distributed hydrologic, ecological, and wildfire risk modeling. Location-specific restoration scenarios are developed

| WBS:                      | 4.1.1.52            |
|---------------------------|---------------------|
| CID:                      | NL0032233           |
| Principal Investigator:   | Dr. Mark Wigmosta   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$681,887           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$220,000           |
| DOE Funding FY18:         | \$261,887           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

based on measured departure in ecological patterns of vegetation structure composition and modeled potential for spread of large wildfires. The Distributed Hydrology Soil Vegetation Model (DHSVM) is used to assess the impacts of the fine-scale forest restoration scenarios on hydrologic conditions, including snowpack and the timing, temperature, and volume of streamflow. DHSVM spatiotemporal outputs are used in a network modeling approach to articulate causal pathways between alternative restoration strategies on ecosystem services that provide input to the Ecosystem Management Decision Support (EMDS) software. EMDS provides multi-objective logic and decision support to select the locations and type intensity of restoration to achieve desired outcomes based on user-defined criteria and our sustainability indicators. EMDS is the USFS

# Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

corporate software solution for decision support and has been used by the USFS and bureaus of the U.S. Department of the Interior since 2006 to evaluate wildfire potential across all administrative units in the continental United States and to establish priorities for allocating fuel-treatment budgets.

These data and models are integrated in a multi-objective analysis framework to assess the extent of forestthinning activities that restore landscape function to reduce high fuel loads while increasing biomass yield and streamflow in a publicly and ecologically acceptable manner. 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. Initial results confirm the need for high-resolution data to properly represent hydrologic and ecological process as well as detailed road network data to estimate delivered costs of biomass for energy. We demonstrated the potential of forest restoration to provide sustainable biomass for energy considering cost, wildfire mitigation, and improved streamflow. Particularly in areas where snowpack supplies late season flows (typical of the western United States), forest restoration can help increase flow during critical salmon-rearing periods while reducing flows in the spring and winter during incubation and emergence.

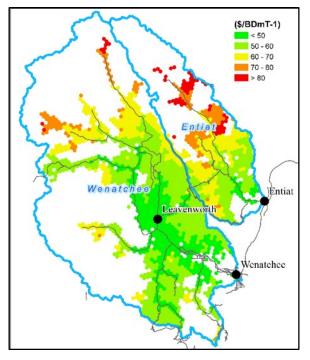


Photo courtesy of Pacific Northwest National Laboratory

# **OVERALL IMPRESSIONS**

- This is a valuable, albeit niche, project characterizing potential win-wins for improved forest management and increased availability of bioenergy feedstock.
- This project addresses a very timely and important goal in developing and demonstrating an analysis framework to prioritize how and where to target forest restoration (timber harvest and thinning) and fuels reduction to have the greatest benefit for bioenergy, reduce severe wildfire risk, increase water yield, and improve ecosystem services. This is aligned with BETO goals. My concern is with the scope of the analysis the team is attempting in one study. Touching on restoration ecology, fire modeling, economics, hydrology, and other analytic frameworks is a risky proposition for a project of this size.
- This project is extremely relevant—forestry biomass has been identified in each of the *Billion-Ton* reports as a major source of biomass. Developing and providing decision-support tools demonstrating that harvesting forest materials can be done sustainably and lead to environmental benefit is essential.

Regarding reducing forest fire risk, additional planning and decision-support tools are needed to assess ecosystem services.

- This project addresses key BETO goals for Analysis and Sustainability.
- This project assesses the potential for synergistic achievement of forest thinning and fire management with bioenergy production while protecting biodiversity. The data from this analysis will provide valuable information to stakeholders about the potential to balance tradeoffs and achieve environmental goals in this system. The team indicated that this forest management is an ongoing process that would allow for repeated harvests throughout time (sustainable production) but did not clearly indicate whether the intention is to move toward controlled burns on the managed lands, which would reduce bioenergy feedstock availability.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Forest restoration is being used to reduce wildfire risk and has been identified as a potentially significant source of bioenergy (0.2–0.6 billion tons in five western states per DOE). As noted, this project is characterizing potential win-wins for improved forest management and increased availability of bioenergy feedstock—specifically, by developing and demonstrating an analysis framework to prioritize how and where to target forest restoration (timber harvest and thinning) to have the greatest benefit for bioenergy, reduce severe wildfire risk, increase water yield, and improve ecosystem services. Beyond forest restoration, the framework can be used to evaluate economic and environmental tradeoffs associated with other forest-derived biomass, estimated in the *2016 Billion-Ton Report* at 103 million and 97 million tons per year of biomass potentially available in 2017 and 2040, respectively.
- Given the broad scope of this project, each task has a designated lead based on expertise. We are primarily using existing models that have been exercised (independently) in the study domain. This work builds on a previous USFS-PNNL collaboration (funded by the State of Washington) to develop a tool to estimate the impact of forest restoration on streamflow but without consideration of biomass yield or decision support. We chose an existing USFS decision-support system to speed technology transfer.
- Future enhancements include simulating the impacts of forest regrowth on biomass yield and the impacts of restoration on smoke and GHG emissions. This will allow consideration of repeated harvests throughout time to estimate sustainable production rates of biomass, continued reduction of wildfire intensity, and improved streamflow and salmon habitat. We can also identify the reduction in smoke emissions with restoration compared to natural wildfires and the reduction in emissions through the collection of forest residue for energy rather than disposal through prescribed burning.

# SYSTEMS INTEGRATION SYSTEMS-LEVEL ANALYSIS

# National Renewable Energy Laboratory

## PROJECT DESCRIPTION

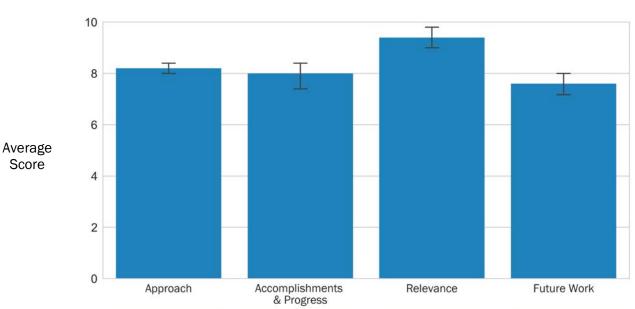
Systems Integration Systems-Level analysis maintains a readily available, established, expert analysis resource for BETO to respond to high-level internal analysis requests. This enables BETO's prioritization, rebalancing, and justification for the distribution of projects and funding across the BETO portfolio. It also enables cross-model coherence for accurate, consistent modeling and analysis results, improves A&S program effectiveness, and supports BETO planning.

Using an interdisciplinary approach in close partnership with BETO, this work encompasses three categories: (1) A&S Program support, (2) emerging analysis, and (3) systems-level analysis.

| WBS:                      | 4.1.2.1             |
|---------------------------|---------------------|
| CID:                      | NL0022704           |
| Principal Investigator:   | Ms. Amy Schwab      |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$2,427,120         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$1,300,000         |
| DOE Funding FY18:         | \$627,120           |
| DOE Funding FY19:         | \$500,000           |
| Project Status:           | Ongoing             |
|                           |                     |

The A&S program support task supports A&S management to improve the A&S portfolio effectiveness by developing frameworks to manage BETO's model portfolio. This helps monitor and communicate the depth and breadth of this complex, multidimensional portfolio while identifying concrete improvements.

The emerging analysis task focuses on maintaining capabilities for quick turnaround or emerging analysis topics. Anticipating trends, issues, and topics, and bringing together experts across the BETO laboratory



# Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

community, this task provides analysis capabilities in BETO's planning processes while providing a conduit for updating modeling assumptions from the latest technology and industry developments.

The systems-level analysis task provides focused, in-depth analysis on key internal topics. Future work on industrial learning curves is aimed at understanding factors influencing a growing bioenergy industry, factors influencing bioenergy technology R&D progress, and how BETO can leverage these factors.

#### **OVERALL IMPRESSIONS**

- This is a critical program for BETO to essentially view a dashboard and understand the interconnections across its modeling efforts, enabling project managers to quickly identify expertise, gaps, and steps forward to address emerging modeling questions.
- This work is crosscutting across all laboratories and BETO headquarters. BETO has developed and maintains a huge complement of models, supporting data, and modeling expertise that enable BETO to provide analytic and quantitative analyses across current issues, identify gaps and weakness to improve analytic capacity, and refine decision support.
- The model mapping carried out in this project is an important agenda with potential to create actionable information for BETO portfolio managers. Is it providing useful information that can be used to shape the program? If not, it warrants evaluation and reshaping.
- The maps generated through this analysis appear to imply there is a lot of overlap in the BETO model portfolio—probably more than there really is. Perhaps it would be worth indicating graphically the currently supported models so that it does not seem like there is so much potential/probable overlap?
- This project encompasses several different efforts to inform the strategic direction of the A&S portfolio. The model map provides useful insight into the interconnections among models and where models reside in terms of their analytic approach and aspects of the supply chain, and it would be made even more useful as a communications tool by further differentiation, perhaps over several versions of the map (e.g., eliminate defunct/no-longer-funded models or color-code models based on specific elements). The proposed effort to enhance and harmonize industrial learning approaches across BETO projects would be a valuable step toward overall harmonization of assumptions and metrics in the portfolio as long as there is buy-in from the modeling/research teams.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate recognition of the value of this model mapping effort.
- The ability of this effort to provide actionable information is evidenced by portfolio actions that BETO has taken based on our initial analysis. As noted in the presentation, the maps presented, which were selected by BETO as the single snapshot depicting the overall portfolio in FY 2017, do not fully capture the multiple dimensions that characterize the models that our effort captured. We plan to work with BETO in the future to ensure that visualizations are effective for the map.
- As mentioned, we presented only two of the variations of maps that were produced and provided as part of this project.

# ECONOMIC ANALYSIS OF RISK

# Idaho National Laboratory

### **PROJECT DESCRIPTION**

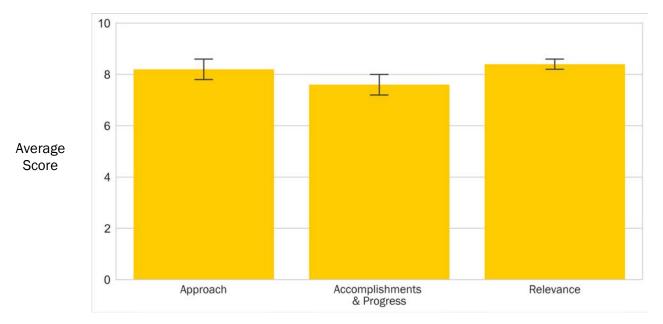
Advancing the cellulosic industry hinges on the ability to quantify risk, and feedstock risk is one of the greatest impediments today. This point repeats itself in stakeholder engagement and literature findings as a key impediment to industry growth. A clear and present need is to identify and reduce risk exposure along the feedstock supply chain; however, today, inconsistent methods for analyzing risks in the feedstock supply chain lead to an investment barrier in the form of high financing costs. Because the industry is in its infancy, the lack of historical data increases perceived investor risks, which amplifies the need for a quantitative, simulation-based approach. Tackling one aspect of risk, the goal of this project is to design and

| WBS:                      | 4.1.2.20            |
|---------------------------|---------------------|
| CID:                      | NL0026663           |
| Principal Investigator:   | Dr. Jason Hanson    |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$1,118,177         |
| DOE Funding FY16:         | \$250,000           |
| DOE Funding FY17:         | \$570,047           |
| DOE Funding FY18:         | \$298,130           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

develop a tool for quantifying cost risk, on an economic basis, in the feedstock supply chain. Project researchers developed the Stochastic Techno-Economic Model (STEM), which simulates possible cost outcomes from which risk can be quantified and then compared across supply chain design alternatives. STEM enables consistent, systematic modeling on an economic basis. Applying the model, researchers have quantified uncertainty in alternative supply chain design configurations, by each unit operation, then translated modeled uncertainty to a logistics distribution of costs to assess risk. The STEM contributes to systems-level risk analysis by generating potential outcomes against which researchers, project developers, financial analysts, or other interested agents can establish mitigation strategies.

# Weighted Project Score: 8.0

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

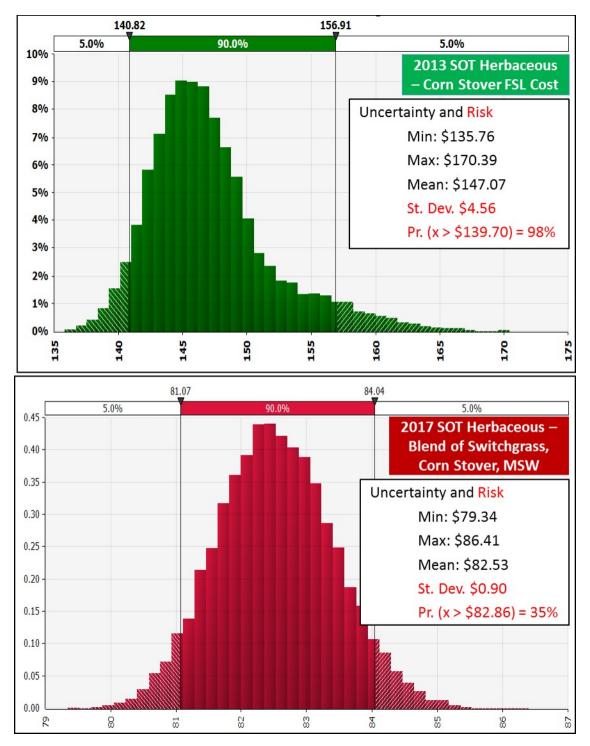


Photo courtesy of Idaho National Laboratory

### OVERALL IMPRESSIONS

• Overall, this is a (policy and investment) relevant project with useful, publicly available products to improve understanding of cost variability and risks.

- The publicly available stochastic TEA STEM will be extremely valuable to industry and researchers to be able to generate comparable supply-chain TEA risk. It will improve transparency for supply-chain participants and identify key areas of risk and opportunity for improvement of supply-chain performance. It was good to know that the team leveraged expertise of experts on deterministic models to help understand different possibilities and uncertainty in data around economics and performance, but it would have been helpful to get more information on the model itself, the sensitivities tested, and the software platform. The histograms of cost for different case studies and the explanation of uncertainty and associated risk provide an easily understandable output with an intuitive interpretation and enable comparisons among feedstocks/blends. It is great to see that the plan includes assessing the integrated land management approach.
- The goal of this research is to design and develop a tool for quantifying cost risk (economic basis) in the feedstock supply chain. The team developed STEM to simulate possible cost outcomes from which risk can be quantified and then compared across alternative supply-chain designs, providing a framework for consistent and systematic analyses. Model development built on past work, including state-of-technology (SOT) reports. Several analyses were conducted, including landscape design alternatives (stover and switchgrass) and herbaceous feedstocks (stover versus a blend). The project contributed to overcoming barriers identified by BETO: to reduce risk, to provide improved understanding of the cost of risk, and to reduce feedstock cost through risk reduction. Barriers addressed include At-B: Analytical Tools and Capabilities for System-Level Analysis; Ft-A: Feedstock Availability and Cost; and At-E: Quantification of Economic, Environmental, and Other Benefits and Costs.
- The STEM simulates possible cost outcomes from which cost risk can be quantified. This is an important goal. Its use of Monte Carlo simulation to characterize probability distributions around point estimates is an appropriate approach to the issue. It is not clear how the probability distributions are being derived given that the input parameters are being drawn from other projects that did not characterize uncertainty. It is also not clear how this model is integrated with others in the BETO portfolio. What is its pathway to impact?

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for your comments.
- The STEM will be hosted on INL servers on the Biomass Feedstock Library page. It will be accompanied by documentation on how the model is built and how the parameters used in the uncertainty model are attained. The reports included there also contain examples of how the STEM has been applied in various applications of alternative feedstock supply chains.
- In terms of impact, two separate analyses where STEM has been used are under review in journal publications. These papers, along with reports generated during the project and hosted on the online site, provide other researchers a way to use the STEM.

# **BIOPRODUCTS TRANSITION SYSTEM DYNAMICS**

# National Renewable Energy Laboratory

## **PROJECT DESCRIPTION**

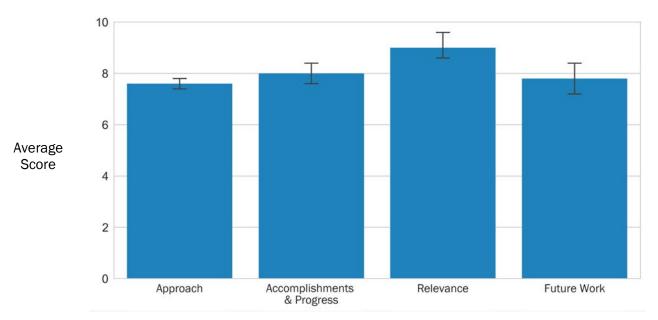
Bioproducts are chemicals derived from a biomass feedstock. They can be produced on their own or as coproducts of a biorefinery that also produces biofuels. Bioproducts have historically been difficult to scale up and bring to market, despite a broad understanding developed within BETO of the various conversion processes that can be used to produce bioproducts. Expanding the bioproduct industry by bringing more bioproducts to market would have a variety of positive impacts. Growth in the bioproduct industry would support the biofuel industry by enabling biorefinery coproducts that yield additional revenue streams, allowing biofuel selling prices to be reduced and expanding the biofuel market. A larger

| WBS:                      | 4.1.2.31            |
|---------------------------|---------------------|
| CID:                      | NL0032347           |
| Principal Investigator:   | Dr. Mary Biddy      |
| Period of<br>Performance: | 10/1/2016-9/30/2020 |
| Total DOE Funding:        | \$700,000           |
| DOE Funding FY16:         | \$51,000            |
| DOE Funding FY17:         | \$200,000           |
| DOE Funding FY18:         | \$249,000           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

bioproduct industry also has the potential to reduce carbon and other emissions associated with the U.S. chemical sector and contribute to increased price stability in some areas of the chemical market by shifting portions of the chemical sector away from reliance on fossil feedstocks. The key barrier to realizing these positive impacts is a lack of knowledge around the factors that prevent or enable bioproducts to reach the commercial market. To date, there has been essentially no research done on how successful bioproducts (commercially produced bioproducts that have captured market share) become successful, why failed bioproducts fail, and the similarities and differences between successful and failed bioproducts.

# Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

The current project addresses this knowledge gap with a decision-support tool that can be used by investors, technology developers, and government agencies to bring more bioproducts to market, thereby simultaneously growing the bioproduct and biofuel industries. Development of the decision-support tool was based on research on the technology development process and success rates in analogous industries, data gathered during previous BETO-funded projects, and a series of interviews with subject matter experts within BETO, the bioproduct industry, and the investment community. This information formed a knowledge base around how bioproducts are developed from applied research to commercial-scale assembly, which was used to build the Bioproduct Transition Dynamics (BTD) model, a system dynamics model that tracks bioproduct development projects from applied research through the "valley of death" of piloting and demonstration to commercial-scale production. The end-of-project goal is to release the BTD, along with supporting documentation, as a transparent open-source model that will inform decisions around bioproduct development and investments and enable more bioproducts to reach the market.

The BTD takes as inputs techno-economic data on specific bioproducts, behavioral parameters for developers and investors, expectations around government support, and exogenous market factors. Model outputs include bioproduct technological progress throughout time, a cash flow statement for the development project, and market share estimates. Following initial model development, a sensitivity analysis was performed on a subset of model inputs to determine, first, if the BTD could be used to answer analysis questions of interest to BETO, and second, which of the inputs considered were most influential on bioproduct success. Results indicate that the BTD can be used to identify scenarios that enable bioproduct development and that "soft" or semiquantitative factors play a large role in determining if a bioproduct will reach the market. A workshop was also held for subject-matter experts and prospective BTD users in July 2018. The workshop covered BTD model logic, input data and assumptions, as well as the sensitivity analysis results and a discussion of potential use cases. Workshop feedback was used to identify additional model development, validation, and application will continue through September 2020.

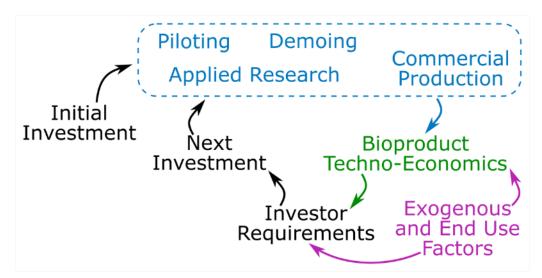


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project, which started in 2016, addresses issues critical to ensuring the success of bioproducts because product transition challenges have not been addressed as much as bioenergy products.
- My layperson interpretation is that the team is trying to forecast (and potentially mitigate) adverse impacts of market flooding (e.g., glycerin from biodiesel industry) and new, higher-value, unique products (e.g., dried distillers grains as feed, bioadvantaged products).

- This project addresses interesting and timely questions related to bringing bioproducts from demonstration through to market maturity. Addressing the valley-of-death challenges faced by bioproducts will shed light on a key but understudied barrier to an integrated and sustainable bioeconomy.
- The project represents needed work. The project fills a research, information, and data gap in identifying factors impacting the development of the bioproduct industry, and it develops a decision-support model, the BTD.
- This project will leverage the extensive expertise in system dynamics of the bioeconomy developed for the BSM to develop a similar approach to analyzing early-stage bioproducts to assess market penetration potential. This is a valuable initial start to this assessment process that has been used to identify the factors with the greatest influence on bioproduct success. It can be used as a starting point to develop the model to more fully address coproducts and the integration of bioproducts into the overall bioeconomy production scenarios.
- At some point, this analysis/model will need to address coproducts with the bioproducts because most bio-based production processes produce multiple products, potentially including fuels. It might not make sense, therefore, to model bioproducts in isolation. Perhaps this should eventually become an early technology readiness level module of the BSM.
- One of the outcomes of the BTD workshop is listed as a new focus of model scope on pilots and demos. This does not seem to match the focus here on overcoming the valley of death, which is about bridging the gap between pilot/demonstration and true commercial scale. The principal driver analysis seems most relevant to a commercial endeavor than a pilot or demonstration, and indeed, this is the rationale for the project's relevance.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their feedback, and we will work to incorporate these suggestions into our future modeling and analysis efforts.

# **BIOECONOMY SCENARIO ANALYSIS AND MODELING**

# National Renewable Energy Laboratory

## PROJECT DESCRIPTION

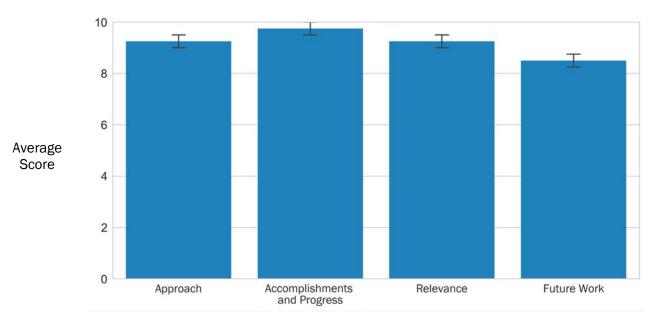
The Bioeconomy Scenario Analysis project uses systems thinking and analysis to assess current and/or prospective techno-economics, R&D, deployment strategies, policy, and market conditions and their impact on the potential development trajectories of the bioenergy industry throughout time. Results from this project include the identification of opportunities and constraints to industrial development; quantification of multiple metrics (energy, economic, environmental); and informing researchers, decision makers, and industry of the steps needed for a sustainable, nationwide biofuel industry. Analyses from this project enable the creation of a bioenergy industry by (1) inciting policymakers to explore scenarios for

| WBS:                      | 4.1.2.32            |
|---------------------------|---------------------|
| CID:                      | NL0033742           |
| Principal Investigator:   | Ms. Emily Newes     |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$1,200,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$750,000           |
| DOE Funding FY19:         | \$450,000           |
| Project Status:           | Ongoing             |
|                           |                     |

nationwide biofuel production and identifying policy actions consistent with pathways for growth; (2) improving the industry's understanding of industry growth potential under different technology and investment conditions and 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 modeling tool used in this project, the BSM, is a publicly available, unique, validated, state-of-the-art, 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. We use models such as the BSM to examine the

# Weighted Project Score: 9.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

implications of policies and incentives as well as their potential side effects. The BSM uses a system dynamics simulation to model interactions and transitions across the supply chain; it tracks the deployment of biofuels given industrial learning and the reaction of the investment community in the context of land availability, projected oil markets, consumer demand for biofuels, and government policies throughout time. Under expected market conditions, analyses using the BSM suggest that the biofuel industry might require significant external actions in the early years to thrive. Interventions that accelerate the industrial learning process (e.g., operation of precommercial and commercial facilities) have been identified as having strong influence in starting the growth of a commercial biofuel industry. Policies that are coordinated across the whole supply chain in BSM foster the growth of the biofuel industry, and production of tens of billions of gallons of biofuels might occur under sufficiently favorable conditions.

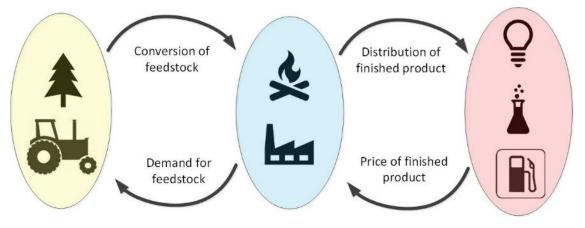


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- Overall, this is a very appropriate project for BETO to continue to fund.
- Insights from their system-of-systems scenario modeling are understandable and useful to policymakers.
- The BSM allows scenario exploration to support decision making, highlighting interactions across systems and evolving markets. The project informs BETO, other stakeholders, and policy decision makers of the implications of policy choices and market developments to enable prioritization and evaluation of various actions and enable researchers to design and analyze the impacts of additional biomass-to-bioenergy scenarios
- The BSM enables the study/assessment of transition dynamics to a bioeconomy (using a complement of tools); generates plausible scenarios for prospective policies, incentives, investments, R&D impacts, and strategies; and enables and facilitates focused discussion among stakeholders
- The project addresses barriers At-A: Analysis to Inform Strategic Direction, At-B: Analytical Tools and Capabilities for System-Level Analysis, and At-D: Identifying New Market Opportunities for Bioenergy and Bioproducts.
- The BSM is a promising newer development in the BETO model portfolio. The researchers have pursued a key goal of identifying specific factors that contribute to cost effectiveness of subsidies so that the subsidies can be better structured and applied. A high-profile research award and uptake in academic research as well as teaching imply methodological rigor as well as potential for future influence. Strategic planning for increased impact beyond research sphere is warranted.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their thoughtful and supportive feedback. We will strive to address their comments in future scenario analysis topics.

# **BIOFUELS NATIONAL STRATEGIC BENEFITS ANALYSIS**

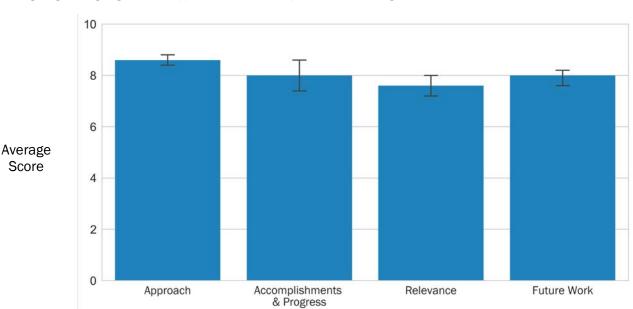
# **Oak Ridge National Laboratory**

# **PROJECT DESCRIPTION**

This project helps DOE assess, quantify, and explain the economic and energy security benefits of biofuels and bioproducts. It identifies system configurations and conditions that advance economic welfare and improve resilience along the biofuel products supply chain. To meet its objectives, the project approach is twofold. First, BioTrans—a mathematical programming model that optimizes long-run investment and operation decisions along the U.S. biofuel/bioproduct supply chain—is used to simulate scenarios of interest regarding market conditions, policy changes, and supply-chain configurations. Second, empirical analysis of historical data is conducted to analyze the dynamics of the gasoline-ethanol price relationship.

| WBS:                      | 4.1.2.41            |
|---------------------------|---------------------|
| CID:                      | NL0024441           |
| Principal Investigator:   | Mr. Paul Leiby      |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$1,041,138         |
| DOE Funding FY16:         | \$200,000           |
| DOE Funding FY17:         | \$300,000           |
| DOE Funding FY18:         | \$341,138           |
| DOE Funding FY19:         | \$200,000           |
| Project Status:           | Ongoing             |
|                           |                     |

During the last merit review cycle (FY 2016–FY 2018), this project generated insights regarding the impact of changing market conditions (reduced oil prices and expanded domestic oil and gas production), policy changes (revised renewable fuels standard [RFS] requirements), and alternative supply-chain configurations on the introduction of advanced biofuels and the energy security role of biofuels. BioTrans was used to explore the role of biofuels in mitigating the cost of oil and biomass supply shocks. Empirical analysis of historical ethanol and gasoline price time series focused on the estimation of the effect of biofuel blending on fuel price



#### Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

volatility. Estimates of the economic value of those volatility reductions were also generated using two different approaches: modern portfolio theory and real option valuation.

The additional work proposed for FY 2019–FY 2021 will extend past the analysis of economic resilience and energy security benefits that focused on biofuels to include new issues and supply-chain configurations that are increasingly viewed as essential to improving the value proposition of advanced biofuels. First, the development of bioproducts as a complement to biofuel production is essential to strengthening the economics of advanced biorefineries. The aspects of the value proposition of multiproduct biorefineries explored in this project will include economic sustainability profitability for farmers and biorefiners, value for consumers, and economic and energy security benefits for the nation. Second, the planned work will explore potential impacts that an octane performance standard, in addition to or in place of the RFS, could have on the biofuel industry.

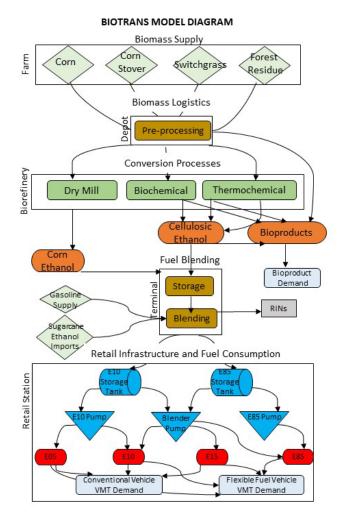


Photo courtesy of Oak Ridge National Laboratory

#### OVERALL IMPRESSIONS

• This project, initially funded by ORNL almost a decade ago, has evolved to improve the economic equilibrium market model BioTrans (which captures farm-to-pump supply-chain connections and petroleum-biofuel interactions). The justification for this project is strong, and results are interesting so far; future work could be strengthened with some minor changes to assumptions (and/or articulation of default assumptions).

- The market price and economic analysis model (BioTrans), strength long-range analysis, 30-year model horizon (year-by-year or comparative statics) solves for optimal investment patterns. The focus themes for the model are the issues of transition to alternative fuels.
- This project helps assess, quantify, and explain the economic and energy security benefits of biofuels and bioproducts. The project identifies system configurations and conditions that advance economic welfare and improve resilience along the biofuel products supply chain.
- This project addresses barriers At-B: Analytical Tools and Capabilities for System-Level Analysis; BioTrans Model; and At-E: Quantification of Economic, Environmental, and Other Benefits or Costs. The project also addresses energy security benefits and the value of fuel price volatility reduction.
- Energy security and economic sustainability considerations are critical, and much of the A&S portfolio focuses on the environmental considerations/arguments surrounding biofuels. There is clearly some dead-weight loss associated with fuel volatility, and quantifying this effect is useful. If increased biofuel blend levels carry increased cost but reduced volatility risk, this quantification could be a key element of the value proposition.
- Although this approach is very interesting, it seems somewhat academic or theoretical, and it is unclear how supply-chain participants would use the modeling approach or results when defining a project or supply chain. The team should think carefully about and communicate how to enable this information to be used to help with deployment and supply-chain development.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you all for the positive comments and for the critiques and suggestions. We are grateful that you took the time to listen to us and review our work with such care.
- Our communication of research findings has typically been through periodic BETO briefings, conference presentations, and peer-reviewed journal publications. The non-BETO outlets mostly reach other researchers and explain why this work is in a technical format. We acknowledge that, to maximize their impact, our results need to be (1) further translated into actionable insights and (2) communicated to supply-chain participants.
  - Translating the results into actionable insights: In the supply shock scenario analysis, it would help to further unpack national aggregate shock costs to show the impacts on different market participants in different regions. We want to convey the effect of different supply-chain configurations (investments) on mean revenue, revenue variability, and resilience to different types of shocks. Flexibility levers (e.g., advanced logistics, biorefinery feedstock flexibility, bioproducts) are one option to enhance resilience. For bioproducts, one planned industry-relevant contribution is to develop general classifications regarding process flexibility and substitutability with petroleum-based alternatives and identify strengths and vulnerabilities associated with the introduction of bioproducts with different levels of those two attributes. The analysis framework can then be applied to any specific bioproduct pathway.
  - Communicating our results in outlets that reach supply-chain participants more easily: We will work to summarize and present our insights in outlets more likely to reach supply-chain participants: articles in trade journals (e.g., *Biomass Magazine*) and/or presentations at more industry-focused conferences. Another potential avenue for increased engagement with industry stakeholders is through further development and publicizing of our current web interactive tool with a focus on key questions that would be of interest for supply-chain participants and making it accessible in the KDF.

# GCAM BIOENERGY AND LAND-USE MODELING AND DIRECTED R&D

# **Pacific Northwest National Laboratory**

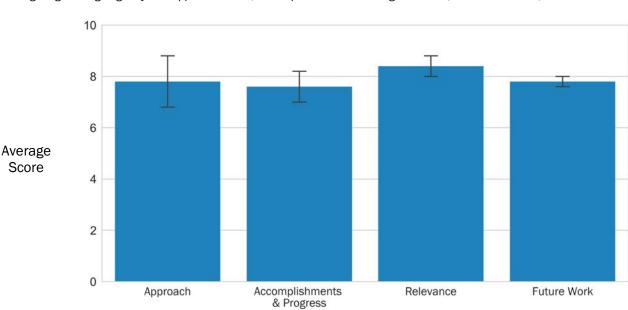
## PROJECT DESCRIPTION

This project serves the BETO A&S platform by providing quantitative analyses and published studies of the potential and impact of bioenergy in the integrated context of global energy and agriculture. Much of the analysis involves developing and using the PNNL GCAM, an established modeling program widely used by DOE, the EPA, academics, and the energy industry. The BETO project leverages the developments of the larger GCAM program to focus on improving modeling capabilities, data, and analysis in key areas related to bioenergy production and use. GCAM has been used by PNNL in international analysis efforts, such as the Intergovernmental Panel on Climate Change (IPCC) and the Stanford Energy Modeling

| WBS:                      | 4.1.2.50            |
|---------------------------|---------------------|
| CID:                      | NL0022708           |
| Principal Investigator:   | Mr. Marshall Wise   |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$450,000           |
| DOE Funding FY16:         | \$150,000           |
| DOE Funding FY17:         | \$150,000           |
| DOE Funding FY18:         | \$150,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Ongoing             |
|                           |                     |

Forum, and it is available and widely used as an open community model. GCAM analysis is complementary to BETO TEA/LCA by providing long-term, multisectoral economic context for bioenergy technologies and systems.

Since the BETO GCAM activities started in 2010, we have developed modeling capabilities and published analyses about lignocellulosic bioenergy crops globally, bioenergy technologies for liquid fuels and power, and bioenergy with CO<sub>2</sub> capture and storage. In recent years, we have focused on integrated economic analysis of bioenergy in the energy demand and transformation sectors. In FY 2017, we published a paper exploring the



# Weighted Project Score: 7.9

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

potential scale and the impacts on energy, land, and emissions of large-scale production and use of biofuels for global aviation to 2050. In FY 2018, we designed and performed an analysis of the competition and potential synergies of electric vehicles (EVs) and bioenergy. Currently in FY 2019, we are studying the economic potential and impact of biopower using GCAM-USA, which models the energy systems in each of the 50 states while maintaining integration with the global model.

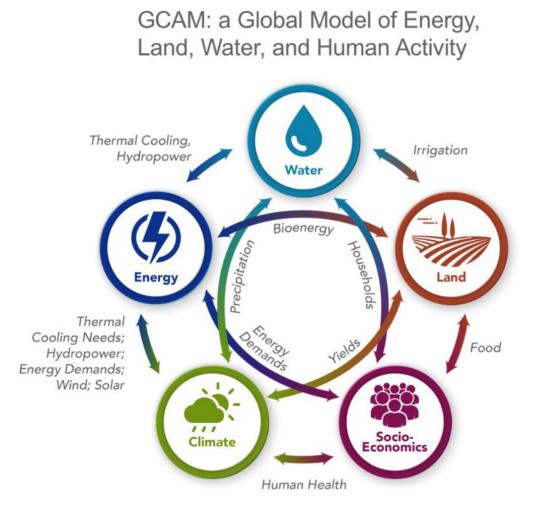


Photo courtesy of Pacific Northwest National Laboratory

# OVERALL IMPRESSIONS

- This established, high-impact program quantitatively tackles specific scenario-related questions associated with bioenergy demand and production in the context of broader agricultural and energy economic systems.
- I had difficulty with this project review. I thought the approach was vague and the accomplishments weak.
- This is important work expanding the GCAM scope and application to include key emerging applications, such as bio-jet and bioelectricity for transport.
- The researchers' evaluation of biopower as a biofuel is relevant, for example, in the California Low-Carbon Fuel Standard policy context. This project fills a key gap in the BETO portfolio by explicitly

studying biofuels in the context of an EV future. Missing these dynamics would ignore a key trend influencing this space, so this is a strong development.

- The fact that GCAM is being used by analysis outside of the project team is a strong sign of its relevance.
- The use of the well-accepted GCAM for broader economy-wide modeling of bioeconomy effects is helpful to better understand the broader impacts of the BETO portfolio.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you to the reviewers for sharing your time and expertise on this effort. As in past peer reviews, your focused questions and comments have been invaluable in helping us plan for future analyses and improve the ways we communicate the results of our project to a broader audience outside BETO.
- Each year, we work closely with BETO to plan project tasks and milestones that are relevant to BETO's current analysis needs and for which GCAM can provide new quantitative insights that are complementary in scope to other BETO analyses. The fact that GCAM is developed as part of a larger, multiclient program provides many opportunities for leveraging model developments, but it also creates challenges for clearly delineating work performed specifically for BETO. We believe that we have been successful in designing and performing relevant bioenergy analyses for BETO and the larger stakeholder community during the past several years.
- A specific concern raised by the review panel is the level of regional resolution in the GCAM modeling. We have achieved much more spatial resolution in our economic modeling of land use within the main GCAM model during the last decade, from 11 world regions to more than 300 with our current water basins. It will always be a conceptual and computational challenge to model economics at a very fine resolution within a global model. Our current strategy for analysis where more resolution is needed is to downscale using geographic information system tools, such as Xanthos for water.
- Because GCAM models many aspects of bioenergy production and demand, the range of possible analyses is broad. This project has had an eclectic mix of analysis topics and papers throughout the years, and this might make it more difficult to discern a long-term plan. Our experience is that being opportunistic to address evolving areas of interest is a fruitful strategy; however, based on reviewer comments, we will also more clearly define a longer-term path for specific analyses and capability improvement.

# WATER RESOURCE MANAGEMENT FOR BIOENERGY AND BIOPRODUCTS

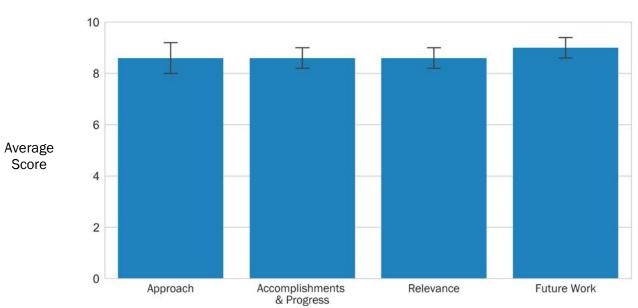
# **Argonne National Laboratory**

# **PROJECT DESCRIPTION**

This project (1) develops an analytic framework and hydrologic models that characterize geospatial water resource needs in the production of bioenergy and bioproducts under landscape design and management and pathway technologies and (2) applies the models and analysis in the United States to understand how growing and processing feedstock affects water use intensity, regional water availability, and water quality at watershed and regional scales. The work aims to (1) evaluate management practices in bioenergy landscapes that protect water resources and increase water-use efficiency and (2) identify scenarios that can improve the water sustainability of advanced bioenergy systems. The output of the project

| WBS:                      | 4.2.1.10            |
|---------------------------|---------------------|
| CID:                      | NL0022889           |
| Principal Investigator:   | Dr. May Wu          |
| Period of<br>Performance: | 10/1/2014-9/30/2020 |
| Total DOE Funding:        | \$2,348,512         |
| DOE Funding FY16:         | \$725,000           |
| DOE Funding FY17:         | \$714,310           |
| DOE Funding FY18:         | \$509,202           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

includes geospatial analyses of national- and regional-scale, county- and watershed-level resolution water footprints and the water availability index of biofuels; a spatial-explicit model, WATER; an energy-water inventory; and a suite of multiscale Soil and Water Assessment Tool (SWAT) hydrologic models that feed into BETO feedstock sustainability analysis, feedstock landscape TEA, and supply-chain sustainability assessment.



### Weighted Project Score: 8.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

# OVERALL IMPRESSIONS

- The assessment of a variety of water resource impacts is critical to informing discussions of the sustainability of various agricultural and industrial practices—especially bioenergy.
- This project is well integrated with other BETO-funded projects and other experts throughout the U.S. Geological Survey
- This project assesses bioenergy feedstocks from the water resource perspective to improve understanding of water quality and quantity; develops an analytic framework/hydrologic models that characterize geospatial water resource needs in the production of bioenergy and bioproducts under landscape design and management and pathway technologies; and applies the models for analysis of the United States to understand how growing and processing feedstock affects water use intensity, regional water availability, and water quality at watershed and regional scales. The goal is to evaluate management practices in bioenergy landscapes that protect water resources and increase water-use efficiency and identify alternative landscape design (LD) that can improve the water sustainability of advanced bioenergy systems.
- This project addresses barriers At-B: Analytical Tools and Capabilities for System-Level Analysis; At-E: Quantification of Economic, Environmental, and Other Benefits and Costs; and At-H: Consensus, Data, and Proactive Strategies for Improving Land-Use Management.
- This work should be feeding into multicriteria analyses elsewhere in the BETO research space. If not, we are missing (1) an opportunity and (2) necessary detail on the water criterion in other efforts. This applies to the multicriteria assessment sustainability analyses in BETO and to the GREET model. Is this work embedded in GREET?
- This speaks to my concern with some of the larger system-level analyses in the portfolio. Can the team be doing a sufficiently rigorous job on each criterion?
- It is important to understand the freshwater demand and implications for water quality of the bioenergy sector, and the WATER model is very comprehensive. Water resource mapping of soil moisture, streamflow, etc., and evidence for water quality/quantity benefits of various management strategies could be very valuable as siting decision criteria for growing/selecting feedstocks and/or for landscape management decisions. It was not clear how the analysis accounts for existing and planned uses of the water that are not in the bioenergy sector, nor if there are interactions among water demand types (i.e., if a shift to growing bioenergy crops reduces water demand from some other crop).

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The project team expresses its deep appreciation to the reviewers for their time, encouragement, and valuable input. We also thank the reviewers for recognizing our accomplishments and providing future directions. Looking forward, we will increase the level of interaction with other water/sustainability tools and models and provide water analysis results that contribute to multifactor tradeoff analysis. We will continue to work with other federal agencies, research institutes, and private sectors to address water use, water resource availability and resulted stress, and water quality with geospatial resolution. Finally, we will stay focused and continue our contributions to BETO as well as to the development of the bioeconomy.
- Water consumption data for corn and soybean irrigation generated from WATER were fed to GREET.
- Thanks for the comments. This water analysis considers existing land use by agricultural sector and forestry sector—the largest water consumption players in non-bioenergy sectors. We have analyzed and will continue to examine the interactions and effects of shifting land use and shifting crop types among these sectors and bioenergy on various freshwater resources across geographic regions.

# INTEGRATED LANDSCAPE MANAGEMENT

# Idaho National Laboratory

# **PROJECT DESCRIPTION**

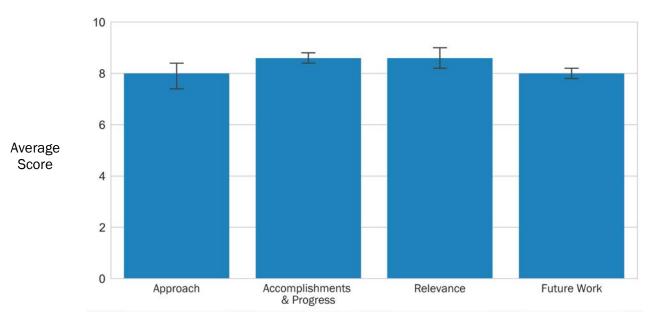
The ILM project represents a path forward to augment biomass feedstock supply chains with herbaceous biomass supplies at reduced access costs while improving sustainability outcomes relative to soil erosion and water quality. The intended outcome of ILM analysis is to support the BETO renewable fuel cost target of \$2.50/GGE by reducing biomass access costs. ILM is a strategy to integrate biomass production practices via sustainable crop residue collection practices and dedicated energy crop production in subfield areas where soil health is not suitable to meet traditional crop yield goals, resulting in economic and environmental waste. In FY 2017, ILM analysis using the Landscape Environmental Assessment

| WBS:                      | 4.2.1.20            |
|---------------------------|---------------------|
| CID:                      | NL0015077           |
| Principal Investigator:   | Mr. Mike Griffel    |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$1,751,051         |
| DOE Funding FY16:         | \$450,000           |
| DOE Funding FY17:         | \$550,000           |
| DOE Funding FY18:         | \$451,051           |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | Ongoing             |
|                           |                     |

Framework (LEAF) showed that significant volumes of biomass are available at state levels for agriculturally diverse states, such as Iowa and Kansas. In Iowa, LEAF modeling coupled with economic analysis during a four-year period indicated almost 60 million metric dry tons of stover from *Zea mays* (corn) could be accessed as a biomass resource with an additional 40 and 113 million metric dry tons of *Panicum virgatum* (switchgrass) and *Miscanthus* × *giganteus* (miscanthus), respectively. During the same four-year period, Kansas producers could potentially generate an additional 1.6 million metric dry tons of stover and 126 and 118 million metric dry tons of switchgrass and miscanthus, respectively. Analysis with additional modeling tools, including the Agricultural Non-Point Source (AGNPS) Pollution Model, developed by the USDA

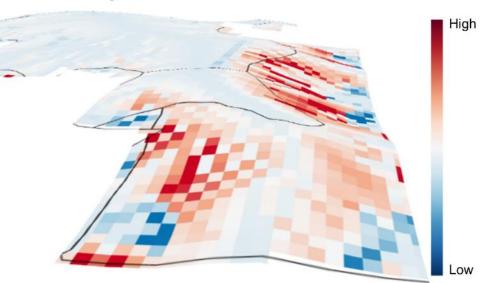
# Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

Agricultural Research Service (ARS), has shown that ILM could significantly reduce sediment and nutrient loading of agricultural watersheds by shifting crop inputs away from vulnerable and unsuitable soil types at subfield levels. AGNPS modeling of the impacts of incorporating perennial energy crop production within the Beaver Creek Watershed in Iowa indicate sediment loading could be reduced by more than 4,000 tons during a four-year period. In FY 2018, a TEA evaluating the impact of ILM designs on economic and sustainability outcomes of agricultural production fields showed biomass access costs could be reduced by 20% while improving economic outcomes at the field level across three Midwest watersheds. To support the TEA, the ILM design portfolio was expanded to include scenarios with efficient subfield geometries; prairie contour strips targeting vulnerable, high-slope areas; and the integration of biomass sorghum production at a wholefield level in lieu of fallow management. An updated soil-erosion modeling software, the Revised Universal Soil Loss Equation 2 (RUSLE2), raster-developed by USDA-ARS, was used to better incorporate the impacts of field topographic features and ILM changes within USDA-defined soil zones. The analysis also shows that soil erosion was reduced in two of the three watersheds, with additional reductions possible by further reducing crop residue recovery rates. Continuing in FY 2019, ILM analysis is focused on developing improved spatial subfield yield variability modeling capabilities and incorporating additional agricultural producer field efficiency metrics in the analysis to better account for the impacts of ILM on field equipment operational efficiency.



Agricultural Soil Loss at a Subfield Scale

Photo courtesy of Idaho National Laboratory

# OVERALL IMPRESSIONS

- This team has a clearly articulated goal and approach to demonstrate through modeling that ILM can reduce biomass feedstock costs at the field level. Results so far indicate that opportunities should exist for farmers to plant bioenergy crops at the marginal fringes of their properties, improving environmental quality and generating revenue.
- The goal of the project is to demonstrate (by modeling) how ILM can reduce feedstock production costs, while maintaining economic and sustainable outcomes, and the project directly supports BETO's fuel cost target (2030) of \$2.50/GGE. Project researchers have provided history indicating that the project is based on earlier work (Sustainable Feedstock Production–Logistics Interface) and leverages (and aims to

improve) LEAF. Farmers, ranchers, landowners, and land managers are potential major suppliers of biomass materials (energy conversion), and the land is the source of those biomass materials.

- This project is pursuing an interesting research question, and its integration of TEA and watershed-scale agricultural analysis is an interesting/relevant approach. Portfolio managers would be well served to ensure that this study is integrated with the Antares analysis as it would offer a useful data source and validation pathway.
- The ILM approach could be an extremely valuable tool for enhancing feedstock production and sustainability outcomes; it requires field validation to ensure that the modeling is an accurate representation of field performance. The team's approach to identifying subfield locations that could be targeted for economic and environmentally beneficial bioenergy feedstock production could be extremely valuable for identifying areas for potential production that will add value for farmers. The team has updated the revised universal soil loss equation (RUSLE), which is a valuable advance beyond the ILM modeling and is successfully used within the project The analysis suggests that applying ILM can reduce feedstock production costs by more than 20%—this would be a significant accomplishment that would greatly enhance the economic viability of more feedstocks (and thereby fuel pathways) going forward if validated through field measurements. Some estimate of statistical significance on the results would be valuable to determine if the differences presented matter regarding environmental performance. Given the potential utility of this modeling approach in real farming conditions, it would be very valuable to do field verification and validation and to implement the proposed subfield management approach in a few instances.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The researchers agree that field validation is important. Efforts to collaborate with projects with available field data will continue.

# **BIOFUEL AIR EMISSIONS ANALYSIS**

# National Renewable Energy Laboratory

# **PROJECT DESCRIPTION**

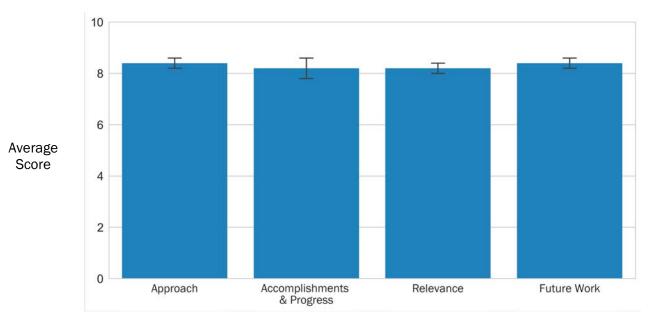
NREL's Biofuel Air Emissions Analysis project is unique and innovative in terms of the tools, approaches, and analyses provided. NREL is the only national laboratory that is actively working at the intersection of federal airquality regulations, air emissions across the supply chain, and process design. Meeting federal air-quality standards is prerequisite to being issued a construction permit. Negotiating the permitting process for a new biorefinery can be onerous and cost investors significant time and money. In a report looking at large-scale projects, 98% of projects incur cost overruns and delays over the project's life. As of 2015, the average delay is 20 months, and the average cost overrun is 80% of the project's capital.

| WBS:                      | 4.2.1.30            |
|---------------------------|---------------------|
| CID:                      | NL0022588           |
| Principal Investigator:   | Dr. Danny Inman     |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$2,172,000         |
| DOE Funding FY16:         | \$558,000           |
| DOE Funding FY17:         | \$650,000           |
| DOE Funding FY18:         | \$614,000           |
| DOE Funding FY19:         | \$350,000           |
| Project Status:           | Ongoing             |
|                           |                     |

Although there are numerous reasons for delayed biorefinery construction, air permitting is fraught with pitfalls because the air permitting process relies on precedence, which the biorefining industry presently lacks. For example, the Tesoro Refining and Marketing Company LLC currently has a bio-oil feed project (in Martinez, California) that has been delayed for 10 months (as of June 5, 2018) because of problems obtaining air permits for the facility. This project is focused on providing much-needed data and analyses that address biorefinery air permitting. This project develops models and quantitative analyses and measures progress toward meeting air-quality regulatory requirements. Biofuels are not necessarily cleaner than fossil fuels in terms of air emissions; however, it is important to emphasize that air emissions from biofuels depend in a large

# Weighted Project Score: 8.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

part on how biomass is produced and converted to biofuels. An accurate air-quality impact assessment requires understanding not only the type and magnitude of air pollutant emissions, but also where and when pollutants are released into the environment, aligning with the latest understanding of how biomass will be produced, collected, and then converted to fuels. Since the initiation of this project, we have been building BETO's capability to meet stakeholders' stated needs to accurately assess potential air-quality impacts by addressing a number of research gaps, including (1) a scarcity of spatially, temporally, and chemically resolved air pollutant emission inventories for the biofuel supply chain(s); (2) a lack of understanding about the types and quantities of air pollutants emitted from advanced biofuel conversion process designs and whether these advanced design cases can meet federal air regulations; and (3) a dearth of quantitative emission estimates on criteria air pollutant emissions from different advanced biomass logistics systems envisioned for biomass feedstocks to supply a large-scale bioenergy industry. In addition to filling research gaps, this project aims to disseminate and communicate our results to the relevant stakeholders at BETO, the national laboratories, and regulatory agencies. To begin to overcome these challenges, we have developed a framework that is designed to assess the air pollutant emissions for several BETO-prioritized advanced biofuel design cases across the biofuel supply chain. One key component of this framework is the Feedstock Production Emissions to Air Model (FPEAM), which allows for estimation of spatially explicit air pollutant emissions from biomass feedstock production, harvest, and transportation.



Photo courtesy of National Renewable Energy Laboratory

# OVERALL IMPRESSIONS

• Overall, this is a well-focused, well-teamed, high value-added project that could help reduce time and financial burdens (and uncertainty) associated with permitting commercial biorefineries.

- This project fills a void in providing a better understanding of emissions data along the supply chain and providing/developing data/emission estimates required for permitting, thereby overcoming a bottleneck in building biorefineries.
- The project addresses barriers At-A: Analysis to Inform Strategic Direction; At-B: Analytical Tools and Capabilities for System-Level Analysis; At-C: Data Availability Across the Supply Chain; ADO-C: Codes, Standards, and Approval for Use; and ADO-G: Co-Processing with Petroleum Refineries.
- This is an interesting project carried out by a well-qualified team. This effort is well connected to other models in the national laboratory space, and the team is working to make the "handshake" more robust. This will be important for other analyses to be able to leverage this work.
- The goal of this project is to provide crucial data, tools, and analyses to the biofuel and air regulatory community to enable the biofuel industry to develop sustainably. Its focus and rigor on criteria emissions accounting from farm to plant fills what would otherwise be a key gap in the BETO portfolio.
- The model aims to ensure that biorefineries will be able to comply with regulations, which is very useful to know at this point in their development. What is not clear is how this modeling will aid in permitting, as the team aims to do. The project is modeling air impacts on a notional basis, whereas a permit would need to be applied to a real facility. Is there a precedent for facilities being permitted on the strength of a model like this?
- If the team is successful in developing the assessment approach and gaining acceptance for a precedent for air pollution permitting for bioenergy facilitating, this project outcome will be very valuable for reducing investor and project risk during commercial facility development. It is not clear if there is an established path for setting precedents using modeling. The proposed release of the FPEAM as a public model and integration with existing spatiotemporal models of air quality will be very useful to industry and researchers.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their helpful and supportive feedback. We will work to incorporate these suggestions in our project plans as we move forward.

# INTEGRATED LIFE-CYCLE SUSTAINABILITY ANALYSIS

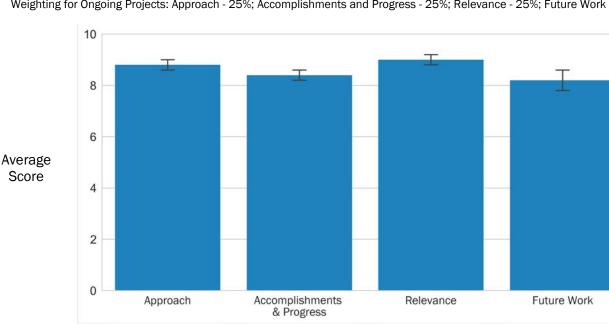
# National Renewable Energy Laboratory

# **PROJECT DESCRIPTION**

The main objective of this project is to provide BETO with a coherent methodology and modeling framework based on LCA and economic input-output analysis, tested and vetted with stakeholders, to better understand the net effects of an expanding U.S. bioeconomy at specific levels. This directly supports a 2019 milestone of BETO's Multi-Year Plan (MYP) and simultaneously addresses a gap previously identified by the DOE BETO peer review. To achieve this, NREL collaborates with developers of the national-level USEEIO model at the EPA and partners with other federal agencies (e.g., USDA), interagency initiatives (e.g., Biomass Research and Development Board), and DOE national laboratories to create an open-

| WBS:                      | 4.2.1.31            |
|---------------------------|---------------------|
| CID:                      | NL0027593           |
| Principal Investigator:   | Dr. Patrick Lamers  |
| Period of<br>Performance: | 10/1/2015-9/30/2019 |
| Total DOE Funding:        | \$1,325,968         |
| DOE Funding FY16:         | \$200,000           |
| DOE Funding FY17:         | \$300,000           |
| DOE Funding FY18:         | \$475,968           |
| DOE Funding FY19:         | \$350,000           |
| Project Status:           | Ongoing             |
|                           |                     |

source model that aligns well with similar efforts, including the Federal LCA Commons and the Sustainable Acquisition Program at DOD. During the review period, following the collection of feedback on the suggested modeling approach from a selected group of practitioners and developers of LCA and input-output models, NREL built a prototype by disaggregating the economic activities associated with and attributed to a selected product of the bioeconomy: corn ethanol. As an important part of the present U.S. bioeconomy and providing a large amount of public, validated economic industry information as well as peer-reviewed literature to compare to, corn ethanol was deemed a suitable test case. Validating the framework through a test case is important because disaggregation is a critical step in creating a representative and accurate framework. By the end of FY



# Weighted Project Score: 8.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

Т One standard deviation of reviewers' scores 2018, the team was able to generate several scenarios for corn ethanol on national and selected regional levels, providing results across multiple environmental and economic impact categories (reaching a "go" decision by DOE BETO).

A second objective of the project is to inform BETO's strategic decision making by engaging in, evaluating, and synthesizing selected global, multilateral activities that develop, compare, or apply metrics, methods, and tools to quantify sustainability effects of bioeconomy products, specifically the International Energy Agency's Technology Collaboration Programme on Bioenergy (IEA Bioenergy) and the Global Bioenergy Partnership (GBEP). This helps to identify gaps, barriers, and critical areas for future BETO bioenergy and sustainability assessments, identify opportunities and challenges to a sustainable U.S. bioeconomy, and contribute to and disseminate BETO information to and from major global bioenergy and sustainability efforts. Across the review period, this project contributed to, among others, a comparison of biofuel life-cycle emissions calculated by LCA tools with regulatory relevance. It found large initial discrepancies among the tools, which could be reduced via a harmonization of default values and allocation methods, indicating a continuous need for global alignment across LCA tools and underlying default values.

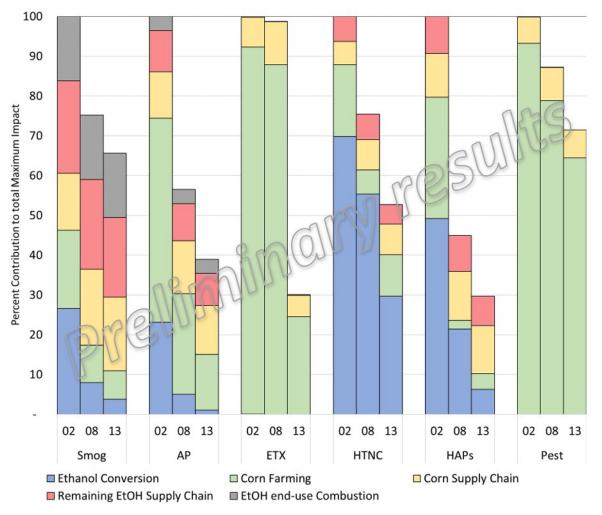


Photo courtesy of National Renewable Energy Laboratory

### **OVERALL IMPRESSIONS**

- Overall, this is a unique project among the BETO projects we have reviewed, and it offers value in improving harmonization and capturing indirect impacts related to the sustainability of bioenergy.
- There is concern that there is so much scope it is hard to address individual parameters rigorously. Dr. Lamers answered this concern directly, stating that this is to some extent an irreducible problem. Other models offer a great deal of rigor on a bottom-up basis. This project is taking a top-down approach, and its results can be usefully compared to those other models.
- This economy-level LCA approach will be very valuable for understanding the impacts of a scaled-up bioeconomy. The ability to assess improvement throughout time and broad regional differences in environmental performance can be valuable to help identify gaps and opportunities for improvement. Regarding the multilateral LCA metrics, tools, and analysis comparisons, this seems more appropriate for (or at least to be done in close collaboration with) the GREET team, which has done a lot of this work on understanding distinctions among GHG LCA tools already. Regarding the conclusion that there is a need for additional global harmonization of data and tools, there are actually good reasons for some of the differences in assumptions and methodology because there are geographic differences as well as valid debate about the best approach for some of these elements (e.g., allocation method). Further, those methods/approaches are sometimes codified by regulations (and are different for regulations in different places). Therefore, it might not be a realistic conclusion or goal to harmonize all metrics and methodologies.
- This project addresses this BETO A&S gap and related MYP A&S milestone, and it provides sufficient background detail to provide BETO with a credible, coherent methodology and modeling framework based on LCA and economic input-output analysis to quantify the net effects of an expanding U.S. bioeconomy at the national and regional levels.
- This project's goal is to inform BETO's strategic decision making by engaging in, evaluating, and synthesizing selected global, multilateral activities that develop, compare, or apply metrics, methods, and tools to quantify sustainability effects of bioeconomy products.
- This project addresses barriers At-A: Analysis to Inform Strategic Direction; At-B: Analytical Tools and Capabilities for System-Level Analysis; and At-E: Quantification of Economic, Environmental, and Other Benefits and Costs.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their constructive feedback, and we appreciate the recognition of the value of this project. The main goal of this effort is to provide BETO with an economy-wide integrated framework that applies a consistent and coherent methodology across multiple environmental and economic metrics. By default, this encompasses a broad scope, but it also purposefully creates a distinction to present BETO-supported, supply-chain-specific, bottom-up models such as GREET that cover fewer metrics. The benefit of the integrated framework is the capability to put product-level effects into an economy-wide context (in relative and absolute terms). Further, we calibrate the integrated model with data generated by and for bottom-up assessments. As such, we automatically review those results and ensure alignment of data and assumptions. A secondary component of the project is to provide scientific support to BETO across multilateral activities that assess the sustainability of bioeconomy products, including, among others, IEA Bioenergy (Task 45) and the GBEP. Rather than harmonizing sustainability metrics, models, and tools, the main intent is to assess respective methods and approaches to improve their transparency so that differences in results and values and their underlying reasons are clearly communicated and can be understood by the various stakeholders interested in these values.

# VISUALIZING ECOSYSTEM SERVICE PORTFOLIOS OF AGRICULTURAL AND FORESTRY BIOMASS PRODUCTION

# **Oak Ridge National Laboratory**

# **PROJECT DESCRIPTION**

Society needs renewable energy and clean water and ecosystem goods and services derived from biodiversity. The goal of this project is to discover how we can manage the production of advanced feedstocks to generate added value through ancillary (non-energy) ecosystem services. Our research develops and uses bioeconomic models to quantify and communicate the costs and benefits of alternative biomass production scenarios. To date, this project has demonstrated the benefits of growing perennial feedstocks in two tributary basins of the Mississippi River and highlighted potential water quality improvements downstream. In addition, we have developed new tools for quantifying, visualizing, and mapping ecosystem services.

| WBS:                      | 4.2.1.40            |
|---------------------------|---------------------|
| CID:                      | NL0022890           |
| Principal Investigator:   | Dr. Yetta Jager     |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$1,456,556         |
| DOE Funding FY16:         | \$350,000           |
| DOE Funding FY17:         | \$400,000           |
| DOE Funding FY18:         | \$406,556           |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | Ongoing             |
|                           |                     |

In our first task, we developed the concept of a total supply curve to visualize stacking values for different ecosystem services associated with growing biofuels. We demonstrated that the value of improved water quality (avoided water treatment cost) exceeded feedstock production cost for at least 40 metric tons of biomass supply in the Arkansas-White-Red river basin. Spatial analysis was used to map where these benefits are experienced.

# Average Score

# Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

These valuation and visualization methods will be used to quantify and visualize ecosystem service portfolios for each of two case studies: one in an agricultural and one in a forestry system. Each requires models to link management decisions related to biomass production to biodiversity outcomes (ecosystem services providing units) and associated values.

For the agricultural system, we are developing ecological models to support the Antares Landscape Design project.

- At the fuel-shed scale, we are implementing the BioEstimate (BioEST) model to understand the effects of biofuel production on a range of native taxa. We reviewed differences in pesticide use in corn and switchgrass. Future research will model where perennials can be grown in Iowa fuel sheds to provide the greatest value to native biodiversity (amphibians, reptiles, insects, mammals, birds).
- At the field scale, we developed an agent-based, tractor-pheasant-hunter model that will identify optimal spatiotemporal harvest strategies to maximize production of high-quality feedstock and recovery of pheasants. Scenarios will compare tractor paths, temporal tradeoffs between nesting success and decomposition of biomass, and spatial strategies for providing refuge.

For forestry, in the forested Pacific Northwest, we are collaborating with PNNL (Wigmosta) and the USFS to develop a decision tool to identify spatial opportunities for selective forest treatments to reduce wildfire and restore listed salmonids. We have developed models of incubation and juvenile rearing survival to evaluate forest-thinning scenarios. Preliminary results show benefits for spring Chinook salmon. A "Wildfire and Wildlife Symposium" is proposed at a joint American Fisheries Society and Wildlife Society meeting in Reno, Nevada. In the future, changes to portfolios of ecosystem services will be valued under alternative spatial-treatment scenarios.

### OVERALL IMPRESSIONS

- This is generally a worthwhile project for ecosystem management, and I'm glad this work is being done. I believe there are clear novel contributions this group can make to inform some next steps on scaling up bioenergy development (e.g., informing resilience and risk calculus), but this message could be clearer to those less familiar with ecosystem services work.
- This project should illuminate paths leading toward the coproduction of biomass, clean water, and utility derived from biodiversity. The goal of this project is to discover how we can manage the production of advanced feedstocks to generate added value through ancillary (non-energy) ecosystem services.
- The project addresses barriers At-E: Quantification of Economic, Environmental, and Other Benefits and Costs; and At-F: Science-Based Methods for Improving Sustainability.
- This project offers an interesting ecological economic modeling for ecosystem services via biomass feedstock production using an ecosystem service valuation approach. In particular, it focuses on biodiversity impacts as indicated by two case-study species. It is important to push on biodiversity impacts, but is there a way to do a more generalized analysis that does not hinge on a highly detailed approach to a couple of key species?
- Not everyone should make a decision-support tool. BETO could consider supporting a large one, but these will not get used if there are a dozen of them and each one is niche.
- This project will provide useful information on how to achieve multiple environmental goals with bioenergy/biomass production. Monetizing these results in the real world, however, will depend on policies such as state payment programs to reduce nutrient loading in rivers/bays or some program that provides revenue to farmers to reward maintenance of recreational opportunities. One recommendation is that these case studies should address key barriers to deployment, and it was not clear if pheasant

conservation is of the same level of importance for local/regional conservation efforts as salmonids are in the West, so selecting and clarifying the importance of these different case-study elements for actual deployment would be helpful.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# COLLABORATIONS TO ASSESS LAND EFFECTS OF BIOENERGY

# **Oak Ridge National Laboratory**

# **PROJECT DESCRIPTION**

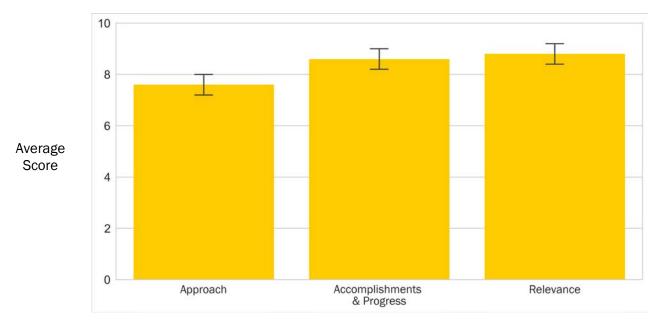
This project aims to (1) develop science-based approaches to support more consistent and accurate assessments of bioenergy effects on land and (2) facilitate public access to BETO sustainability research and relevant data on sustainability standards and indicators. As a stretch goal, the project strives to shift the LUC debate toward the opportunities and benefits attainable by integrating bioenergy and improved land management, or beneficial LUC. The project's approach supports BETO to clarify, quantify, and communicate the costs and benefits of an expanding U.S. bioeconomy by focusing on consistent definitions for land cover, disturbance, and management practices; explicit baseline data; evidence-based testing of

| WBS:                      | 4.2.1.41            |
|---------------------------|---------------------|
| CID:                      | NL0026709           |
| Principal Investigator:   | Mr. Keith Kline     |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$1,257,373         |
| DOE Funding FY16:         | \$250,000           |
| DOE Funding FY17:         | \$350,000           |
| DOE Funding FY18:         | \$382,373           |
| DOE Funding FY19:         | \$275,000           |
| Project Status:           | Sunsetting          |
|                           |                     |

hypotheses; and analytics to identify relationships among observed changes and potential driving factors. We (1) conduct research and develop publications in collaboration with other international researchers; (2) contribute strategically to relevant reports and tools being developed by third parties; and (3) established a sustainability portal on the KDF website to facilitate access to information on standards, indicators, and LUC research. Assessing a feedstock's effects on land and indirect land-use change (ILUC) is challenging. Model estimates and assumed LUC relationships continue to have a significant bearing on most indicators of sustainability. A review of 50 regulatory and voluntary sustainability frameworks applicable to the bioeconomy found LUC/ILUC to represent the greatest sustainability risk. Project outcomes include the

# Weighted Project Score: 8.4

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

following: During the past two years, the project's research and outreach efforts have generated more than 20 publications, 50 presentations, and significant contributions to dozens of reports by partners, such as the IEA's *Technology Roadmap: Delivering Sustainable Bioenergy*, the GBEP's *Technical Report: Attribution of Impacts to Bioenergy Production and Use for the Implementation of the GBEP Sustainability Indicators for Bioenergy (GSI)*, the climate calculator tools, and others. The project has begun to shift the debate toward identifying opportunities for beneficial LUC as reflected in work that collaborators will continue through IEA Bioenergy, the Food and Agriculture Organization, and other entities. By documenting and testing alternative conceptual frameworks for understanding LUC, and by promoting science-based methods, we expect the project impacts to increase throughout time as better data become available. Publications and methods will reduce uncertainties about costs and benefits associated with an expanding U.S. bio-based economy on land. New KDF web pages on sustainability, standards, and indicators will facilitate access to an expanding body of research aimed at quantifying these effects (see: https://bioenergykdf.net/content/sustainability-and-standards-home).

Fig.: Over the past two years, the project contributed to 21 journal articles and 24 other reports ranging from IEA Bioenergy publications to a book chapter on the challenges to measuring LUC.

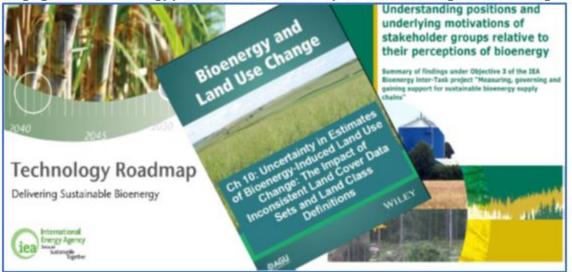


Photo courtesy of Oak Ridge National Laboratory

### **OVERALL IMPRESSIONS**

- This group has demonstrated clear value to the BETO portfolio by being one of the few groups to actively engage with international efforts and by pushing modelers to question, defend, and incorporate real-life evidence as much as possible when approximating very complex sustainability concerns (in this case, LUC).
- This project addresses the important topic of cost-benefit assessments of bioenergy impacts on land. The team presents a valuable analysis of drivers of LUC and food prices and potential cherry-picking or narrowness in previous analyses. Understanding how and/or whether bioenergy production is impacting food prices (and other indirect effects) will be critical to the public perception and success of bioenergy products. It would be helpful to acknowledge diverse points of view and valid points of contention in the analyses that remain to be resolved.
- This is a sunsetting project.

- The project aims to develop science-based approaches to support more consistent and accurate assessments of bioenergy effects on land, facilitate public access to BETO sustainability research and relevant data on sustainability standards and indicators, and inform the ILUC and LUC debate.
- This project aims to facilitate collaboration and evidence-based analysis around LUC, which is an estimable goal. It has yielded many publications, though it is not clear whether they are all uniquely the product of this project. It has also yielded a great deal of international collaboration and interaction, which creates value for BETO and EERE. The project PI is clearly well networked and influential globally. The primary thrust of this work appears to be facilitating BETO's participation in IEA Bioenergy and GBEP conversations. If this is the intent, then it has been successful in this regard.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for acknowledging the value of our efforts to address the challenging LUC debate through science-based approaches, statistical analysis of evidence, and the provision of documentation to improve model input values and assumptions. By engaging various perspectives in this process, we aim to improve overall understanding and broaden the "ownership" of final products and results of analysis. Regarding a question on outreach and public access to project results, we note that more than 50 presentations were made by team members during the past two years, and the KDF team reports that the project's new website for sustainability indicators received more than 2,200 visits in the first three months since release.
- We should clarify that we fully agree with a reviewer regarding the need to acknowledge diverse points of view. Diverse perspectives and points of contention, such as the issues associated with shifts in U.S. feed supplies and uses, are addressed in an approach. Such perspectives are explicitly acknowledged and examined in past papers, with several being highlighted in the 2017 paper in *Global Change Biology Bioenergy* on "Biofuels and Food Security: Priorities for Action." Also, diverse perspectives were sought and are being represented among coauthors in several final reports and papers in preparation (see 13 papers listed in the peer-review presentation).

# CARBON CYCLING, ENVIRONMENTAL & RURAL ECONOMIC IMPACTS OF COLLECTING & PROCESSING SPECIFIC WOODY FEEDSTOCKS IN BIOFUELS

# **Consortium for Research on Renewable Industrial Materials**

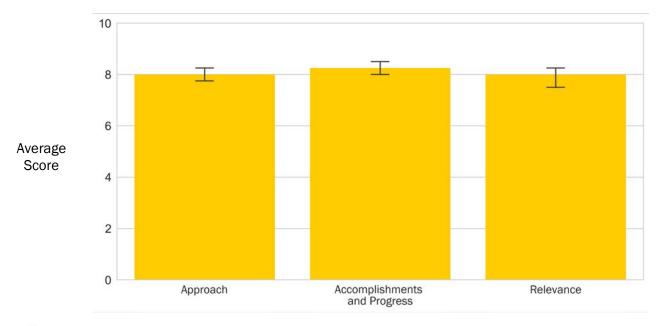
## **PROJECT DESCRIPTION**

The goal of this project is to understand the carbon flows for woody biomass allocated for bioenergy products relative to no bioenergy, including the role of wood products, and an evaluation of the implications for different forest management systems.

| WBS:                      | 4.2.1.60            |
|---------------------------|---------------------|
| CID:                      | EE0002992           |
| Principal Investigator:   | Dr. Steve Kelley    |
| Period of<br>Performance: | 8/31/2010-3/31/2019 |
| Total DOE Funding:        | \$1,430,535         |
| Project Status:           | Sunsetting          |

# Weighted Project Score: 8.1

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 ${f I}$  One standard deviation of reviewers' scores

### OVERALL IMPRESSIONS

- This Consortium for Research on Renewable Industrial Materials program has been evaluating connections between what type of biomass is grown, how it is harvested, and what it is used for—with a focus on biomass residues and durable wood products from three regions (Pacific Northwest, Southeast, Northeast).
- Analytic findings on the fate of carbon under different regions and harvesting scenarios help inform researchers and policymakers and select findings have been incorporated into GREET (the gold-standard LCA model for biofuels).
- This is a sunsetting project.
- The objective of this project is to assess the potential quantity and economic accessibility of CO<sub>2</sub> management of the U.S. bioeconomy through BECCS. The project provides foundational work for FY 2019 projects (1) Bioeconomy Carbon Flux Assessment and (2) Harnessing the Bioeconomy for Carbon Drawdown: Potential and Innovation Needs.
- The project addresses barriers At-A: Analysis to Inform Strategic Direction, At-C: Data Availability Across the Supply Chain, and At-D: Identifying New Market Opportunities for Bioenergy and Bioproducts.
- This project provides valuable insight into the life-cycle GHG emissions associated with various woody material production pathways and fates. I was glad to see a direct connection with the GREET team highlighted to ensure that the new data generated are incorporated into that model.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The statement of work does not include an economic evaluation of alternative woody biomass feedstocks.
- Working with the GREET team is very valuable.

# **BIOMASS PRODUCTION AND NITROGEN RECOVERY**

# **Argonne National Laboratory**

# **PROJECT DESCRIPTION**

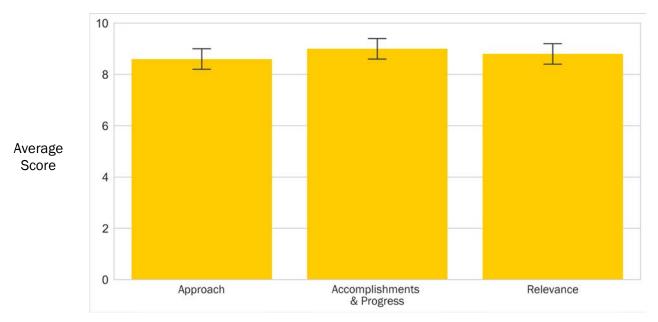
This project aims to bolster the cost-competitiveness of bioenergy through the valuation of ecosystem services produced by bioenergy crops on marginal land in an integrated landscape design. It does so by (1) generating primary data from field experimentation to quantify the ecosystem services produced by bioenergy crops grown in marginal land; (2) modeling at a small-watershed scale two water-quality-enhancing landscape designs, integrating bioenergy with grain crops and conservation; and (3) expanding this approach across a range of Midwestern settings through a TEA conducted in collaboration with INL. A multiyear primary field data-collection effort shows clearly favorable results, in particular for soil water

| WBS:                      | 4.2.2.10            |
|---------------------------|---------------------|
| CID:                      | NL0022598           |
| Principal Investigator:   | Dr. Cristina Negri  |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$2,350,000         |
| DOE Funding FY16:         | \$600,000           |
| DOE Funding FY17:         | \$630,000           |
| DOE Funding FY18:         | \$600,000           |
| DOE Funding FY19:         | \$520,000           |
| Project Status:           | Sunsetting          |
|                           |                     |

nitrate and GHG reduction, in the bioenergy plots compared with the commodity crops. The results, therefore, provide a rationale for working with other stakeholders and Natural Resources Conservation Science to include bioenergy buffers as a conservation practice. Modeling analyses include the development of a method to assess marginal land, the analysis of the effectiveness of saturated bioenergy buffers in improving the hydrogeochemistry of nutrients and erosion sedimentation, and LCA of emissions. Valuation of ecosystem services has demonstrated that the replacement of commodity crops in marginal farmland with perennial bioenergy crops can provide an advantageous value proposition for producers, given the pricing for the lignocellulosic material and the calculated value of ecosystem services, such as water quality improvement.

# Weighted Project Score: 8.8

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

Outcomes from the project are anticipated to be a modeling framework to guide the transformation of the agricultural landscape to a future state of integrated bioenergy and commodity crops, with improved crop yields and ecosystem services, a better economic outlook for rural communities, and reduced water-quality issues realized at the local to national (e.g., Gulf of Mexico) scales.

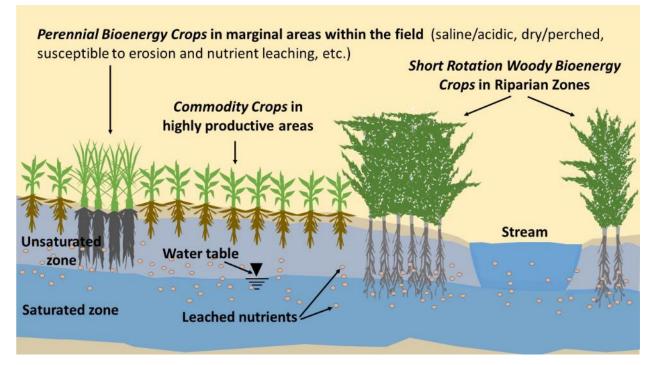


Photo courtesy of Argonne National Laboratory

### **OVERALL IMPRESSIONS**

- This project, which has existed in some form for almost a decade, valuably integrates modeling and fieldwork to understand and improve ecosystem services (and overall sustainability) through incorporating energy crops, with unique insights for potential development of ecosystem service markets.
- This is a sunsetting project.
- This project aims to bolster the cost competitiveness of bioenergy through the valuation of ecosystem services produced by bioenergy crops on marginal land in an integrated landscape design and to investigate the integration of bioenergy buffers into the agricultural landscape and evaluate the associated economic factors and associated ecosystem services.
- This project addresses barriers At-E: Quantification of Economic, Environmental, and Other Benefits and Costs; At-F: Science-Based Methods for Improving Sustainability; and At-H: Consensus, Data, and Proactive Strategies for Improving Land-Use Management.
- This project offers an interesting and well-designed approach to designing a bioenergy-integrated landscape to produce environmental services. The analysis hinges on a strong integration of modeling and field testing, scaling up from farm to watershed. It also takes an interesting approach to integrating yield with ecosystem services to evaluate the economics of these integrated systems alongside conventional cultivation as well as alternate conservation alternatives. I encourage the researchers to

integrate with other, similar BETO-funded efforts to leverage, rather than overlap, efforts across the portfolio.

- My concerns are:
  - This group is taking on both breadth and depth in its research. This is not inherently problematic as long as it does not sacrifice rigor anywhere or duplicate efforts elsewhere in the pursuit of comprehensiveness.
  - The TEA hinges on ecosystem services valuation. This is valid, but it does not offer real financial benefit unless a market emerges for the services being created.
- This project executes an extremely valuable field implementation of the team's approach to identifying subfield marginal lands that can be leveraged to produce bioenergy feedstocks while reducing nutrient runoff and enhancing field economics. The team has undertaken several field analyses of biodiversity effects of the subfield management approach, including analyses of soil biota and canopy insect diversity. The combination of modeling/analysis to identify the field locations and field experimentation is demonstrating the value of this ILM approach and is an exemplary project for this type of work.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the summaries of the project, which was initiated in FY 2011.
- We are engaged with other researchers as appropriate, given the various approaches, goals, settings, etc., of different project teams. To address the two concerns: (1) Each task and activity of this unique field study is carefully thought out and necessary for this system-level investigation. We are addressing critical questions at the interface between production and ecosystem services, with a focus on the marginal areas of the agricultural landscape. We maintain a detailed approach to both the collection of fundamental field data and the calculation/modeling of ecosystem services benefits and economic value. (2) Examples of water quality trading systems offer a good set of insights (e.g., Chesapeake Bay, Ohio River), and in the next funding cycle we intend to further the understanding of the value of trading through public-private partnership.

# **BIOENERGY SUSTAINABILITY: HOW TO DEFINE AND MEASURE IT**

# **Oak Ridge National Laboratory**

# PROJECT DESCRIPTION

The objective of this project is to propel the U.S. bioenergy industry toward implementation of cellulosic biomass systems that maximize benefits (e.g., rural jobs, water quality, biodiversity) while minimizing negative impacts. Although there is strong consensus regarding the need for sustainability, there is little agreement about the methods or metrics that can measure it. The first phase of our project, "Bioenergy Sustainability: How to Define & Measure It," worked to characterize environmental and socioeconomic costs and benefits of cellulosic bioenergy production in the context of stakeholder priorities. We applied indicators of progress toward bioenergy sustainability in three different landscapes: east Tennessee

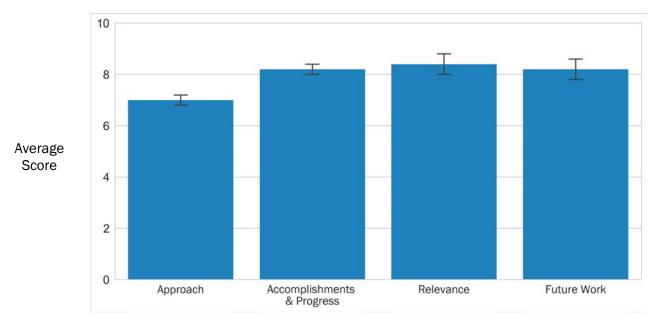
| WBS:                      | 4.2.2.40            |
|---------------------------|---------------------|
| CID:                      | NL0022601           |
| Principal Investigator:   | Dr. Esther Parish   |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$3,061,907         |
| DOE Funding FY16:         | \$750,000           |
| DOE Funding FY17:         | \$800,000           |
| DOE Funding FY18:         | \$861,907           |
| DOE Funding FY19:         | \$650,000           |
| Project Status:           | Ongoing             |
|                           |                     |

switchgrass-to-ethanol production, southeastern U.S. bioenergy wood pellet production, and Iowa ethanol production from corn stover and switchgrass. A checklist of 35 environmental and socioeconomic indicators and these three case studies were used to develop an overall approach for assessing sustainability:

- Work with stakeholders to establish a set of goals based on the bioenergy project context and scope
- Select and prioritize a set of sustainability indicators that can inform decision making relative to those goals

# Weighted Project Score: 8.0

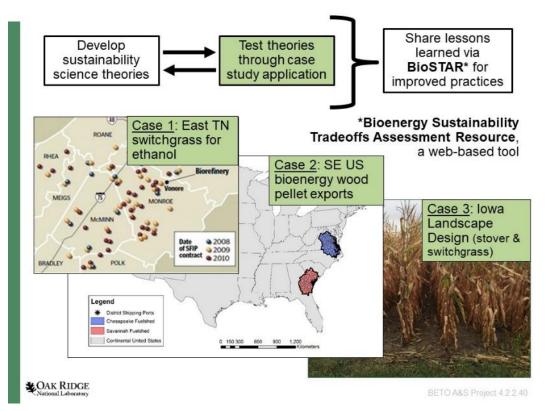
Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $\square$  One standard deviation of reviewers' scores

- Establish baseline and target values for each indicator to assess future sustainability outcomes relative to a reference case of no bioenergy production
- Characterize indicator trends using empirical measurements, surveys, and/or computer models
- Analyze potential tradeoffs between environmental and socioeconomic indicators under a set of defined alternative future scenarios
- Use results to identify good practices.

We designed the Bioenergy Sustainability Tradeoffs Assessment Resource (BioSTAR) to allow stakeholders to view the results of our sustainability case studies and/or conduct a sustainability assessment for their own bioenergy project. Since March 2017, we have published 19 papers about sustainability theory, our case study results, and successful engagement with Iowa stakeholders. The new three-year phase of our project was funded in October 2018 and focuses on the quantification, aggregation, prioritization, and visualization of sustainability indicators for improved understanding of the potential tradeoffs and synergies between environmental and socioeconomic priorities. We are developing the underlying sustainability theory needed to assess these tradeoffs and synergies at the fuel-shed scale (i.e., the scale of the entire landscape supplying cellulosic biomass to a biorefinery). We are leveraging research by other DOE laboratories, the USDA, EPA, U.S. Geological Survey, and universities to develop a starting set of national-scale spatiotemporal sustainability indicator data sets that can be used to characterize baseline conditions and cellulosic feedstock sustainability trends anywhere in the continental United States. These new data sets and methods will be incorporated into our web-based BioSTAR tool so that DOE, industry, and other researchers can holistically quantify costs and benefits and analyze tradeoffs of U.S. biomass production options, integrating environmental and socioeconomic indicators of sustainability tailored to local conditions and stakeholder priorities.





## OVERALL IMPRESSIONS

- This ambitious program is working to compile and simplify the presentation of complex sustainability metrics over various scales, regions, and metrics.
- The abstract provides ample detail about the history and genesis of work, the relevance of the research contributing to a better understanding of sustainability issue/theory, and metrics. The primary objective is a bit altruistic in a sense that the goal to propel the U.S. bioenergy industry toward implementation of cellulosic biomass systems that maximize benefits (e.g., rural jobs, water quality, biodiversity) while minimizing negative impacts could be the goal for any project in this space. It would be nice to have more definitive goals identified in the presentation. A desired outcome is to provide science-based data and web-based analytic tools (e.g., BioSTAR) to holistically analyze tradeoffs of U.S. biomass production options by integrating environmental and socioeconomic indicators of sustainability tailored to local conditions and stakeholder priorities.
- This is clearly an important and timely issue, and it is relevant to many national and international discussion in the bioenergy space. It is not clear that the model described can be generalized. Can it be applied to new cases other than the case studies under consideration? Thirty-five indicators are very comprehensive. It would be hard to rigorously assess them in a single case study—let alone build a generalized model capable of doing so for all possible cases.
- This is a valuable effort in terms of better understanding how target sustainability performance criteria can inform feedstock selection and potentially landscape-level design, and it will be even more valuable when available publicly. It might be challenging to implement at a national level because of the site-specificity and target-setting requirements outlined. If some fundamental overall tradeoffs were evaluated for different feedstocks, that could help with upfront screening even absent detailed site data and target setting. Knowing there are many existing sustainability certification schemes and approaches for varying audiences, the team should think carefully about and communicate whether and/or how BioSTAR differs from existing certification/sustainability schemes (including the one being developed under the EE0007088 project) in terms of audience/utility and any complementarities.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

Thank you for the thoughtful comments acknowledging the ambitious objectives set forth by this project. Specific project goals are summarized as milestones. A key clarification is that the BioSTAR tool is being developed in parallel with three case studies. Each case study is useful and addresses specific BETO strategic goals while providing the team with examples for testing BioSTAR's usefulness. BioSTAR is a visualization tool designed to illustrate tradeoffs among a set of user-defined indicators. BioSTAR incorporates some aspects of a calculator to facilitate estimation of indicator values, but the tool focuses on making it easier to understand and compare options without losing the details behind each source of indicator data. BioSTAR output could be used to illustrate the degree to which desired metrics are met or not, including defined certification requirements, but BioSTAR was not designed for certification purposes. Users determine indicators and targets, making the BioSTAR platform adaptable to any existing standard or certification. An evaluation of individual indicators is done using other models outside of BioSTAR. The starting checklist of indicators presented in BioSTAR is based on earlier project publications. The team reviewed indicators from various sustainability certification schemes (and other sources) and then worked with U.S. bioenergy stakeholders for several years to deliberately narrow the focus to a set of essential, practical measurements that could be repeated across multiple bioenergy projects. But we agree that most studies will not measure all 35 indicators, and we have developed and published an indicator selection framework that allows users to choose from any set of indicators as they determine the most important indicators for their situation. In summary, this project has: (1) developed a sustainability assessment approach based on a decade of research; (2) tested the approach through case studies of bioenergy production in three different U.S. landscapes; and (3)

prepared a prototype web-based visualization tool (BioSTAR) designed to help researchers and educators visualize indicator baselines, targets, trends, and tradeoffs among targets for particular cases of cellulosic bioenergy production.

# SHORT-ROTATION WOODY BIOMASS SUSTAINABILITY

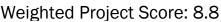
# **Oak Ridge National Laboratory**

## **PROJECT DESCRIPTION**

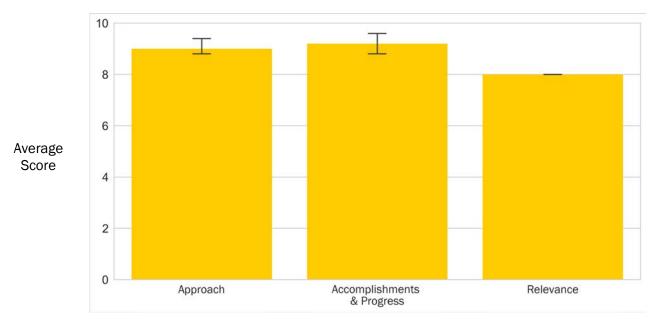
The southeastern United States is projected to be an important region to produce loblolly pine as an SRWC for bioenergy. SRWC production differs from traditional forestry (i.e., pulpwood and sawtimber) because more frequent rotations can increase ground disturbance, and greater weed control and fertilization might impair water quality; however, the environmental effects of growing loblolly pine in a short-rotation system have not been evaluated at a watershed scale. Further, current forestry best management practices (BMPs), developed for traditional forestry, have not been tested for SRWC production. In this study, we used a combined watershedscale experiment and a watershed-modeling approach to

| WBS:                      | 4.2.2.41              |
|---------------------------|-----------------------|
| CID:                      | NL0025180             |
| Principal Investigator:   | Dr. Natalie Griffiths |
| Period of<br>Performance: | 10/1/2014-9/30/2018   |
| Total DOE Funding:        | \$1,489,884           |
| DOE Funding FY16:         | \$345,000             |
| DOE Funding FY17:         | \$345,000             |
| DOE Funding FY18:         | \$799,884             |
| DOE Funding FY19:         | \$0                   |
| Project Status:           | Sunsetting            |
|                           |                       |

examine the environmental sustainability (i.e., effects on water quality, water quantity, soil quality, and productivity) of SRWC production in the southeastern United States. The watershed experiment used a beforeafter, control-impact approach. Baseline conditions in three adjacent watersheds in South Carolina were monitored for two years, and then 50% of two (treatment) watersheds were harvested, planted with loblolly pine seedlings, and managed for SRWC production (i.e., multiple herbicide and fertilizer applications to achieve high yields). Environmental responses were measured for six years after loblolly pine were planted; approximately halfway through the approximate 10-year rotation.

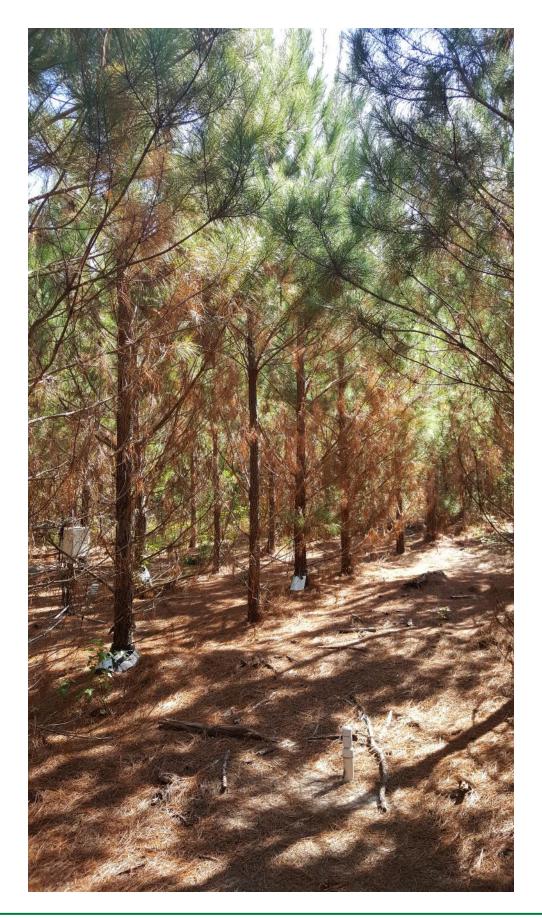


Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

The intensive silviculture plan resulted in rapid tree growth. After the sixth growing season, carbon sequestration by the loblolly pine was 6–14 years ahead of standard timber plantations, and water use (i.e., evapotranspiration) was similar to a 10- to 20-year-old loblolly pine stand. Watershed modeling results suggest that during multiple rotations, SRWC production will result in slightly more reduced evapotranspiration and slightly more increased streamflow than conventional forestry; however, structural differences in the watershed models sometimes resulted in inconsistent results. Ecosystem nitrogen dynamics changed during six years of tree growth. During the first two growing seasons, nitrate leaching rates were high, and there was a corresponding increase in groundwater nitrate concentrations (to less than 2 mg N/L). Despite the elevated groundwater nitrate, stream-water nitrate concentrations remained low and unchanged through the sixth growing season. Groundwater modeling suggests that elevated nitrate in groundwater should have reached the stream after six years. Therefore, biotic processes (e.g., denitrification) might have removed this nitrate. Denitrification measurements that were initiated in the last two years of our project found that this microbial process was likely important in removing elevated nitrate, especially in the organic-rich, riparian-zone streamside management zones separating the pine plantations from the streams. Overall, the minimal effect of SRWC production for bioenergy on stream water quality suggests that current forestry BMPs are effective at protecting surface waters in the coastal plain landscape even with high levels of fertilization and herbicide application associated with SRWC production.





Photos courtesy of Oak Ridge National Laboratory

### **OVERALL IMPRESSIONS**

- This project focuses on the nutrient, carbon, and water fluxes in a short-rotation woody biomass plot and sheds valuable insights on nutrient-loading policies and denitrification dynamics in the subsurface.
- This combined field and modeling analysis to assess the environmental performance of intensive SRWC production in the Southeast is well implemented and provides a significant advancement of our understanding of the viability and sustainability of this production system. The replication at the watershed level is (probably necessarily) low; nevertheless, the teams have amassed a valuable set of data on SRWC performance. Although this approach used current state-of-the-art cultivation practices, these practices leverage chemical inputs rather heavily. Given that sustainability is a fundamental goal of these bioenergy production systems, it would have been nice to see a treatment with a more environmentally friendly management regime (i.e., reduced chemical inputs) to assess performance and sustainability differences.
- This is a sunsetting project.
- Current forestry BMPs, developed for traditional forestry, have not been tested for SRWC production. This study uses a combined watershed-scale experiment and a watershed-modeling approach to examine the environmental sustainability (i.e., effects on water quality, water quantity, soil quality, and productivity) of SRWC production in the southeastern United States.
- This project determines whether current forestry BMPs are adequate to protect water and soil resources.
- This project addresses barriers At-C: Data Availability Across the Bioenergy Supply Chain and At-E: Quantification of Economic, Environmental, and Other Benefits and Costs.
- The high temporal and spatial resolution as well as the sophisticated field techniques applied to the fieldmonitoring element of this research is yielding a valuable data set. This field testing is well integrated with the agronomic modeling, making the overall research project very coherent. The field trials carried out in this research are yielding strong and promising results as to the efficacy of the BMPs evaluated through this research.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Thank you for all these comments. We agree that watershed-scale experiments are very difficult to replicate. Our original study design included two treatment watersheds, each with a different management regime; however, it was decided to focus on one management treatment in two watersheds based on the inherent variability among watersheds and because adding multiple experimental treatments would make interpreting the results more difficult. We pushed the system in terms of the amount of fertilizer applied at the watershed scale because we wanted to measure potential maximum responses. We also wanted to see if standard BMPs would work at high fertilizer application rates. Although we did not include different management scenarios at the watershed scale, we did use different levels of herbicide and fertilizers at the plot scale to examine the effects on the ecosystem nitrogen budget.

# SPATIALLY RESOLVED MEASUREMENTS OF ENVIRONMENTAL SUSTAINABILITY INDICATORS FOR BIOENERGY

# **Oak Ridge National Laboratory**

# **PROJECT DESCRIPTION**

A suite of environmental indicators has been identified to evaluate the environmental sustainability of bioenergy production systems (i.e., water quality and quantity, soil quality, GHG, biodiversity, air quality, productivity). Measurement of many of these environmental indicators requires manual sampling in the field. Often, these measurements can be time and labor intensive to collect and thus limited in spatial and temporal resolution. Environmental sensors have improved understanding of temporal variability of some indicators, but spatial variability is still understudied. Coupling environmental sensors with unmanned vehicles provides the ability to measure environmental indicators at high spatial

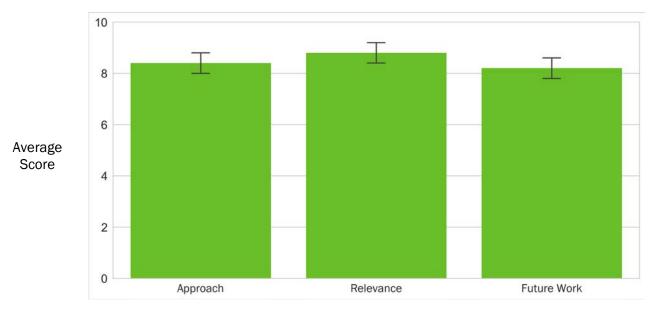
| WBS:                      | 4.2.2.44              |
|---------------------------|-----------------------|
| CID:                      | NL0035013             |
| Principal Investigator:   | Dr. Natalie Griffiths |
| Period of<br>Performance: | 10/1/2018-9/30/2021   |
| Total DOE Funding:        | \$350,000             |
| DOE Funding FY16:         | \$0                   |
| DOE Funding FY17:         | \$0                   |
| DOE Funding FY18:         | \$0                   |
| DOE Funding FY19:         | \$350,000             |
| Project Status:           | New                   |
|                           |                       |

resolution. The goal of this project is to quantify spatially resolved environmental sustainability indicators in a bioenergy feedstock production landscape using state-of-the-art and commercial, off-the-shelf water-quality sensors coupled with unmanned surface vehicles (USVs).

This new project, which began in FY 2019, will focus on developing a USV-water-quality platform for measuring nitrate concentrations at a high spatial resolution. The USV-water-quality platform will be tested in nearby lotic and lentic water bodies to assess measurement accuracy compared to traditional measurements

# Weighted Project Score: 8.4

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f ar I}$  One standard deviation of reviewers' scores

(i.e., grab sampling). After development and testing of the USV-water-quality platform, the system will be used to assess spatial patterns in stream water nitrate concentrations in the BETO-sponsored Antares Landscape Design project. Bioenergy feedstock production coupled with conservation practices have the potential to improve water-quality conditions in the agricultural Midwest, where nitrate pollution is a significant concern. The USV-water-quality platform will be used to assess the efficacy of saturated buffers, a conservation practice implemented within the Antares Landscape Design project, at reducing nitrate inputs. The USV-water-quality system will also be used to examine spatial patterning in water quality that might arise because of variation in bioenergy feedstock plantings, conservation practices, and hydrologic inputs (e.g., tile drains) within the two Antares focus watersheds. Overall, this project will evaluate the ability of sensors coupled with USVs to advance understanding of a key environmental sustainability indicator by providing valuable, spatially resolved water-quality data within a bioenergy production landscape.



Photo courtesy of Oak Ridge National Laboratory

#### OVERALL IMPRESSIONS

- This project is a novel effort to leverage new technology to improve the potential frequency, cost effectiveness, labor efficiency, and spatial resolution of farm runoff water-quality data.
- I would have liked more discussion on the current and near-term competing alternatives to provide the water sampling service provided by this USV system.
- This project will advance field measurements for water quality by deploying and testing the use of inexpensive, automated vessels for sampling water quality at high spatial and temporal resolution with

low cost. If successful, these sensors would enhance the ability of researchers to cost-effectively acquire much-needed data to evaluate benefits/impacts of various land management strategies on nutrient runoff and water quality. In addition to cost and performance assessments indicated in the project plan, I strongly suggest some evaluation of reliability, durability, and maintenance of performance throughout time because the long-term performance will significantly affect the overall cost to run these sensors.

- This is a new FY 2019 project.
- The goal of this project is to quantify spatially resolved environmental sustainability indicators (water quality and quantity, soil quality, GHG, biodiversity, air quality, productivity) in a bioenergy feedstock production landscape using state-of-the-art and commercial, off-the-shelf water-quality sensors coupled with USVs. Coupling environmental sensors with USVs provides the ability to measure environmental indicators at high spatial resolution.
- This project addresses barriers At-C: Data Availability Across the Supply Chain; and At-E: Quantification of Economic, Environmental, and Other Benefits and Costs.
- This is an interesting, novel research/engineering project. I'm glad to see it in the BETO portfolio because it stands to serve other BETO projects well if the technology being developed aids in broader field data-collection campaigns.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for these comments. Similar approaches (coupling USVs and/or unmanned aerial vehicles [UAVs] with water-quality measurement systems) have been described in the literature; however, we are not aware of any studies that have used USVs to measure nitrate concentrations in freshwater, and we are also not aware of any studies that have USVs to measure water quality when addressing scientific questions related to bioenergy sustainability. These are the objectives of our study. Most studies on USV/UAV-water-quality sensor systems that we reviewed in the literature focus on describing the technology and associated measurements, but few have used this technology to address specific research questions. USVs have been used to measure temperature, conductivity, turbidity, salinity, and chlorophyll in rivers, and UAVs have been equipped with water-quality (temperature, conductivity, dissolved oxygen, pH) sensors or sampling devices to collect water for later analysis in the laboratory. Most USVs that have been used for water-quality measurements are larger systems for deployment in larger water bodies (i.e., lakes, rivers). The USV system we selected was designed for bathymetric mapping and is one of the few USV systems we found that was small enough to navigate smaller bodies of water but large enough to hold nitrate sensor payloads.
- Thank you for these excellent comments and suggestions. We will incorporate an assessment of reliability, durability, and maintenance in our cost-benefit analysis (FY 2019 Q4 milestone).

# ENABLING SUSTAINABLE LANDSCAPE DESIGN FOR CONTINUAL IMPROVEMENT OF OPERATING BIOENERGY SUPPLY SYSTEMS

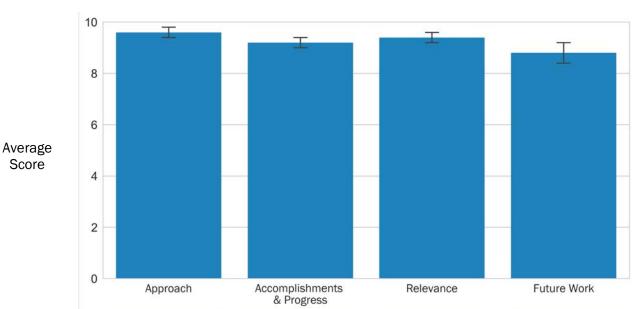
#### Antares Group, Inc.

#### **PROJECT DESCRIPTION**

When fully developed, documented, and demonstrated in three commercially relevant bioenergy supply sheds, the landscape-design activities, associated enabling tools and practices, and the field-level sustainability and logistics system results will advance the state of the art of sustainable bioenergy landscape design processes that will support current and future cellulosic biorefineries and the emerging bioenergy and bioproduct industries. Through

| WBS:                      | 4.2.2.60           |
|---------------------------|--------------------|
| CID:                      | EE0007088          |
| Principal Investigator:   | Mr. Kevin Comer    |
| Period of<br>Performance: | 4/1/2016-3/31/2021 |
| Total DOE Funding:        | \$4,974,990        |
| Project Status:           | Ongoing            |
|                           |                    |

outreach and information resources developed by the project team, the template created by this project can be adapted and implemented elsewhere and will offer a path to shared benefits for a broad range of federal, state, local, and industrial stakeholders. This project will use new and emerging subfield analytic software that will enable management decisions via precision agronomics. This will allow for the identification of optimum areas to incorporate perennial energy crops and conservation practices into corn- and soybean-producing fields in a manner that is both economically and environmentally beneficial. The foundation of the project's multistage stakeholder outreach plan is to leverage existing federal, state, and local conservation programs, coupled with a transformative approach of integrating herbaceous energy crops into the bioenergy supply mix to supplement agricultural residues. The project team will seek to implement a modified conservation grasslands approach on a pilot program basis to allow for the establishment and harvest of up to 2,000 acres of warm-



#### Weighted Project Score: 9.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${f I}$  One standard deviation of reviewers' scores

season grass energy crops that allow landowners to retain their conservation program benefits while harvesting and selling their grass crop. Additional conservation practices will be implemented and monitored, including the establishment of up to 15,000 acres of cover crops. A multiyear comprehensive field research, testing, and monitoring program will be conducted on targeted fields within the project's activities.

The best and most immediately relevant opportunities to develop and demonstrate innovative and impactful landscape design practices for bioenergy systems exist within the feedstock supply sheds of operating bioenergy projects. This project will be conducted in the biomass feedstock supply sheds serving POET-DSM's Project LIBERTY biorefinery in Emmetsburg, Iowa, and formerly DuPont Cellulosic's biorefinery in Nevada, Iowa (the plant recently sold to Verbio for renewable natural gas production from herbaceous biomass feedstocks). These are areas where LUC is already underway but is still early in its evolution in supporting the supply chains of groundbreaking cellulosic biorefineries. The project will build from information available from these operating bioenergy systems and collect additional data necessary for addressing barriers and stakeholders' objectives. The project's activities are also coordinated with the Iowa Department of Agriculture and Land Stewardship and are aligned with their aggressive efforts through the Iowa Nutrient Reduction Strategy to reduce nutrient runoff that contributes to Gulf hypoxia and other negative impacts to water quality. The project team is also implementing precision agriculture strategies to improve profitability and sustainability of biomass harvest operations and decision-making processes.



Photo courtesy of Antares Group, Inc.

#### OVERALL IMPRESSIONS

- This is an incredibly valuable project to develop new tools and approaches for landscape design to improve profit, biomass supply, and sustainability, with the ability to develop, test, and validate models on large real plots of agricultural land.
- As one of the largest programs (in terms of financial resources, partners, and acreage), this project has been appropriately evolving as a key partner to many other BETO-funded programs.

- This is a valuable project. The project provides a valuable resource to other projects in the portfolio to collect data and lends itself to landscape design (three bioenergy supply sheds), testing and developing equipment, and access to expertise and lessons learned.
- This project advances the state of the art for sustainable bioenergy landscape design processes, and it will develop and demonstrate new tools and approaches for planning and implementing sustainable landscape design strategies aimed at simultaneously improving farm profitability, environmental sustainability, and future sustainable biomass supply production, thereby improving the viability of future herbaceous biomass supply systems and projects.
- This project addresses barriers At-B: Analytical Tools and Capabilities for System-Level Analysis; At-C: Data Availability Across the Supply Chain; At-E: Quantification of Economic, Environmental, and Other Benefits and Costs; At-F: Science-Based Methods for Improving Sustainability; and At-G: Social Acceptance and Stakeholder Involvement.
- This project exhibits a strong and well-designed integrated use of empirical field assessment of corn stover and perennial grass cultivation, including use on buffer strips integrated with common and well-supported modeling frameworks (such as the SWAT model). Its focus on concrete case studies in service of broader questions is commendable. I do see some redundancies between this project and others in the BETO portfolio, but this should be an opportunity to better integrate this project's methods, frameworks, and case-study sites across the portfolio to take advantage of potential synergies.
- This is a significant and comprehensive field effort to experimentally test approaches to leveraging marginal lands for economically and environmentally beneficial feedstocks for the bioeconomy, including the development of novel field equipment that will advance the viability of residue harvesting. Although representing a large investment, this project is providing significant real-world value and is well integrated with national laboratory projects to enable data collection, validation of modeling, and field testing of landscape management approaches. My only recommendation on any of the project components is that the team should carefully assess whether there is true value in developing a new sustainability certification scheme as outlined in the presentation given how many existing voluntary certification schemes there are, and if the team determines it is somehow uniquely valuable, the uniqueness should be clearly explained as part of the description of the approach.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

## **BIOFUELS INFORMATION CENTER**

#### National Renewable Energy Laboratory

#### PROJECT DESCRIPTION

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 (EISA) that requires DOE to develop a "Biofuels and Biorefinery Information Center."

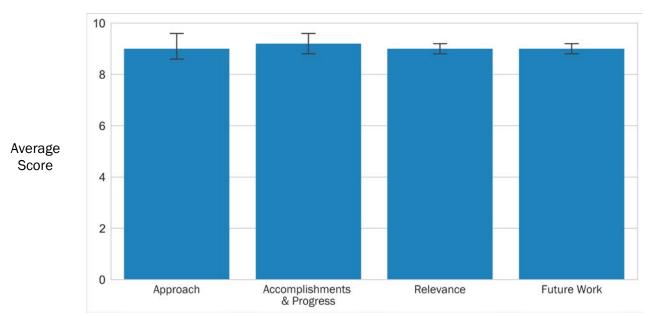
The BIC task supports biofuel pages on EERE's most visited website, the Alternative Fuels Data Center (https://afdc.energy.gov/), as well as the Bioenergy Atlas tools (https://nrel.gov/gis/biomass). This task results in more than 800,000 web page views (an instance of an Internet user visiting a web page) per year. In FY 2017, the

| WBS:                      | 6.3.0.1             |
|---------------------------|---------------------|
| CID:                      | NL0016477           |
| Principal Investigator:   | Ms. Kristi Moriarty |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$1,420,000         |
| DOE Funding FY16:         | \$110,000           |
| DOE Funding FY17:         | \$500,000           |
| DOE Funding FY18:         | \$410,000           |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | Ongoing             |
|                           |                     |

task expanded to include the USDA's Biofuels Infrastructure Partnership (BIP) and the annual *Bioenergy Industry Status Report*. The USDA BIP expanded infrastructure for E15 (gasoline blend with 15% ethanol) and/or E85 (gasoline blend with 51% to 83% ethanol) to approximately 1,400 stations, and NREL collects and analyzes all infrastructure and sales data collected by the 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, costs to install new equipment) and sales data (price and volume for E10 [gasoline blend with 10% ethanol], E15, E85, and diesel by month). The *Bioenergy Industry Status Report* provides key bioenergy metrics in one place. Topics covered include biofuels (ethanol, both starch and



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oxed{I}$  One standard deviation of reviewers' scores

cellulosic; biobutanol; biodiesel; and renewable hydrocarbons), renewable natural gas, biopower, and bioproducts. Reports were published in 2013, 2015, and 2016, and the 2017 report is under review.

The task also supports the PI's time to engage stakeholders on infrastructure and deployment of biofuels. This includes leading, membership, and participation in the following roles: member board of advisors at the Fuels Institute, voting member for multiple UL standards committees, cochair of the infrastructure team at Agriculture Auto Ethanol, member of Society of Automotive Engineers Fuel Grade Assurance Protocol Committee, and member of Coordination Research Council's Ultra-Low Sulfur Diesel Corrosion Committee. The PI routinely responds to industry inquiries to assist in deployment of biofuels.

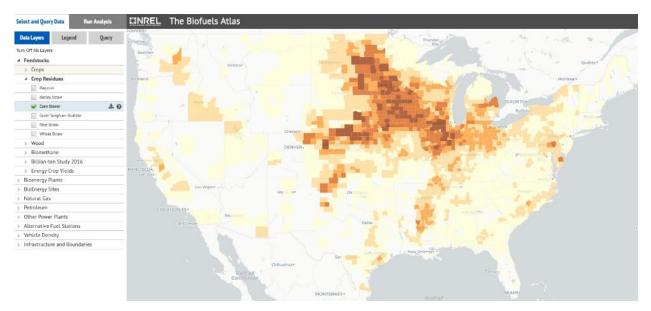


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This program was created in response to EISA 2007 Sec. 229, but it has turned into an invaluable resource to characterize the myriad barriers to domestic biofuel deployment.
- The purpose of the BIC task is to provide relevant data, information, reports, and web-based tools to all bioenergy stakeholders. The establishment of the BIC was mandated under Title II, Sec. 229 of EISA.
- This project addresses barriers At-B: Analytical Tools and Capabilities for System-Level Analysis; At-C: Data Availability Across the Supply Chain; At-G: Social Acceptance and Stakeholder Involvement; and ADO-C: Codes, Standards, and Approval for Use.
- The BIC is practical, serves a clear demand that would otherwise be unfulfilled, and is a good use of DOE money.
- Aggregating data and making them accessible is an important goal because they reach key, nontechnical players in the bioenergy system. A strength of this project is its interaction with end-market commercial actors. This key piece of the story is missed by BETO otherwise.
- The BIC is an extremely valuable resource that is leveraged extensively by the stakeholder community to help make informed market decisions and understand costs. This program is highly valuable and a very efficient use of BETO resources, and it should be continued with further redundancy (i.e., additional deeply engaged personnel) to ensure continuity and performance.

#### **RECIPIENT RESPONSE TO REVIEWER COMMENTS**

• I thank the reviewers for their helpful and supportive feedback.

### **BIOENERGY KNOWLEDGE DISCOVERY FRAMEWORK**

#### **Oak Ridge National Laboratory**

#### PROJECT DESCRIPTION

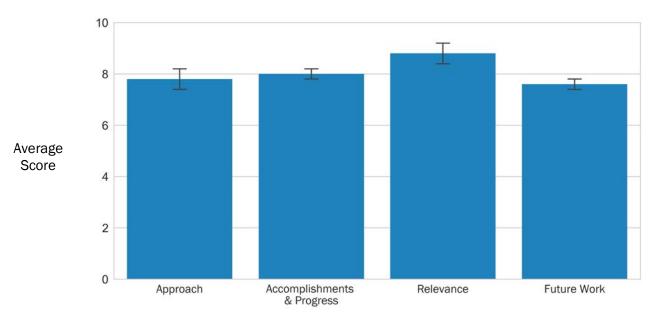
Many issues in the biofuel supply chain, from production to delivery, need to be addressed to foster a viable biofuel industry. Infrastructure issues related to generation, distribution, and delivery of biofuels include finding the optimal locations to site a biorefinery to minimize cost with adequate availability of feedstock resources nearby. The Bioenergy KDF is a collaborative platform for knowledge collection, curation, and discovery to support DOE's effort to develop a sustainable biofuel industry. The Bioenergy KDF facilitates expanded research opportunities by providing a means to synthesize vast amounts of information from across the bioenergy supply chain. The Bioenergy KDF enables data harmonization from different

| WBS:                      | 6.3.0.2             |
|---------------------------|---------------------|
| CID:                      | NL0022893           |
| Principal Investigator:   | Mr. Aaron Myers     |
| Period of<br>Performance: | 10/1/2007-9/30/2022 |
| Total DOE Funding:        | \$917,000           |
| DOE Funding FY16:         | \$250,000           |
| DOE Funding FY17:         | \$300,000           |
| DOE Funding FY18:         | \$187,000           |
| DOE Funding FY19:         | \$180,000           |
| Project Status:           | Ongoing             |
|                           |                     |

sources and serves as a source of authoritative and benchmark data sets and key topics.

#### Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- This KDF project, which has been ongoing for more than a decade, continues to provide clear value to the public and researchers through making data and visualization/analysis tools available to the public.
- To me, this is more of a resource and communications program than "analysis," but it is worth funding, nonetheless.
- This project provides access to knowledge, data, and tools at one site. The Bioenergy KDF is a collaborative platform for knowledge collection, curation, and discovery to support DOE's effort to develop a sustainable biofuel industry.
- This project bringing formerly unavailable data or opaque tools to sunlight is an important goal. For example, the BSM is a key element of EERE/BETO strategic positioning and impact. Keep an eye on what is being used and focus where the demand exists.
- I believe a geospatial data repository would be very useful for a variety of reasons. It would enable ongoing hosting of data sets that are otherwise hard to find and would offer both increased traffic to the KDF site as well as a mechanism for discovery of research via links on the KDF site. The challenge will be the cost of the storage and computing power required.
- The KDF is a useful resource for finding BETO work quickly and easily, and significant improvements have been made recently to facilitate finding related work via landing pages. Continuing to enhance the KDF to enable long-term retention of data sets and generate DOI numbers will help maintain relevance. The KDF is a great way to crowdsource appropriate data relevant to bioenergy.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Thank you for the feedback. We think the reviewers presented interesting ideas and viewpoints, and we will look to address these moving forward.

## ADVANCED DEVELOPMENT AND OPTIMIZATION



### ADVANCED DEVELOPMENT AND OPTIMIZATION OVERVIEW

The Advanced Development and Optimization (ADO) Program develops, tests, and verifies engineering-scale, integrated biorefinery process performance to reduce technology uncertainty and to enable industry-led, subsequent scale-up activities. In addition, ADO develops novel methods to expand end-user acceptance of biofuels and bioproducts and identifies new, robust market opportunities.

ADO conducts integrated systems research by combining technology components, unit operations, or subsystems; testing those under integrated operations; and verifying the integrated process at the engineering scale. Engineering scale refers to production systems that employ new process technologies to produce small volumes of products, learn about the performance of new technologies, and accelerate robust system optimization. Engineering scale, in general, offers the first view into continuous operation at a scale where components or unit operations are assembled and operated together in an integrated environment. Integration at the engineering scales provides data and process capability learning that enable private stakeholders to subsequently scale up process technologies. Engineering-scale verification data are critical to evaluating research-and-development (R&D) techno-economics and sustainability progress.

## ADVANCED DEVELOPMENT AND OPTIMIZATION SUPPORT OF OFFICE STRATEGIC GOALS

The strategic goals of the ADO Program Area are to:

- Develop and test bioenergy production technologies through verified proof of performance in engineering-scale systems and relevant environments
- Research ways to enhance scaling and integrate bioenergy production processes
- Identify innovative end uses.

## ADVANCED DEVELOPMENT AND OPTIMIZATION SUPPORT OF OFFICE PERFORMANCE GOALS

The performance goals for the ADO Program Area are as follows:

- By 2022, verify integrated systems research at the engineering scale for hydrocarbon biofuel technologies that achieve a mature modeled minimum fuel selling price (MFSP) of \$3/gasoline gallon equivalent (GGE) with a minimum 50% reduction in emissions relative to petroleum-derived fuels.
- By 2030, verify integrated systems research at the engineering scale for hydrocarbon biofuel technologies that achieve a mature modeled MFSP of \$2.50/GGE with a minimum 50% reduction in emissions relative to petroleum-derived fuels using economically advantaged feedstocks to produce renewable fuels and bioproducts.

## ADVANCED DEVELOPMENT AND OPTIMIZATION APPROACH TO OVERCOMING CHALLENGES

The ADO approach to overcoming challenges and barriers generally falls into three broad categories:

- 1. Technology and program interfaces
- 2. Systems research and integrated testing
- 3. Co-optimization of fuels and engines.

The ADO Program Area's approach is based on research, development, and testing through cooperative partnerships with private industry and academia, national laboratories, and other U.S. and international agencies and organizations.

The U.S. Department of Energy (DOE) Bioenergy Technologies Office (BETO) has identified the following technical challenges and barriers to be addressed by ADO to achieve its strategic and performance goals:

- Process integration
- Feedstock supply-chain infrastructure
- First-of-a-kind technology development
- Technology uncertainty of integration and scaling
- Codes, standards, and approval for use
- Codevelopment of fuels and engines
- Coprocessing with petroleum refineries
- Materials compatibility and equipment design and optimization.

## ADVANCED DEVELOPMENT AND OPTIMIZATION: ANALYSIS AND MODELING



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### INTRODUCTION

The Advanced Development and Optimization (ADO): Analysis and Modeling Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place from March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 10 projects were reviewed in the ADO: Analysis and Modeling session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$8,092,031 (fiscal year [FY] 2016–FY 2019 obligations), which represents approximately 0.90% of the BETO portfolio reviewed during the 2019 Peer Review. During the Project Peer Review meeting, the principal investigator (PI) for each project was given 30 minutes (depending primarily on the funding level) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the Project Peer Review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the ADO: Analysis and Modeling Technology Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Dr. Siva Sivasubramanian as the ADO: Analysis and Modeling Technology Area review lead, with contractor support from Mr. Remy Biron and Mr. Joshua Messner (Allegheny Science & Technology). In this capacity, Dr. Sivasubramanian was responsible for all aspects of review planning and implementation.

### ADO: ANALYSIS AND MODELING OVERVIEW

ADO conducts integrated systems research up to and including the engineering scale. ADO efforts focus on understanding the relationships between and within unit operations and discovering research-and-development (R&D) gaps for further technology development. In support of BETO's goals to reduce minimum fuel selling price and achieve other BETO programmatic milestones, ADO identifies and leverages potential biofuel pathways to hydrocarbon fuels developed in the Feedstock Supply and Logistics (FSL), Advanced Algal Systems, or Conversion R&D programs. This includes developing testing protocols and performing the necessary verification testing. Results of verification testing, shared across BETO, inform future R&D priorities.

The Analysis and Modeling session reviewed projects that interact with experimental work and challenges anticipated to exist at the large scale or across bioenergy industries and markets. The resulting analytical and modeling products can be used to refine research and engineering strategies or to investigate product properties and how that might impact existing and future infrastructure and markets.

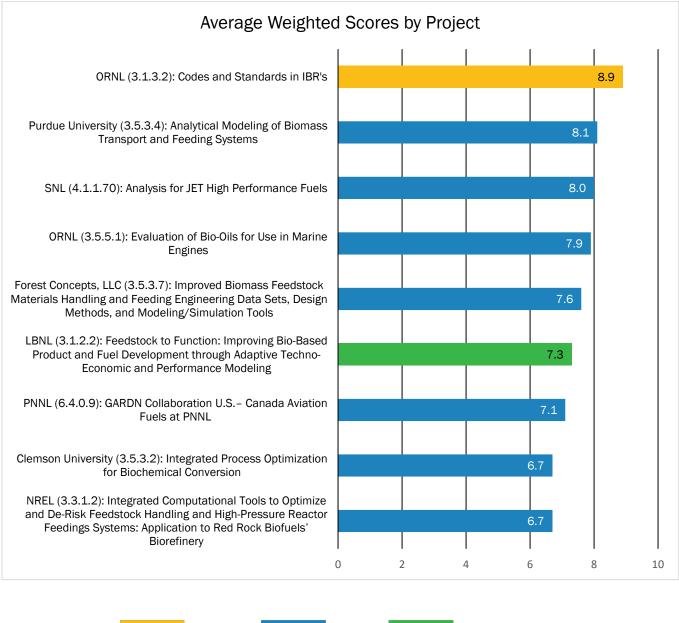
## ADO: ANALYSIS AND MODELING REVIEW PANEL

The following external experts served as reviewers for the ADO: Analysis and Modeling Technology Area during the 2019 Project Peer Review.

| Name           | Affiliation            |
|----------------|------------------------|
| Lucca Zullo*   | VerdeNero, LLC         |
| Mike Fatigati  | Taylor Energy          |
| Daniel Lane    | Saille Consulting, LLC |
| Mark Warner    | Warner Advisors, LLC   |
| Raghubir Gupta | Susteon Inc.           |

\* Lead reviewer

## TECHNOLOGY AREA SCORE RESULTS



Sunsetting Ongoing New

### ADO: ANALYSIS AND MODELING REVIEW PANEL SUMMARY REPORT

#### Prepared by the Advanced Development and Optimization: Analysis and Modeling Review

In general, developing broad, general-purpose industrial modeling tools, or modeling complex phenomena with broad applicability to industrial processes, is a prime target for government-funded research. The BETO portfolio in this area is quite broad, spanning from empirical studies to extremely fundamental ones using *ab initio* and first-principle methods and including the development of validation tools and specific applications of the emerging field of machine learning. This varied portfolio appears balanced across such a broad spectrum.

The review panel found that all projects are supportive, at least qualitatively, of BETO goals as expressed in the BETO *Multi-Year Plan* (MYP). There was consensus, however, that at times the link to the quantitative goals of the BETO MYP was either weak or somewhat forced. This is not necessarily a negative review.

Many projects are at an early or fundamental stage, and although they provide a positive benefit to the industry, the benefit might be challenging to evaluate as a specific contribution to the goal of \$3/gasoline gallon equivalent.

We also had consensus that the presentation format and time limits were not conducive to properly communicating the value and status of the projects. In particular, the format of the presentations consumes too much space in boilerplate information regarding the project budget, timeline, and other programmatic information that could probably be presented as a session summary by the BETO program director before the PIs' presentations.

The PIs' answers to the reviewer comments made it clear that much relevant information was omitted because of space and time constraints. Some of this information was critical to provide a fair and informed assessment of the projects. Not surprisingly, the reviewers found that the techno-economic analysis (TEA) was one of the weakest parts on most projects. Given the broad potential impact, this was not considered a particularly significant weakness. Instead, the panel identified deficiencies with industrial practitioners' participation and validation methods as more substantial weaknesses needing more immediate correction.

#### IMPACT

We noted three main themes in the portfolio of research. All have a significant impact, although the immediacy of their effects on the industry is different.

The first is that of empirical or semiempirical studies. These have a straightforward and often clearly quantifiable impact. Among them, we found that the Oak Ridge National Laboratory (ORNL) study on fire propagation in biomass storage facilities is of particular relevance because it led to immediate but straightforward and actionable solutions to a real problem affecting industry safety. Also from ORNL, the work on evaluating the use of bio-oils in marine engines was particularly well received. The industry has always struggled to find a viable and straightforward pathway for the exploitation of pyrolysis oil, and this analysis lays an original and impactful approach that provides clear possible economic viability without much of the complexity associated with upgrading to fuels for road applications. A commercially viable pathway to deploy bio-oils is exceptionally significant.

Second, the more fundamental first-principle mathematical modeling applied to the analysis of performance and design of biomass feeding systems was well represented in different projects. Given the known impact that biomass handling has on a biorefinery's ability to reach its design goal, this is significant research with clear implications. Nonetheless, the panel felt that the impact, though qualitatively apparent, is not immediately quantifiable. Third, some projects are dealing with still unresolved fundamental issues. There is agreement on the promise of the discrete element method (DEM) as a technique to approximate the complex behavior of biomass particles, but significant work is needed to fully assess the correct predictive envelope of the method and provide fully validated results.

The qualitative impact of modeling exercises is challenging to evaluate without appropriate validation data and techniques; thus, the panel was appreciative of the Forest Concepts, LLC project aiming to develop a quantitative method to measure flow properties in biomass and felt that much more work and emphasis in this area is needed.

The use of multiple nested or parallel modeling techniques—such as DEM, computational fluid dynamics (CFD), and the finite element method (FEM)—to address the entire slate of equipment and processes used in biomass handling are pragmatic approaches to achieving an adequate level of fidelity but add considerable complexity. In other industries, these modeling techniques are mature but remain the domain of specialists. These techniques often support the development and design of new equipment but are used sparingly in operations given the level of expertise and computer resources used.

As these programs evolve, we encourage more direct involvement with equipment manufacturers and the development of simpler, higher-level derived modeling tools that could be used more extensively by practitioners, as outlined in the Clemson University project on Integrated Process Optimization for Biochemical Conversion. We believe this type of layered approach and the direct involvement of equipment manufacturers significantly improves the impact of these projects. Also, although we welcome the direct participation of biorefinery operators and the development of the modeling tools in the context of their operation, we hope that the general lessons learned can be transferred to the broader industrial community and not remain confined to specific operations.

The panel was extremely intrigued by projects using *ab initio* chemical simulation and machine learning to scope molecules of interest with functionality for biofuel applications. We understand that these are relatively early-stage projects, and in the case of machine learning, the leveraged technology is still relatively immature. We believe these approaches and projects have substantial potential, and we encourage their continuation. Validation data and extension of the predictive envelope remain key metrics to expand to address more practical applications.

As discussed earlier, the direct impact to the BETO MYP, though clear to all, is not particularly easy to quantify. We felt that these tools could provide powerful screening. Although there is no substitute for the direct evaluation of a molecule for suitability to a task, these tools can help weed out unsuitable ones and lead to more effective, faster, and economically efficient development.

#### INNOVATION

The review panel did not find a lack of innovation in the portfolio. The exploration of relatively new computational methods such as machine learning and the creative use of DEM to simulate biomass flow are innovative and examples of integrating maturing technologies into a more sophisticated analytical framework.

As mentioned, data validation remains a relatively weak area of this portfolio. Given its importance and complexity, we believe this is a significant innovation opportunity, as demonstrated by the Forest Concepts project. As the portfolio evolves and expands, we encourage BETO to devote resources to more projects explicitly addressing gaps in data validation.

The use of distributed parameter modeling (DEM, CFD, FEM) techniques can achieve its full potential when applied to designing new biomass handling equipment and not only to optimizing existing ones, which is the most significant focus today. This goal requires a substantial leap in data validation techniques, as clearly understood by the PIs.

The use of molecular modeling tools—whether based on machine learning or *ab initio* calculations—to develop screening tools is also innovative and of great interest. We hope that as the work progresses, these tools are more directly integrated into the conceptual framework of a biorefinery by the introduction of links to the synthesis route and type of biomass feedstock.

#### **SYNERGIES**

Modeling efforts are synergistic because modeling is not a solution to a problem; it is a tool. Several projects model biomass flow using a combination of DEM, CFD, and FEM techniques and higher-level metamodels that are synergistic, and lessons—especially in the selection of tools and the approximation used—can and should be shared among projects and programmatic areas.

Screening tools aimed at molecular properties have clear possible synergies with other BETO programs—in particular consortia such the Co-Optimization of Fuels & Engines (Co-Optima)—although these possible or actual synergies were not always explicitly mentioned. The scope for synergies is substantive and not ignored by the PIs.

The modeling of fire in a biomass storage facility and the exploration of bio-oils as marine fuels are very focused projects, yet the PIs demonstrated extensive and broad capabilities that are relevant to many other aspects of the BETO program, and we hope BETO can leverage these capabilities in other areas.

The panel agreed that the TEA of the impact of these projects was wanting, and more detail would have been desirable. In some cases, such details were absent because of the limiting format of the presentations. The panel appreciates the difficulties in expressing a quantitative economic value for some projects at the current state of development, and this should prompt a more general discussion of appropriate TEA metrics, especially in the very early stages of these projects.

Further, we discussed whether some financial metrics used by BETO are the most appropriate. Nonetheless, we expect at least a qualitative and aspirational statement of the potential economic impact. Because individual projects fit into larger, more complex projects and development goals, such a statement becomes a critical assessment of the synergistic project value.

#### FOCUS

The projects in this programmatic area focus on addressing well-defined problems in BETO's larger programmatic area and are well aligned within the MYP. The panel was somewhat concerned with the possibility of projects losing internal focus either because of pushing the teams outside their sphere of competence or because of overambitious goals.

An example of the first problem is the project presented by Forest Concepts. The development of the measurement cell is an excellent effort and an example of innovative research both responsive to the BETO goals and capable of advancing the state of the art in this sector. The part of their project dealing with modeling, on the other hand, is less exciting and appeared to be included to fill perceived gaps in responsiveness to the funding opportunity announcement (FOA) rather than because it is essential. We believe that BETO could exploit the natural synergies existing in the program. BETO should then guide such a project to direct work where expertise is the strongest and foster collaboration with some other efforts among those who have higher expertise and can place an emphasis on modeling.

An example of a potentially overambitious effort is the National Renewable Energy Laboratory (NREL) project to model the feedstock handling and the high-pressure reactor of the Red Rock Biofuels biorefinery. We felt that attempting to model both the feedstock handling and the gasifier might be an overreach given the time and budget of the project and the acknowledged knowledge gap in several areas.

We found the screening tools using either machine learning or *ab initio* methods still too narrowly focused on a small set of physical properties and with a relatively weak link to the bioprocessing pathway and specific biomass types. These deficiencies in broader focus are nonetheless justified by the early stages of development and the complexity of the problem. They do not detract from the current value of the work but indicate needed future developments.

It should be clear that these problems are nonetheless minor and easily mitigated by guidance and coordination from BETO program directors. Such guidance is critical. The development of modeling tools and techniques is always fraught with risk when it comes to focus: on one hand, the work needs to be broad enough to serve a large audience and fulfill larger programmatic goals in solving shared problems; on the other hand, projects often need to be specific enough to provide a solution for one problem at hand and demonstrate that they can address real case studies.

#### TECHNOLOGY DEVELOPMENT PIPELINE

The panel found no substantial fault with the technology development pipeline, which strikes a balance between projects of immediate impact and the development of tools with a longer time horizon. We identify three themes:

- 1. Screening tools and systems for faster progress
- 2. Advanced modeling of biomass systems
- 3. Validation and measurement tools.

We believe this last area is particularly importance, and we hope to see in it more projects and with increased emphasis in the future. Within the broad strokes of this classification, we believe that the technology portfolio could be expanded. Without prejudice for modeling and optimization efforts carried within other programmatic areas, other technologies and consortia supported by BETO could benefit from the more systematic modeling and analysis approach presented in this technology area.

In the view of the panel, the project that was the least aligned in this portfolio was the project on the Green Aviation Research and Development Network (GARDN) U.S.-Canada Aviation Fuels at Pacific Northwest National Laboratory (PNNL) because it did not fit any clear technology pipeline. The project was not devoid of scientific merit nor was the panel concerned about its execution; it is an excellent example of international collaboration, which the panel considered very positive. The project did not provide any new insight or expand the scope of existing insights, however. The project ultimately stood alone without a clear objective to follow further down the path. In projects where new modeling approaches are being developed, BETO should ensure that they can maximize the impact on industry by ensuring complexity and computer resource demand do not become limiting factors. In these cases, metamodeling techniques—such as that proposed by the Clemson University project—appear to be a valuable approach.

Last, as machine learning and extensive data set analysis technologies continue to improve, we welcome and encourage continued and expanded investment in this area.

#### RECOMMENDATIONS

Our recommendations can be summarized as follows:

- The programmatic area is essential and needs to be continued and expanded.
- Modeling work should, in general, contain a stronger emphasis on data validation. Projects specifically focused on collecting needed experimental data—via new measurement techniques or instrumentation—should be included in the technology area.

- More industry and industrial practitioner input is necessary, including from equipment manufacturers, domain experts in the area of physical fuel properties, and others. In projects aiming to model specific sections of the biorefinery, the ultimate goal should be the design of new equipment, not only the optimization of existing ones.
- During the peer review, it would be beneficial to include an introduction by the program directors explicitly illustrating the logic behind the selection of the various projects, how BETO sees them fitting into the overall program, and, in the case of sunsetting projects, how the final results match initial expectations.
- The presentation format used by the PIs should have less boilerplate information. Such information could be presented as part of the proposed directors' overview. In general, the presentation format should allow for more relevant technical details to be included. It was a common occurrence for panel members to upgrade their initial assessment of the project based on the live presentation and questioning of the presenter.
- The area of tools for screening options, such as the selection of optimal molecules for a given performance, should be expanded because it is of great value and can take advantage of rapidly evolving areas of computer science such as machine learning. It should, however, more explicitly include links to biorefinery feedstock and routes. We believe that the value there is not that of predicting the best molecule or pathway but rather to support the early and rapid identification of bad ones.
- TEAs are often absent or marginal, reflecting the inadequacy of the standard metrics used by BETO for this area. Such deficiency needs to be corrected with the development of new and more flexible metrics.

## ADO: ANALYSIS AND MODELING PROGRAMMATIC RESPONSE

#### INTRODUCTION/OVERVIEW

At BETO, we appreciate the participation of the review panel and the feedback received from both the review panelists and the steering committee during the Project Peer Review meeting in March 2019 and the Program Management Review meeting in July 2019, respectively.

The review panel classified the ADO Analysis and Modeling Technology Area portfolio of nine projects into three groups:

- 1. Empirical or semiempirical studies comprising codes and standards (ORNL) and evaluation of bio-oils (ORNL). The review panel highlighted that these projects have a straightforward and quantifiable impact by providing actionable solutions to the industry.
- 2. Fundamental first-principle mathematical modeling applied to the analysis of performance and design of biomass feeding systems projects consisting of Clemson University, Forest Concepts, Purdue University, and NREL. These projects focus on understanding operational challenges and help achieve reliable operations at design capacities. The reviewers noted that the impact of the research work in this area is significant with clear implications. In addition, they observed that the impact is qualitatively apparent, and because of the early nature of these projects, at present the immediate impact cannot be quantitatively ascertained.
- 3. *Ab initio* chemical simulation and machine-learning projects, including the projects from Lawrence Berkeley National Laboratory (LBNL) and Sandia National Laboratories. These projects address the identification of molecules with functionalities and relevant properties using computer-aided tools and techniques.

With respect to maximizing the impact of the ADO Technology Area, the program will consider the following actions:

- Validate mathematical models with relevant operating data to ensure high fidelity of these models
- Encourage industrial participation via a consortium such as the Feedstock-Conversion Interface Consortium (FCIC)
- Continue *ab initio* methods and machine-learning projects to realize their full potential
- Evaluate the importance of developing reduced-order (simplistic) mathematical models to enable wider adoption by stakeholders.

In terms of innovation, the panel provided the following suggestions:

- Integration of synthesis routes of molecules and types of biomass feedstocks using *ab initio* methods and machine learning should be pursued
- Expansion of modeling projects beyond optimization of existing equipment to new designs could help reach the full potential of this research and should be encouraged
- Development of improved data validation methodologies to ensure high fidelity of the mathematical models should be investigated.

The ADO program will implement the following actions:

- Pursue the idea of integrating synthesis routes of molecules with types of biomass feedstocks
- Consider the suggestion to expand the modeling projects to handle newer designs in addition to modeling the performance of existing equipment
- Emphasize improved validation techniques to ensure the accuracy of mathematical models.

The review panel observed that, given the similar nature of projects classified among the three groups mentioned previously, the projects are synergistic in nature and sharing lessons learned could be beneficial to current as well as future projects. In addition, the panel recommended that TEA metrics enabling critical assessment of synergistic values be considered. We will strongly encourage all our project participants to collaborate and share their learnings among themselves, as appropriate, and publish their results using proper channels for public dissemination.

The review panel commented that, in general, the ADO Analysis and Modeling portfolio of projects focuses on addressing problems and barriers of BETO's larger programmatic area and is well aligned with the MYP. The review panel cautioned the likelihood of some projects losing their internal focus because of the possibility of extending beyond their core competencies or being overambitious in their goals. We will provide the necessary guidance and assistance on an ongoing basis to ensure that the focus and objectives of these projects stay intact and are not lost. We appreciate the feedback of the review panel.

The review panel did not observe any substantial flaw with the technology development pipeline. They observed that the current portfolio strikes a balance between projects having an immediate impact on achieving the goals of BETO and those considering a longer-term viewpoint. The review panel suggested coordination with other program areas within BETO to garner greater benefits from systematic modeling and analysis approaches. In addition, the panel suggested the development of reduced-order models to increase the adoption of results obtained from modeling projects without requirements of increased computing resources to handle complex models. The ADO Technology Area, as needed, will coordinate with other programs in BETO to maximize the benefits resulting from modeling projects and analysis techniques. We agree that the development of reduced-order or simplistic models will be of great use to enable wider adoption, and this will be further evaluated with existing projects as well as identifying opportunities through additional funding mechanisms.

#### Recommendations

The review panel provided the following recommendations:

- The projects in the ADO Analysis and Modeling subprogram are essential and need to be continued and expanded
- Increase emphasis on improved validation procedures for the mathematical models
- Enhance participation and collaboration with industrial practitioners
- Revise the presentation template to better inform the value and status of each project
- Provide flexible TEA metrics for projects that are in early stages of development.

The ADO team will strive to increase industry participation through consortia activities such as the FCIC and impress upon the PIs the mathematical modeling projects to validate their models using relevant operating data to ensure high fidelity of these models. The ADO team will also coordinate with other programs in BETO to address the recommendation of revising the presentation template and development of flexible TEA metrics appropriate for early-stage projects.

#### Conclusions

We take this opportunity to thank all the members of the review panel for their thorough, insightful, and constructive review of the portfolio of projects presented in the ADO Analysis and Modeling session. The panel concluded that the primary strength can be attributed to a diverse portfolio of projects spanning from empirical studies to extremely fundamental ones using *ab initio* methods and including the development of validation tools. The review panel's overall positive comments, performance rating of various projects, and identification of areas for improvement demonstrate that the ADO Technology Area is well managed and achieving the goals of BETO.

## FEEDSTOCK TO FUNCTION: IMPROVING BIO-BASED PRODUCT AND FUEL DEVELOPMENT THROUGH ADAPTIVE TECHNO-ECONOMIC AND PERFORMANCE MODELING

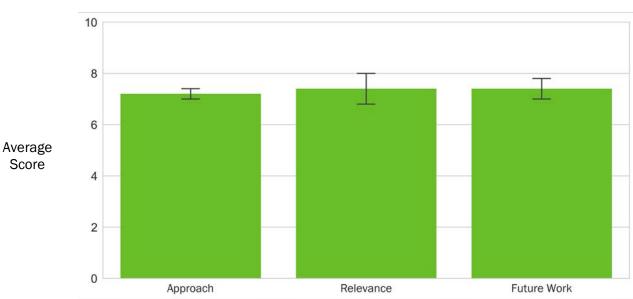
#### Lawrence Berkeley National Laboratory

#### **PROJECT DESCRIPTION**

This project aims to develop the foundation for an adaptive computational tool that predicts bioproduct and biofuel properties for validation and certification and determines the cost, benefits, and risks of promising new and uncertified pathways and their blending effects. Many high-potential biofuel and bioproduct pathways are developed by mimicking the carbon number and chemical structures of commercially available products. Experimental property testing of these pathways is usually conducted years after initial bench-scale experiments are complete because of high experimental costs or high volume requirements; however, neglecting to conduct property testing early in the pathway development cycle

| WBS:                      | 3.1.2.2             |
|---------------------------|---------------------|
| CID:                      | NL0034839           |
| Principal Investigator:   | Dr. Vi Rapp         |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$350,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$350,000           |
| Project Status:           | New                 |
|                           |                     |

can lead to investments spent on scaling up the production of bioproducts and biofuels that do not perform as expected.



#### Weighted Project Score: 7.3

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 ${f I}$  One standard deviation of reviewers' scores

The comprehensive Feedstock to Function tool developed in this project will incorporate supervised machine learning to predict desired properties of high-potential bio-based molecules early on in technology validation and certification processes. Capabilities of the tool will be demonstrated and validated by predicting high-value properties of alternative jet fuel pathways. Coupled with a lightweight TEA and life-cycle assessment (LCA) model, this tool will enable bioproduct and biofuel developers and researchers to streamline bioproduct and biofuel scale-up, overcome experimentally and kinetically derived property bottlenecks, identify cost and emissions bottlenecks, and potentially de-risk investments needed to scale up fuel production for the technology certification process. Further, the Feedstock to Function tool could be a surrogate for high-throughput experimental property testing to derive insights on desired properties for individual or blended biobased molecules and enable rapid evaluation.



Photo courtesy of Lawrence Berkeley National Laboratory

#### **OVERALL IMPRESSIONS**

- These sorts of online tools will offer industry tremendous opportunities to fine-tune efforts prior to much in the way of R&D expenditure.
- Focus on the development of the tool should really be on the ability to allow rapid "failure" of the potential project rather than only on the selection of molecules—the ability to eliminate options early on in the process will be critical to speeding up R&D efforts.
- I was initially skeptical about the project's final ability to provide a significant improvement in the long adoption cycle of new biofuel molecules, but the quality of the presentation and the arguments made by

the presenter changed my mind. This is a worthwhile exercise in using rapidly advancing machinelearning technology to extract otherwise hidden information from large data sets.

- Although identifying possible suitable classes of molecules for an intended application might not help the adoption cycle considerably, identifying which molecules or class of molecules might not work could save considerable time spent on unproductive research and allow the researchers to focus earlier on targets that are more likely to deliver the desired performance.
- This modeling exercise can establish the framework not only for a predictive tool but also for a design tool for a new class of molecules amenable to novel production pathways.
- In general, this tool can provide learning for developing more general tools for physical property prediction and evaluation based on machine learning, and therefore its value might transcend.
- The TEA/greenhouse gas (GHG) part is currently the weakest.
- LBNL is developing a flexible, open-source tool to predict physical and chemical properties of highpotential molecules (fuels, fuel coproducts, and other bioproducts) derived from biomass and evaluate the cost, benefits, and risk of promising bio-based molecules or biofuels to enable faster, less expensive bioprocess optimization, certification, and scale-up.
- This project is in a novel area that has the potential to add value of focusing technical efforts in the early phase of process development.
- Early selection of potential products will reduce the development cycle time and cost.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the feedback. As we make progress with the tool, we will be sure to incorporate your recommendation to focus on the tool's ability to assist with "rapid failure" and screening of molecules to eliminate options early in the R&D process.
- Thank you for your comment. We are glad you value our project and property prediction of molecules. Regarding the TEA/GHG prediction, significant progress has been made on the development of this portion of the tool. We have completed the analysis of five jet fuel routes and established methods for allowing users to vary key input parameters and generate updated results in real time. Because the success of any biofuel pathway depends on its ability to (1) be economically competitive and (2) qualify for Renewable Fuel Standard categories/low-carbon fuel standard credits, the addition of the TEA/GHG module allows industry decision makers to quickly screen both end molecules and production pathways for viability.
- As a previous reviewer stated, this tool will offer industry tremendous opportunities to fine-tune efforts early on in the R&D process as well as to assess costs associated with production, the potential GHG footprint of different production routes, and the sensitivity of these key metrics to varying input parameters (e.g., biomass pretreatment method, product yield, on-site energy demand).

## CODES AND STANDARDS IN INTEGRATED BIOREFINERIES

#### **Oak Ridge National Laboratory**

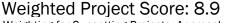
#### **PROJECT DESCRIPTION**

Reports of recent fires in corn stover handling and storage areas have highlighted the increasing challenges of fire hazards (real and perceived) for commercial-scale biomass handling facilities. At the commercial scale, the volumes of feedstock required for a biorefinery exceed that of any existing biomass handling facilities, particularly for herbaceous biomass. The challenges of mitigating fire risk in such large-scale biomass handling and storage areas have not been fully addressed. A goal of this project is to engage industry in proactively addressing fire risks while not overburdening industry development. In previous research in this project (2014–2016), we worked with industry stakeholders to conduct biomass commodity

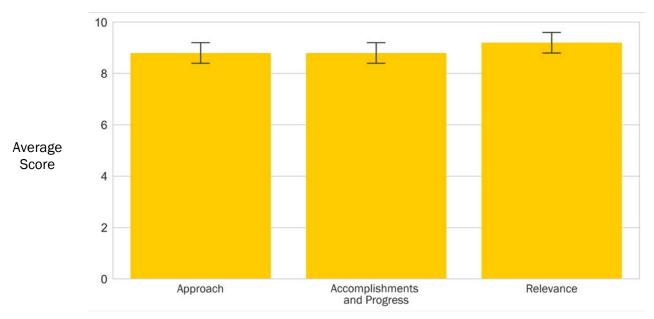
| WBS:                      | 3.1.3.2             |
|---------------------------|---------------------|
| CID:                      | NL0026705           |
| Principal Investigator:   | Dr. Erin Webb       |
| Period of<br>Performance: | 10/1/2014-9/30/2019 |
| Total DOE Funding:        | \$1,623,000         |
| DOE Funding FY16:         | \$780,000           |
| DOE Funding FY17:         | \$440,000           |
| DOE Funding FY18:         | \$195,000           |
| DOE Funding FY19:         | \$208,000           |
| Project Status:           | Sunsetting          |
|                           |                     |

classification tests at UL in Northbrook, Illinois, to determine how to classify corn stover and switchgrass bales in sprinkler design standards. We found that biomass bale fires tend to be more severe (faster growth, hotter) than expected and will require larger sprinklers than previously thought.

Industry stakeholders then asked us to investigate fire risk in biomass bale storage to identify storage strategies to reduce the probability and severity of these fires. Working with industry and rural firefighting stakeholders and engineers at UL, we developed corn stover bale stack fires to determine how fire grows and spreads within a stack of corn stover bales. Previous tests at UL were focused on fire in an individual bale, whereas these tests were designed to study fire spread through a stack of bales. We discovered that fire tends to grow and spread



Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

along the vertical channels between columns of bales. We demonstrated in a series of small-scale stover fire tests conducted by UL and Iowa State University that if these vertical channels can be blocked, the fire growth and spread is dramatically slowed, giving responders a better chance to contain the fire. A new staggered stack design was developed to eliminate top-to-bottom vertical channels. Although this new staggered stack could increase costs by reducing the stacking efficiency, we hypothesize that the benefits of reducing the fire risk in stover bale storage yards will exceed the increased stacking costs.

Another benefit of the experiments conducted in this project has been an increased awareness of how dangerous large bale stack fires are to responders. Instability of bale stacks during a fire and rapid fire growth pose significant risks to firefighters. After observing fire tests conducted in this project, Nevada, Iowa, fire officials modified their response procedures to create a collapse zone around stacks on fire to protect firefighters from falling bales. They have already implemented these new procedures and applied them in May 2018 during a large lumber stack fire that posed similar threats (stack instability and quick fire growth).

In FY 2018–FY 2019, our goal is to disseminate the knowledge gained in this project to key stakeholder groups. We will submit a journal manuscript documenting the results of the corn stover stack fire tests to advance discussion of bale stack fires within the research community. We will also prepare and submit an article on lessons learned in improving the safety of firefighters responding to bale stack fires so that approaches being implemented in Nevada, Iowa, can be adopted in other biomass-growing regions. Finally, we will apply an existing corn stover logistics simulation model to evaluate tradeoffs between reduced fire risk and increased costs of implementing a staggered stacking design.



Photo courtesy of Oak Ridge National Laboratory

#### OVERALL IMPRESSIONS

• This is an outstanding project that has immediately applicable, real-world impact.

- The information needs to be disseminated broadly and quickly.
- Most people in the industry think of biomass fires (1) in the abstract or (2) in terms of wet smoldering; this work has the added benefit of demonstrating how much of an issue biomass fires can be and at the same time provides easily understandable, usable solutions.
- This is an excellent project on fire prevention. Fires are not caused by poor moisture in herbaceous biomass stockpiles but by arson and lightning.
- This is a well-guided empirical analysis of a real risk with clear economic consequences that leads to relatively simple and practical solutions for outdoor fires.
- It would be interesting to know how this cost compares to the standard practice and include a detailed assessment of fire risks, which appears to be large but is mostly defined in qualitative terms.
- This project is aimed at reducing the fire risk in biomass storage by developing strategies to slow the spread of unavoidable fires.
- This is a good example of enabling research that will help drive conformity and improve operation within the bioeconomy.
- An investigation into and determination of appropriate biomass handling standards is unrealistic for individual ventures to take on.
- Wide publication of these results and recognition is very important.
- The dissemination/implementation of the information developed in this project will be pertinent to reliable, dependable biofuels production.
- It is unfortunate that the team was not able to partner with the arsonists of past fires for early data collection regarding flame propagation, which results in duplicating efforts.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The project team thanks the reviewers for their constructive and encouraging comments. We agree with the reviewers' suggestions that this information needs to be more broadly disseminated and that the costs of implementing fire risk mitigation approaches should be evaluated. We are working on that now in the latter half of FY 2019. We also agree with the reviewers that fire detection technologies should be implemented at biomass storage sites, and we will consider this approach in our cost simulations.
- A reviewer noted that reducing fire risk has impacts on safety that cannot be measured by cost alone. We could not agree more, and we are improving the safety of firefighters and surrounding communities, which is the most rewarding outcome of this project for us. We will take this advice and review other risk literature to develop additional metrics for our simulations of fire events in biomass supply chains.
- One reviewer asked how we can be confident that the new stacking approach will work at a large scale. The tests we conducted in this project were done with the largest stacks that we could safely set fire to. These stacks were designed to replicate a section of a commercial-scale stack, and we are confident that the tests were large enough for us to learn how fire moves through a stack of bales. We acknowledge that there will remain some uncertainty in how well this approach works at the industrial scale until a fire occurs in a larger stack using the new stacking design.

## INTEGRATED COMPUTATIONAL TOOLS TO OPTIMIZE AND DE-RISK FEEDSTOCK HANDLING AND HIGH-PRESSURE REACTOR FEEDINGS SYSTEMS: APPLICATION TO RED ROCK BIOFUELS' BIOREFINERY

#### National Renewable Energy Laboratory

#### **PROJECT DESCRIPTION**

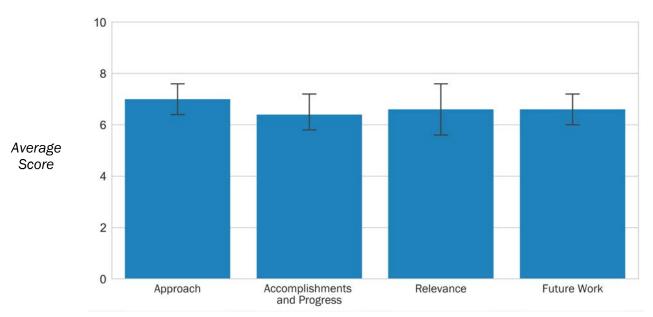
Biomass feedstocks exhibit inherent heterogeneity and vastly different materials properties from common granular feedstocks, for which many solids handling unit operations were designed. These features have proven a significant impediment to the implementation of robust, continual biomass feeding systems for second-generation biorefineries. To address these challenges, we are developing integrated, experimentally validated

| WBS:                      | 3.3.1.2              |
|---------------------------|----------------------|
| CID:                      | EE0008253            |
| Principal Investigator:   | Dr. Jonathan Stickel |
| Period of<br>Performance: | 3/1/2018-2/28/2021   |
| Total DOE Funding:        | \$1,799,999          |
| Project Status:           | Ongoing              |

simulations for several common feed handling and reactor feeding systems. We are building on previous investments of DOE that developed state-of-the-art modeling and simulation tools under the Consortium for Computational Physics and Chemistry, the FCIC, and other BETO-funded projects. We are leveraging and extending these tools to model the solids handling processes that constitute the front end of the Red Rock Biofuels (RRB) gasification and Fischer-Tropsch conversion process. This key partnership will facilitate experimental validation of the simulations as well as provide immediate impact whereby the resultant models will be used to optimize and de-risk commercial-scale deployment of the RRB process. Specifically, we are developing simulations for the feed hoppers, compression screw feeder, and conveyor pyrolyzer units employed in the RRB process. We will inform the parameterization of these models for feedstock-specific

#### Weighted Project Score: 6.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

scenarios by multimodal characterization of the structure, physical properties, and flow behavior of various feedstocks. Once validated, this simulation toolkit will be generalized to aid in optimizing and de-risking other biomass conversion processes that use these common solids handling reactor feeding units. In addition, we will provide correlations that can be used to adjust optimal operating conditions based on feedstock parameters. We have a uniquely qualified team (a national laboratory, a university, and three corporations) to undertake the computational tasks and corresponding validation experiments. Completion of the project will constitute substantial progress toward understanding and overcoming the barriers associated with handling and feeding biomass, which will facilitate and de-risk the commercial-scale deployment of second-generation biorefineries.

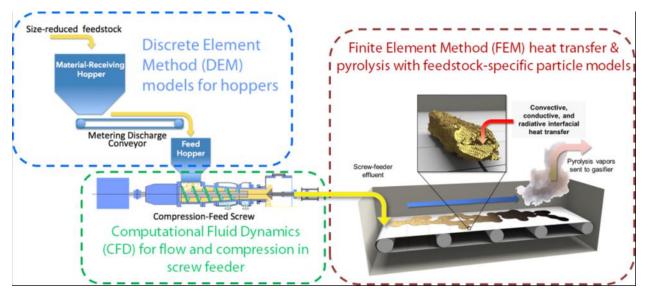


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- A fundamental question in this project is that it is trying to both address an industrial optimization problem while addressing the novel use of complex computational techniques across three different unit operations.
- As a scientific endeavor, this is quite challenging, and although the potential exists to optimize the reactor feed line and performance, the project is overambitious.
- Validation of the model with experimental data is not clear, and real assessment of economic value is missing at this point.
- There are nuggets of interest (e.g., the screw feeder), but the overall project is disjointed and lacking the ability to make a strong case for itself.
- In addition, the quality of the gasification modeling is somewhat limited.
- We would like to see direct involvement of equipment manufacturers.
- This project, led by NREL involving a multi-institutional team, is aimed at developing physics-based models for feed handling and feeding biomass solids to the RRB gasifier.
- This is an ambitious project with multiple challenges in modeling the physics and most importantly validating the model to be used for design/optimization of the RRB plant.

- This project is good enabling research to support general bioeconomy commercialization.
- The heavy reliance on one specific project and computational models could limit the broad applicability of the results.
- This project might reduce the time required to resolve problems of biomass feed handling and transport.
- This project addresses a real need to help de-risk feedstock handling challenges.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that our project is challenging and ambitious, but we feel that the role of national laboratory projects is to address challenges of this magnitude. Although we will do our best to achieve the goals we proposed, there is always risk associated with scientific research. We expect to provide significant new methods and insights for feedstock feeding, even if we are not completely successful at using our models to optimize RRB's process. Experimental validation of the computational models is a key part of our work plan, and we apologize if that was not clear in the presentation. The equipment manufacturers Jenike & Johanson and Valmet are team members on this project. In addition, RRB has facilitated discussions between the team and TCG, the gasification-reactor vendor for RRB. Economic assessments performed by RRB have identified that reducing downtime associated with failures in the feeding system is critical to achieving economic targets; thus, success in this project will provide substantial economic benefit.
- Because of the constraints of the FOA, we need to focus our scope to the unit operations of one vendor and use one set of computational tools. This approach, by its nature, cannot be comprehensive; however, this project will connect nicely with other computational projects being funded by BETO.

# INTEGRATED PROCESS OPTIMIZATION FOR BIOCHEMICAL CONVERSION

#### **Clemson University**

#### **PROJECT DESCRIPTION**

The main objective of this research project is to develop analytical tools to enable a biorefinery to identify an optimal integrated process design that ensures a reliable, cost-effective, sustainable, robust, and continuous feeding of biomass feedstocks to achieve the design throughput of the reactor.

| WBS:                      | 3.5.3.2             |
|---------------------------|---------------------|
| CID:                      | EE0008255           |
| Principal Investigator:   | Dr. Sandra Eksioglu |
| Period of<br>Performance: | 4/1/2018-3/31/2021  |
| Total DOE Funding:        | \$1,149,999         |
| Project Status:           | Ongoing             |
|                           |                     |

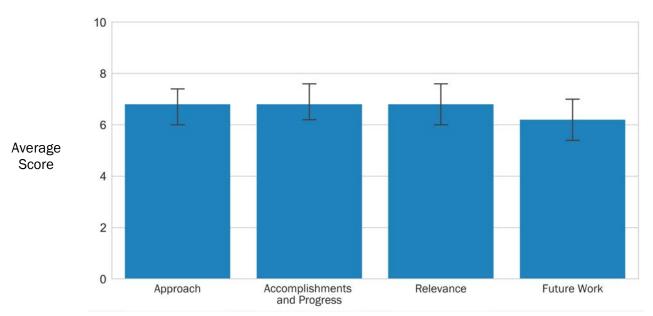
This project will develop and integrate several analytical models that are expected to improve the performance of

the proposed feeding system design (from biomass grinding to the pretreatment reactor throat design). The proposed feeding system design incorporates additional processes than current practices followed by the industry. These processes (fractional milling, high-moisture pelletization and cooling) positively impact the uniformity of the feedstock and improve the reactor's time onstream.

The analytical models proposed include DEM and mathematical optimization models. DEM models will provide functional relationships between biomass characteristics (such as particle size, shape, distribution, moisture) and biomass flowability and the failure mode of equipment. Modeling efforts also include the development of functional relationships that capture the effect of temperature and pressure on feedstock handling. We will incorporate these functions into mathematical models to optimize the performance of the

#### Weighted Project Score: 6.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

proposed process. The optimization models will identify (1) optimal process parameters to ensure uniform particle sizes and uniform material flow with reduced fine particles; (2) optimal queue location and size to optimize costs, equipment use, and throughput; and (3) blendstocks that optimize costs and the reactor's performance in the face of biomass quality variations. Analytical results from the models will be validated at a process demonstration unit at one dry ton/hour for two weeks. This technology will be tested on corn stover, switchgrass, and miscanthus.

The analytical models will be integrated into an alpha version of a cloud-based decision-support system that will be available on the web free of charge. This decision-support system will serve as a training tool for bioenergy stakeholders (industry practitioners, government, academia, etc.).

This research is expected to deliver an optimized feeding system design. This system considers processes starting with biomass grinding, then the pretreatment and the reactor's throat. The system will deliver a consistent feedstock that meets biochemical conversion specifications as designed by NREL at one dry ton/hour for two weeks. We expect that the optimized system will maintain the reliability of the reactor to 90% for biomass with 10%–30% moisture levels and 5%–15% ash content. The optimized design will potentially result in tighter particle size distributions, reduced fines, reduced grinding energy consumption, improved flowability, etc.

Another outcome of this research is a decision-support system that will enable decision makers to undertake sound actions and impact stakeholders in the short, medium, and long terms.

## **Discrete Element Modeling of Switchgrass**

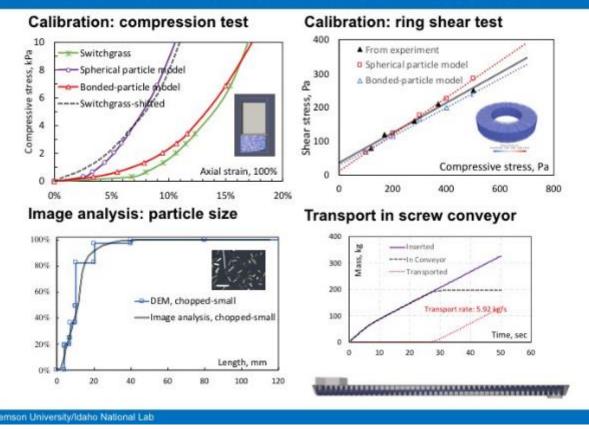


Photo courtesy of Clemson University

#### OVERALL IMPRESSIONS

- This project addresses a significant problem. The approach is intriguing—nested or hierarchical models—and promising; however, it has not yet sufficiently proven to be able to provide quantitatively correct results.
- The impact of some key process variables (e.g., moisture) is not yet explained explicitly, but the potential ability of using glued spheres to model the geometric complexity and size variability of biomass is extremely interesting.
- This is a complex tool, and it is not likely to be used on a routine basis for plant-level studies; however, it could become an excellent tool in the hands of designers of new handling equipment. Requirements from that audience should be included.
- The next phase of the project is critical to proving whether a practical toolkit for industry practitioners can be developed.
- The commercialization strategy is unclear. Equipment manufacturers appear as a prime audience but are missing from participation.
- This project aims at developing a DEM to optimize feeding to a biomass conversion reactor.
- The majority of the project work focuses on heavy-duty computer modeling with two-week testing at Idaho National Laboratory (INL) to get experimental data for model validation.
- This is a good example of basic research to support industry commercialization.
- The focus on the critical nature of assumptions and requirements for confirmation was clear.
- This is an intensive modeling approach to develop an optimized feedstock handling and supply system model with significant uncertainty regarding a pathway to market.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Although quantitatively correct results are challenging for any model, our DEM model efforts aim to provide quantitative relationships between biomass characteristics and equipment performance for planned processing equipment. The model has been calibrated for switchgrass and shown quantitative agreement with experimental data of compression and ring shear tests. Additional calibrations of other biomass materials are planned. The DEM models also need to be validated to provide quantitative accurate results of biomass handling and flow in different processing units. Such an effort is underway.
- Key process variables (e.g., moisture) are being considered in the DEM model through a new cohesion model. This will allow the modeling of moisture and fine content effect.
- The optimization team and the DEM modeling team are working closely together for the next phase to develop a framework for system-level optimization. The final product is intended to be more practical.
- Although we hope the models and the resulting tools will have broader applicability and commercial values, the current focus is still on model and capability development.

# ANALYTICAL MODELING OF BIOMASS TRANSPORT AND FEEDING SYSTEMS

# Purdue University

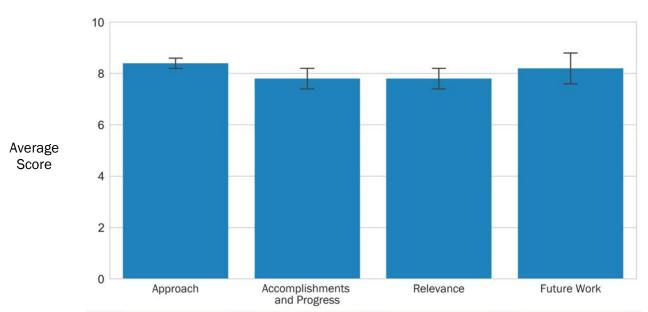
# **PROJECT DESCRIPTION**

Major improvements in lignocellulose pretreatments and enzyme, microbial, and thermochemical catalysts, together with demonstrations of these technologies in reactor volumes ranging from 1–20 m<sup>3</sup> or larger, have proven to be key concepts in cellulose conversion. The BETO programs carried out in cooperation with industry have demonstrated pathways and process designs that decrease enzyme loadings; broaden substrate range; and enhance

| WBS:                      | 3.5.3.4             |
|---------------------------|---------------------|
| CID:                      | EE0008256           |
| Principal Investigator:   | Dr. Michael Ladisch |
| Period of<br>Performance: | 3/1/2018-2/28/2021  |
| Total DOE Funding:        | \$1,190,000         |
| Project Status:           | Ongoing             |
|                           |                     |

titer, rate, and yield using industrial microorganisms; however, the movement of lignocellulosic biomass solids between and within unit operations of a biorefinery remains a challenge because of the difficult materialhandling characteristics of solid forms of biomass materials and aqueous slurries formed from these materials during pretreatment, hydrolysis, and fermentation.

Our team consists of Purdue University, INL, Argonne National Laboratory (ANL), Forest Concepts, and AdvanceBio. We are addressing the analytical modeling of corn stover in the forms encountered in a biorefinery: loose material, pellets, and slurries at high-solids loadings. Our goal is to develop strong and innovative computational and empirical models that rigorously represent the flow performance of biomass materials and enable a deep understanding of how particle and equipment characteristics impact biomass flow.



## Weighted Project Score: 8.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

Ultimately, these models will be used to predict operational envelopes for stable feeding of biomass into a biorefinery reactor.

Dry solids feeding is being modeled using two computational techniques: DEM and FEM. These models will account for the effects of moisture, temperature, and pressure on feedstock handling and use measurements at conditions encountered when these materials are processed at temperatures between ambient and 200°C, pressures up to 20 bar, moistures ranging from 15%–85%, and solids loadings of 150 to more than 300 g/L as defined by conditions in the biorefinery. LCA and TEA, carried out in cooperation with ANL, will provide metrics for how process changes impact GHG reduction and costs.

The resulting models, together with experimental verification in INL's Process Development Unit, will be applied to predict optimal control points and to simulate process variability for continuous feeding into a biorefinery reactor. Key to model development is the measurement of properties at conditions that are encountered in the plant. These measurements are being carried out at Purdue University and in the INL laboratory as well as pilot equipment including pressure vessels. Specialized rheometry systems for measuring flow properties, imaging methods, and NREL's laboratory analytical procedures for particle characterization are providing measured parameters necessary for the modeling research. The near-term impact of this work will come from validated models that predict flow behavior during feeding, define critical operating ranges, and provide a quantitative basis for new equipment designs that will help to alleviate the operational reliability issues experienced by the DOE-supported pioneer biorefineries.

- This is an excellent project with specific and measurable results that will have impact on industry.
- The inclusion of stover slurry rheology characterization (and potential modeling?) is outstanding and needs to be shared widely with industry because this is an area that causes problems with scaling processes across industry.
- Overall, this project outlines a clear use of a powerful analytical tool to provide a predictive framework to increase the reliability and amount of biomass throughput in a biorefinery. The oral presentation managed to eliminate some doubt about the wisdom of considering pelletized biomass.
- The conveyor analysis is the most interesting part because it is of general interest and useful to processors that might use other devices (e.g., stirred tanks), which might be used for liquefaction as an alternative to the proposed screw reactor. The use of a screw reactor for liquefaction is intriguing— mainly because it might work at much higher dissolved solids percentages than conventional methods. It is likely—although not a given—that the tradeoff is more mechanical complexity and increased operating and capital cost.
- I would like to see as future work some level of comparison with other approaches to liquefaction. This could be at a relatively high level but should be enough to provide a practitioner confidence in further pursuing the proposed liquefaction approach.
- Explicit involvement of equipment manufacturers would be desirable to increase awareness and use of these models.
- This project addresses the development of engineering solutions to alleviate biomass feeding problems in reliable biorefinery operation.
- This project has an excellent balance of computational modeling and experimental testing with a very strong project team.
- This project has the potential to produce good background research and is well managed.

- Limiting the project to corn stover and an unusual process configuration somewhat constrains the ultimate applicability of the results.
- This program appears to be more about the development of a model for the sake of model development than the actual development of a robust feedstock supply system.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for these comments. We plan to share results with industry through presentations and papers.
- Two approaches are under consideration for the liquefaction: (1) liquefaction with maleic acid in the screw reactor and (2) batch liquefaction with enzymes. Both are being modeled. Additionally, the equipment manufacturer is a partner on the project, and it is worth noting that the INL system was reverse engineered from larger equipment for ease of scale-up of results.
- Modeling is directed to corn stover because this is the primary herbaceous feedstock used by the pioneer biorefineries. Regarding process configuration, both batch (enzymatic) and continuous (screw reactor with maleic acid) are considered. We expect that the modeling approach can be used for other materials, but that would need to be verified in a future project.
- The focus of this project is on developing a modeling approach that will give guidance on how to feed corn stover more robustly. The models are expected to predict which material properties and operating conditions will result in acceptable screw torques and material bulk densities.

# IMPROVED BIOMASS FEEDSTOCK MATERIALS HANDLING AND FEEDING ENGINEERING DATA SETS, DESIGN METHODS, AND MODELING/SIMULATION TOOLS

# **Forest Concepts, LLC**

# **PROJECT DESCRIPTION**

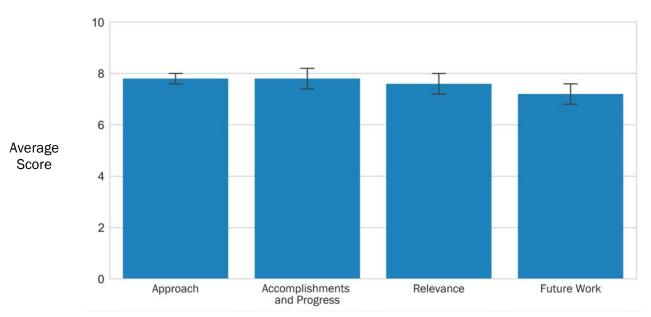
The overarching objective of this project is to contribute to the design and operation of reliable, cost-effective, continuous feeding of biomass feedstocks into a reactor of an integrated biorefinery. The overarching goal comprises two sub-goals: (1) develop and validate a comprehensive computational model to predict mechanical and rheological behavior of biomass flow to enable the systematic and reliable design of a biomass handling/conveying system;

| WBS:                      | 3.5.3.7            |
|---------------------------|--------------------|
| CID:                      | EE0008254          |
| Principal Investigator:   | Dr. James Dooley   |
| Period of<br>Performance: | 6/1/2018-1/31/2021 |
| Total DOE Funding:        | \$1,479,033        |
| Project Status:           | Ongoing            |
|                           |                    |

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, as well as external mechanical properties, including temperature and pressure. The project team includes Forest Concepts, Pennsylvania State University, and Amaron Energy. 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. Amaron Energy provides a case study site for validation of project outcomes. New equipment to be developed includes a 250-mm cubical triaxial tester (CTT) to provide biomass mechanical property data, a 300-mm wall friction tester to quantify the

# Weighted Project Score: 7.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

interaction of biomass with materials of construction, a large gas pycnometer to quantify biomass particle density, and other laboratory devices to ensure simulations are populated with biomass-specific data. Biomass materials used in the project include milled wood chips and corn stover.

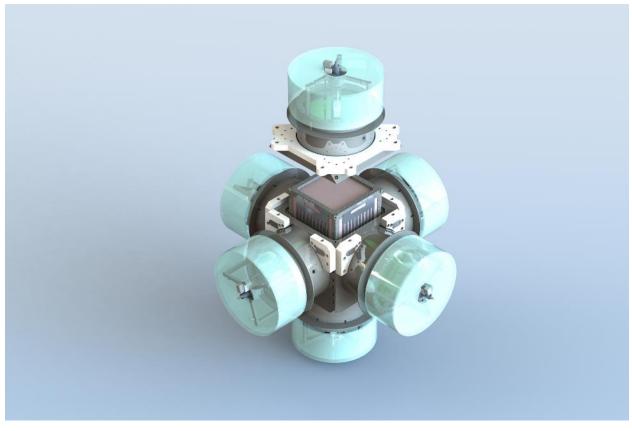


Photo courtesy of Forest Concepts, LLC

- This project has significant potential for physical property measurement of large particle biomass. A focus on the correlation of results from the developed technology to results from the "original," smaller technology should be of primary importance because this will be critical to the application of the measurements in an area where the smaller technology has been dominant in the past.
- This work is commendable because it is driven by a vendor that has correctly identified the need to improve the ability of measuring bulk flow properties of biomass material and proposed the development of an enhanced laboratory device (CTT) to carry out such measurements.
- The results are validated using a flow model of a hopper. This is a very valuable effort that might have impact beyond the scope of this project because it can help define a general approach to experimentally measure the flowability of bulk biomass.
- The project would benefit from a better explanation of the scientific basis and a more descriptive treatment of how measurements from the CTT inform flow simulations.
- I strongly recommend participation of vendors and equipment manufacturers in the modeling exercise.

- This project is aimed at developing a measurement technique to better understand biomass particle flow in biomass feed systems.
- The development of a CTT is planned to alleviate the limitations of the current system developed by Penn State.
- This is a well-focused project with a good mix of hands-on industry experience and well-qualified academic staff with a thoughtful approach to addressing biomass handling issues.
- This project appears well defined and managed.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Statistically valid experiments with matched sets of biomass material will be used to correlate the output of the new large CTT with existing systems at Penn State University, which is planned for early in Budget Period 2.

# EVALUATION OF BIO-OILS FOR USE IN MARINE ENGINES

# **Oak Ridge National Laboratory**

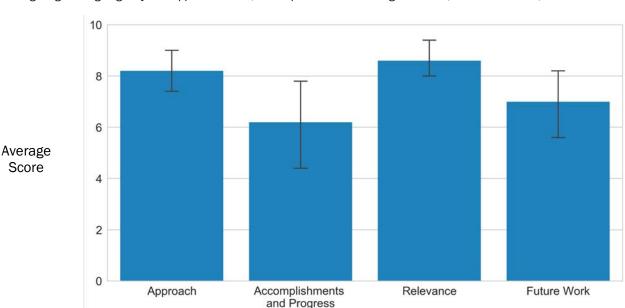
### PROJECT DESCRIPTION

This project is in the second year of a multiyear effort to determine the feasibility and impact of biofuels (especially bio-intermediates) as viable fuel candidates for marine engines. The engines used to power cargo vessels, cruise liners, and many service vessels are fueled with a residuum heavy fuel oil (HFO). This low-quality fuel is highly viscous and contains high levels of sulfur (~3.5 vol %) and appreciable levels of water and sludge. Before it can be burned in the engine, the HFO must be heated to reduce the viscosity to enable proper flow characteristics. This fuel must also be processed onboard to remove the entrained water and sludge. When burned, HFO produces high levels of sulfur and particulate emissions. In fact, the

| WBS:                      | 3.5.5.1             |
|---------------------------|---------------------|
| CID:                      | NL0033568           |
| Principal Investigator:   | Dr. Michael Kass    |
| Period of<br>Performance: | 10/1/2017-9/30/2020 |
| Total DOE Funding:        | \$200,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$200,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Ongoing             |
|                           |                     |

sulfur emissions from one ship are equivalent to those produced from 50 million cars in one year. The level of HFO used in one year by marine ships is roughly equivalent to the sum of diesel used on highways in the United States.

The International Maritime Organization has set aggressive emission targets to reduce fuel sulfur content from 3.5% to 0.5% in 2020. Likewise, in the United States, the California Air Resources Board and other state agencies have regulations limiting the sulfur content of fuel used in coastal regions to 0.5%. This requirement will force ship operators to either operate on more expensive fuels, such as low-sulfur HFO, liquified natural



# Weighted Project Score: 7.9

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

gas, or distillate fuels; or, they can incorporate expensive emissions-control systems. Low-cost biofuels, especially bio-intermediates, are potential low-sulfur alternative fuels. The bound oxygen is also a known pathway to particulate matter reduction, and their inherently low viscosity means that less energy is required to achieve proper flow characteristics, thereby improving overall efficiency. This effort addresses several key technical barriers associated with and expanding a renewable resource to improve energy independence.

The general research plan is to (1) determine the feasibility of bio-intermediates as blends with HFO and (2) assess the impact of bio-intermediates on ship fuel systems and engine performance. Initial empirical studies have focused on obtaining rheological (flow) properties of HFO and its blends with bio-intermediates. A fast-pyrolysis bio-oil derived from softwood was obtained and blended with HFO to assess and confirm miscibility. These blends remained miscible even when heated. Viscosity measurements were also performed on bio-intermediate HFO blends. A key (and unexpected) finding was that the addition of 5% bio-oil dramatically reduced the viscosity of HFO at ambient temperature. Polymerization of bio-oil HFO blends was not observed. These results are highly encouraging. The research team also begun compiling literature on relevant bio-oil combustion in engines, and a determination of the combustion characteristics of bio-oil HFO blends will begin in the current quarterly period. Future work is planned to determine the compatibility of bio-intermediates with fuel handling systems and to conduct engine-based experimentation to determine combustion characteristics and the emissions profile.



Photo courtesy of Oak Ridge National Laboratory

- This is an outstanding concept and approach with a clear identification of a critical need (low-sulfur fuels, no progress toward supply), and shortcuts are needed to further process bio-oils and can lead to the rapid commercialization of specific technologies once desired properties are identified.
- There is high potential for global impact if major risks can be assessed and addressed.
- This could finally be a practical application of bio-oils that is not hampered by exceedingly high upgrading costs.

- A clearer definition of the suitable bio-oil—a description that has been used for a vast variety of somewhat different liquids obtained from biomass—would be very useful. That, in turn, could help with more focus on the TEA, which is missing.
- This is a high-impact project of great interest and excellent effort.
- This project is aimed at determining the technical feasibility of using bio-oils (raw or slightly processed/stabilized) in marine engines.
- Marine engines currently use HFO, and bio-oil could be a great replacement considering upcoming sulfur regulations.
- This project is targeted at finding potential ways to blend bio-based oils into marine fuel, which is a major source of worldwide pollution.
- The work is generating key data to perform an empirical screen.
- This is a logical extension of the use of bio-oils and biocrude, which appear to be underused at present.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for supporting feedback. This effort has been focused on the technical feasibility aspect of bio-intermediates as a marine fuel. As we progress, we will continue to evaluate issues related to supply, including infrastructure needs and scale-up.
- Determination of a suitable bio-oil will be important. It is our thought that the marine application will be suitable for a broad range of bio-oils. Our initial studies have focused on softwood-derived bio-oils, and we plan on assessing their compatibility as a function of properties, such as water content, oxygenates, total acid number (TAN), and other variables. Our plan is to define the boundaries associated with water and chemistry that are suitable. A result would be a determination of suitable bio-oil properties.
- Yes, this is an accurate assessment of the project goals.
- Yes, the research team's immediate focus is on assessing the impact and compatibility of bio-oil with HFO. Early studies have emphasized miscibility and viscosity, and we are extending these to include compatibility (i.e., corrosivity) and lubricity.
- Yes, our study appears to be the first to look at blends of bio-intermediates with HFO for engine use. In our literature search, we were only able to find a study that looked at blends for burner applications. Unfortunately, that source did not evaluate the properties we are interested in.

# ANALYSIS FOR JET HIGH-PERFORMANCE FUELS

# **Sandia National Laboratories**

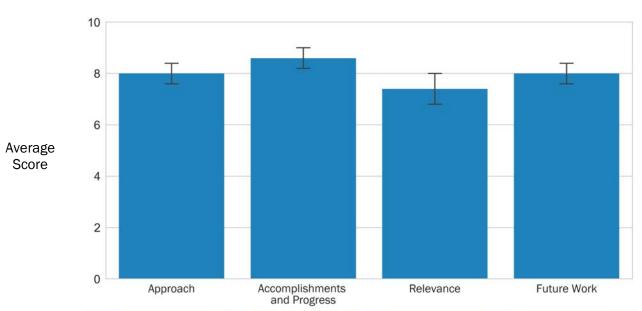
### **PROJECT DESCRIPTION**

Successful large-scale deployment of "drop-in" alternative jet fuels has been limited by their high cost of production compared to conventional fuel. Conventional jet fuels are limited by the crude oils from which they are made, the refinery technologies that can be applied, and the critical requirement to make consistent, on-spec fuels from hundreds of different feedstocks in hundreds of different refineries around the globe. These restrictions severely limit the opportunity to produce higher-performance jet fuels without massive investments in new refining equipment, and perhaps not even then.

| WBS:                      | 4.1.1.70            |
|---------------------------|---------------------|
| CID:                      | NL0033867           |
| Principal Investigator:   | Dr. Anthe George    |
| Period of<br>Performance: | 1/31/2018-9/30/2018 |
| Total DOE Funding:        | \$100,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$100,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Ongoing             |
|                           |                     |

Biomass resources and conversion technologies offer an

opportunity to make types of components not accessible through petroleum refining and for the investment in making them to result in added production capacity, something that not even a costly retrofit of existing refineries could match. Simultaneously, if these new components can be designed to confer performance advantages, there is evidence that the benefits could offset at least some of the current cost differential. Through a recent workshop on jet engine fuel optimization, jet engine manufacturers defined the benefits they most desire: better operability, more efficient fuel combustion, and increased range payload. Therefore, we have the guidance needed to develop cost-competitive, sustainable, high-performance fuels (HPFs).



## Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

We began by benchmarking conventional jet fuels and relating key performance attributes to the properties of their various components on a molecular level. Based on this knowledge, we then proposed bio-based alternatives with the potential to optimize the combination of benefits sought by engine manufacturers and aircraft operators; this was based on published properties, structure-property correlations, and *ab initio* methods.

This presentation provides preliminary findings of the multiteam efforts on the identification of molecules, determination of their energy content, development of the Jet fUels blenD Optimizer tool (JudO) tool to determine "drop-in" blending, and how to achieve required energy content through Pareto front analysis of fuel composition. We also present preliminary results on the performance benefits of notional high-performance jet fuels.

Next steps in this work include:

- Improvements to the JudO tool by adding fuel attributes to meet drop-in ASTM requirements
- Molecule structure-property relationships on further key jet-fuel properties and associated structureproperty trends
- Production of data on the laboratory-scale feasibility of HPFs, focusing on alkyl cycloalkanes and refined analysis of their value propositions.

This work will provide guidance on where R&D efforts in this space should be directed.

- This project has the potential to assist industry with the identification of highest-value molecules for future work and could help shortcut failures and reduce the waste of resources. It does speculate with novel and previously unresearched molecules, but that should be the point of tools like this. I look forward to seeing the final product.
- The concept of designing a high-performance fuel *ab initio* based on desired characteristics to deliver specific benefits to a user is powerful, and the PIs make a compelling case in the project.
- The critical limitation at this time is that a clear dollars-per-gallon production cost target that makes the fuel economically viable has not been included. It is a relatively minor weakness at the early stage of this project, but it will become increasingly more relevant as the project advances.
- The approach is appropriate and applies to molecules regardless of their origin—fossil or bio—and it is intriguing that potentially superior performance might be obtained by bio-derived molecules. The different reduction state of the bio-derived molecule makes this consideration regarding the process pathway even more critical as the project evolves and will determine its increased or diminished relevance for the BETO mission.
- Nonetheless, these caveats on the economics should not prevent the team from seeing where the real value of these tools lie: the team provides a target, and it is up to other R&D efforts to see if such a target is realistic and reachable, both technically and economically. By providing a target that can fulfill required performance criteria, these tools, though they do not guarantee success, do ensure that R&D efforts are focused on molecules and the class of molecules that can indeed perform as required.
- This study was designed to understand the impact of various high-energy-density molecules on the performance of the jet fuel.

- The work followed a strategic and scientifically based approach to determine which bio-based compounds would have the best chance of positively contributing to jet fuel blends.
- The presenter did a good job of methodically explaining the process in an understandable manner.
- The current availability or whether the compound could be produced was not addressed, but it would add value.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We are sincerely grateful to the reviewers for their insight and their efforts in reviewing our program. We acknowledge the notes regarding the strengths of this aspect of the Co-Optima effort, and we limit our comments to the weaknesses sections of the review. In general, we note the comment that this is a small piece of work and that it would benefit from an expanded scope. Many of the comments pertain to work that was beyond the scope of this effort, which would nevertheless be valuable to accomplish.

# GARDN COLLABORATION U.S.-CANADA AVIATION FUELS

# **Pacific Northwest National Laboratory**

### **PROJECT DESCRIPTION**

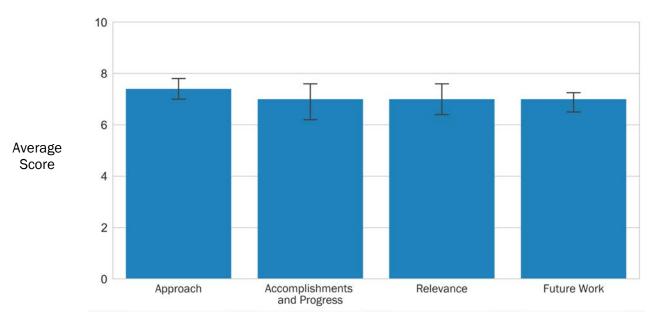
GARDN is a nonprofit organization funded by the Business-Led Networks of Centres of Excellence program of the Government of Canada and the Canadian aerospace industry. GARDN funds collaborative projects that can reduce the environmental footprint of the next generation of aircraft, engines, and avionics systems, and it helps members from academia and industry bring their innovative ideas to life. The Assessment of Likely Technology Maturation (ATM) pathways used to produce biojet from forest residues consortium, within GARDN, is tracking the performance and life-cycle impacts of forest residues to jet fuels via fast pyrolysis, catalytic fast pyrolysis (CFP), and hydrothermal liquefaction (HTL),

| WBS:                      | 6.4.0.9             |
|---------------------------|---------------------|
| CID:                      | NL0033748           |
| Principal Investigator:   | Ms. Corinne Drennan |
| Period of<br>Performance: | 1/1/2018-9/30/2019  |
| Total DOE Funding:        | \$200,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$200,000           |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Ongoing             |
|                           |                     |

involving partners from stakeholders of biojet fuels. PNNL was invited to participate in the ATM consortium for expertise in each conversion pathway as well as in hydrotreating, jet fuel preparation (e.g., fractionation, meeting specifications), and capturing life-cycle inventories associated with conversion processes. The consortium, led by NORAM and the University of British Columbia, includes the Canadian government CanmetENERGY laboratories, PNNL, (S&T)<sup>2</sup> Consultants Inc., and SkyNRG, with support from the Boeing Company, Bombardier Inc., Air Canada, and WestJet Airlines Ltd.

#### Weighted Project Score: 7.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

BETO, already coordinating on sustainable aviation fuels with Canada and Mexico, supported the majority of PNNL's participation in the ATM. In FY 2018, PNNL completed hydrotreating of the bio-oils biocrude from each liquefaction process (fast pyrolysis, CFP, and HTL), provided conversion performance data and biojet fuel products for fuel analysis, and provided general technical support in examining the three supply chains. A comprehensive report for the ATM's research is expected to be published in 2019. Through the collaboration, the ATM has demonstrated the feasibility of hydrotreating technology for upgrading bio-oils biocrudes from current thermochemical conversion technologies and established a model international collaboration network for building methodology and analysis of the complete supply value chain for biojet fuels from a single representative forest residue feedstock through conversion, upgrading, and fractionation. This international collaboration provides important experience and information to stakeholders of biojet fuels and will accelerate the acceptance of biojet fuel from biomass thermal chemical conversion processes.

#### OVERALL IMPRESSIONS

- This appears to have been a very short project that almost seems to have been designed to highlight the unsuitability of these feedstocks for aviation fuels; it might have been a result of the schedule or of the materials provided, but the overall gist seems to be that it is validating a negative result (i.e., do not consider this use). Hopefully the final report will be clearer and offer a broader explanation of the commercial applicability of the feedstocks.
- In general, this project has several points of merit. One is that it appears to demonstrate that the production of jet fuel from woody biomass is not a particularly attractive proposition. From a technical perspective, the comparison among different types of bio-oils is valuable because it highlights critical differences that are relevant when considering these materials regardless of the final application.
- A more detailed TEA would have been desirable, and the amount of hydrogen (H<sub>2</sub>) upgrade necessary hints to a considerable hit on the GHG profile unless only renewable H<sub>2</sub> is used. A more detailed discussion on the GHG profile would have been needed.
- The conclusion on whether further investigation is warranted—and under which conditions—is not clear.
- This project, funded under GARDN, asked PNNL to participate in the ATM pathways to produce biojet fuel from forest residues.
- PNNL evaluated various hydrotreating options for pyrolysis oil to produce biojet fuel. PNNL found that the pyrolysis oil was not the best feedstock.
- This background research project focused on pathways from biomass to biojet fuel, accessing the overall sustainability.
- This project is of nominal overall value to industry.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Thank you for the considerations and comments. We agree that disseminating information about the differences between different bio-oils is important. A detailed TEA and LCA will be published this year. It is important to frame the results of this work in the context of woody biomass conversion via fast pyrolysis, CFP, and HTL. The results presented do not hold for the feedstock or conversion technology alone. For example, high-quality jet fuel is obtainable from woody biomass but by using a different conversion approach. Liquefaction technologies have the potential to produce quality jet fuel using different feedstocks or by blending different feedstocks with woody biomass.

# ADVANCED DEVELOPMENT AND OPTIMIZATION: INTEGRATION AND SCALE-UP

anna



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# INTRODUCTION

The Advanced Development and Optimization (ADO): Integration and Scale-Up Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place on March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 26 projects were reviewed in the ADO: Integration and Scale-Up session by six external experts.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately \$322,323,910 (fiscal year [FY] 2016–FY 2019 obligations), which represents approximately 37.5% of the BETO portfolio reviewed during the 2019 Project Peer Review. During the Project Peer Review meeting, the principal investigator (PI) 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 approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the Project Peer Review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the ADO: Integration and Scale-Up Technology Area full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Ms. Liz Moore as the ADO: Integration and Scale-Up Technology Area review lead, with contractor support from Mr. Remy Biron (Allegheny Science & Technology). In this capacity, Ms. Moore was responsible for all aspects of review planning and implementation. Mr. Joshua Messner also assisted with technical and logistic aspects of the review.

# ADO: INTEGRATION AND SCALE-UP OVERVIEW

The ADO Technology Area conducts integrated systems research up to and including the engineering scale. ADO addresses components and systems scalability capable of handling industrially relevant and economically advantaged feedstocks to produce renewable fuels and bioproducts. Engineering-scale verification also provides biofuels and bio-oil intermediates for testing and certification to ensure that those products can seamlessly integrate with existing distribution infrastructure. It also enables petroleum refineries to evaluate the effect of coprocessing biobased intermediates and reduces technical uncertainties for how biobased intermediates can be integrated into existing operations.

The ADO: Integration and Scale-Up session reviewed projects that focused on first-of-a-kind or early investigations into integrated systems and use of industrially relevant materials. ADO recognizes the critical need to transition from a controlled bench environment to the variability likely to be encountered as technologies progress toward the commercial scale. At these scales, in addition to the process optimization and intensification that can occur, quantities of materials needed for product testing and acceptance can be produced.

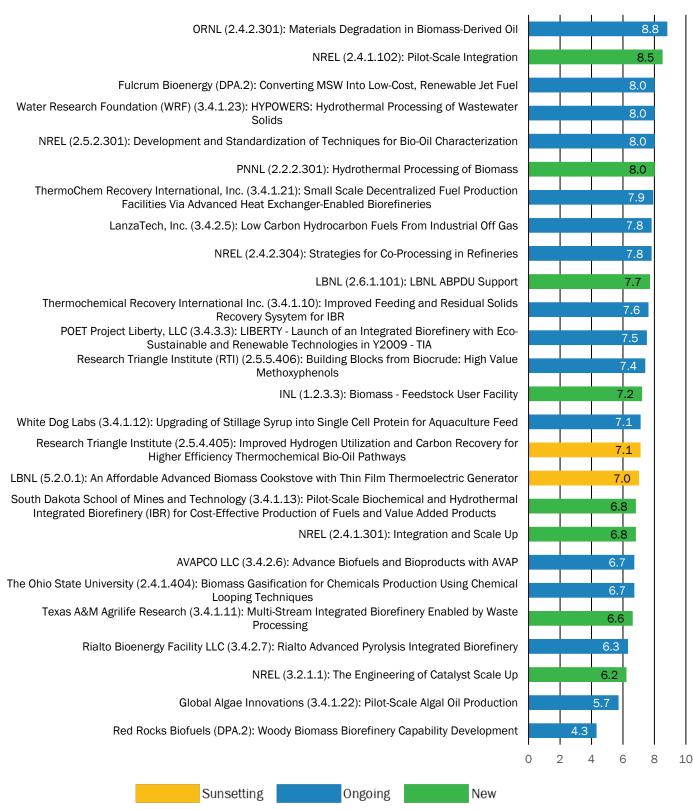
# ADO: INTEGRATION AND SCALE-UP REVIEW PANEL

| Name             | Affiliation                     |
|------------------|---------------------------------|
| Raghubir Gupta*  | Susteon Inc.                    |
| Michael Fatigati | Independent consultant          |
| Daniel Lane      | Saille Consulting, LLC          |
| Mark Warner      | Warner Advisors, LLC            |
| Andrea Slayton   | Slayton Technical Services, LLC |
| Luca Zullo       | VerdeNero, LLC                  |

\* Lead reviewer

# **TECHNOLOGY AREA SCORE RESULTS**

# Average Weighted Scores by Project



768

# ADO: INTEGRATION AND SCALE-UP REVIEW PANEL SUMMARY REPORT

#### Prepared by the Advanced Development and Optimization: Integration and Scale-Up Review Panel

ADO (previously known as Demonstration and Market Transformation) at BETO serves as a critical interface between the BETO research-and-development (R&D) projects and the deployment of advanced bioenergy technologies for end use. This team has been organized to manage the translation of R&D into technology demonstration and integration through well-established processes for project definition and execution using competitive solicitations. ADO is currently managing a diverse set of projects in its portfolio of technology areas (biochemical, thermochemical, etc.), technology-readiness levels (TRLs) (4–8), and feedstocks used (wood, stover, waste). Key barriers to market adoption of the technologies remain, including unfavorable market drivers such as low prices of oil and natural gas and no price on carbon emissions, as well as technology challenges associated with long-term reliable and robust operations of pilot plants, feedstock logistics, costs and long-term supply contracts, conversion and separation costs, and, most importantly, financing of demonstration and first-of-a-kind commercial facilities.

On behalf of the review panel, we thank the ADO team for the invitation to review the projects. It was a great learning experience for the panel members. We sincerely hope that comments provided by the review panel members on the individual projects are helpful in shaping better outcomes for the projects in the future.

#### SCOPE

From the panel's review of 26 projects in the ADO: Integration and Scale-Up portfolio, it was clear that ADO is managing engineering-scale systems development to verify and validate technologies in relevant environments (with real feedstocks and under realistic operating conditions) using engineering prototypes developed from the knowledge gained in early TRL R&D projects. In addition, ADO is providing a critical link to other BETO platforms, such as the Agile BioFoundry, Co-Optimization of Fuels & Engines (Co-Optima), Feedstock-Conversion Interface Consortium (FCIC), Chemical Catalysis for Bioenergy Consortium (ChemCatBio), Bioprocessing Separations Consortium, and DISCOVR Algae Consortium. Application of learnings from these targeted consortia to technical development and verification is a critical function that ADO is undertaking to reduce the overall cost of conversion and technology risk for commercial deployment.

ADO is also overseeing the BETO user facilities and connecting them with users to advance the technologies funded by BETO from the laboratory/bench scale to the pilot scale. These facilities include the biochemical conversion facility at the National Renewable Energy Laboratory (NREL), feedstock user facility at Idaho National Laboratory (INL), bio-oil testing for corrosion facility at Oak Ridge National Laboratory, Advanced Biofuels and Bioproducts Process Development Unit (ABPDU) at Lawrence Berkeley National Laboratory (LBNL), thermochemical pilot plant at NREL, biomass cookstove facility at LBNL, and the hydrothermal liquefaction (HTL) facility at Pacific Northwest National Laboratory (PNNL). In addition, ADO is putting concerted efforts in developing methods and tools at the national laboratories (e.g., NREL) that can be leveraged by other BETO projects. These include analytical methods development for the characterization of bio-oils, process modeling tools, and techno-economic analysis (TEA) and life cycle assessment (LCA) methodologies. Enabling and cross-cutting technologies such as corrosion testing, analytical methods development, and feedstock handling are critical for the success of the entire portfolio. In sum, risk management associated with the development and deployment of new bioenergy technologies through technology verification and validation is ADO's primary role in BETO.

# IMPACT

DOE investment through cost-shared projects to scale up the technologies from the bench to pilot and pilot to commercial demonstration is critical for future private investment in these technologies. The ADO team, through its structured project management practices, has generally done a very good job.

The POET (Liberty) project in the ADO portfolio is essentially in commercial operation, although some longterm operability issues are being addressed. Two other projects—Fulcrum BioEnergy (using waste gasification) and Red Rock Biofuels (RRB)—are at commercial demonstration scale, which are part of the Defense Procurement Act projects. These projects should be in operation by next year, if everything goes as planned. The success of these projects is critical to demonstrating the technology and to attracting commercial interest and investment capital for future deployment of the underlying technology.

Several other technology projects are at the pilot scale. This program review shows that these small pilot-scale projects are moving along well and form a good basis for taking them to commercial demonstration. These projects include chemical looping biomass gasification at Ohio State University, continued process and technology improvements at ThermoChem Recovery International, Inc. (TRI), treatment of biorefinery wastes at Texas A&M and South Dakota School of Mines and Technology, and the production of coproducts along with biofuels at Research Triangle Institute (RTI). Successful execution of these projects is critical to determining their merit for future investment to take them to the next scale.

The peer review noted that several projects awarded under the Project Development for Pilot- and Demonstration-Scale Manufacturing of Biofuels, Bioproducts, and Biopower (PD2B3) funding opportunity announcement (FOA) underwent a very structured stage-gate review. Based on the results, some projects were discontinued after Budget Period 1 and others moved forward to Budget Period 2. The currently ongoing projects in this category are making good progress to qualify for commercial demonstration. DOE funding was critical for them to undertake front-end engineering and design and permitting activities to attract project financing for commercial demonstration plants. Examples include LanzaTech, which is converting ethanol into jet fuel; biosludge conversion to fuels by the Water Research Foundation using PNNL's HTL technology; and AVAPCO, which is converting ethanol into nanocellulose and jet fuel. Commercial demonstration of some of these technologies will pave the way for their market acceptance and widespread deployment.

#### INNOVATION

With ADO's mission of technology verification and validation, major technology innovations through the projects are not expected. With ADO's emphasis on the use of real feedstocks under relevant conditions and promoting the use of national laboratory user facilities for pilot testing, however, the review panel noted several engineering innovations in various projects. For example, process intensification work done at TRI by integrating advanced heaters and novel particle-flow designs promise significant process improvement in future TRI biomass gasification projects. The production of coproducts along with biofuels is a desired pathway to enhance the attractiveness of bioenergy technologies. Several projects are pursuing new catalysis and process designs to meet this goal. Some modeling work done at NREL and other places is providing insights into solving operational problems and improving process designs.

## PROJECT MANAGEMENT

The review panel made the following observations on ADO's project management practices:

• The use of an independent engineer for project validation is a very good practice that allows for checking the claims made by project performers through on-site visits and rigorous analysis. The timing of these validations could be improved to avoid excessive delays in the project schedule. Some delays were apparently caused by project performers not having a clear understanding of validation requirements. BETO should consider including information about the independent engineer validation process as an appendix in various FOAs.

- It was not clear how learnings from individual projects (both successes and failures) were shared with the wider community and other project performers. There are industry best-practice guidelines to share these findings.
- It was not clear how much support ADO/BETO provided to the project participants in technology transfer. Researchers are heavily focused on solving technical problems without much understanding of business aspects and industry relevance. Having a small technology-transfer team at BETO (similar to Advanced Research Projects Agency-Energy but focused and at a much smaller scale) would be helpful to guide the projects to generate industry interest.
- Value chain analysis in some of the projects was missing. For example, if ethanol is a feedstock to produce biojet, analysis of long-term cost and availability of ethanol should be an important part of the project. Also, the final product has certain specifications for selling, so the final process step must include a separation/purification box to obtain those specifications.
- For some projects, the development of coproducts appeared to greatly increase the complexity and potentially the capital cost. Although the cost per gallon of gasoline produced through these coproduct pathways was attractive, getting the investment capital to build the entire plant could be difficult because of high overall capital costs.
- For some projects, the price used by project presenters for gasoline or diesel as a selling price was not the commodity price that could be achieved by the seller on the market. The presenters did not always appear to know the difference between the "cost at the pump" and what they could sell the product for. ADO should provide some guidelines to the project to fix this anomaly.
- In general, transitioning from one budget period to the next took significantly longer than planned. If BETO has certain administrative processes for review and approval, these need to be included in the FOA for planning the budget periods.
- ADO/BETO should develop uniform guidelines for conducting TEA and LCA studies for all projects. For reference, the National Energy Technology Laboratory uses well-defined guidelines for TEAs in all their projects under the carbon dioxide (CO<sub>2</sub>)-capture portfolio. Further, the assumptions and methodologies used for TEAs must be clearly defined and stress-tested (even if only shown to DOE), including coproduct valuation, market assessment, fully loaded costs, and use of tornado diagrams to prioritize future R&D work.
- Most projects provided a goal of meeting \$3/gasoline gallon equivalent (GGE) as a target to meet the *Multi-Year Plan* (MYP) goals without providing enough specifics. For most projects, no real effort was made to quantify how much the project could contribute toward reducing costs. Further, this target was set a few years ago. With changes in market conditions, ADO/BETO should revisit this goal because making biofuels might not be the best market driver for using biomass.
- Some laboratory projects funded through annual operating plans (AOPs) need industry context. For example, process models must be validated with relevant experimental data. The catalyst scale-up project should include a commercial catalyst manufacturer to share industry practices. This work at the national laboratories will significantly benefit from strong industry partnerships from an early stage. Process modeling is not a substitute for industry input.

#### RECOMMENDATIONS

The Peer Review Panel makes the following three recommendations:

**Recommendation 1:** ADO/BETO should develop guidelines for uniformly conducting TEA studies for all projects using a systems approach. The assumptions and methodology used for these TEAs must be clearly

defined and stress-tested, including coproduct valuation and market assessment to constantly ask, "Does this technology make economic sense?" These TEAs should be used to prioritize future R&D work.

**Recommendation 2:** Project validations using independent engineers should be continued but with clearer directions provided to project performers.

**Recommendation 3:** Projects at the pilot scale must include a value chain analysis from raw material procurement to offtake agreements for the final product(s).

The overall assessment of the Peer Review Panel was that ADO is doing a good job of demonstrating and validating integrated biorefinery technologies by focusing on the evaluation of performance at the pilot, demonstration, and pioneer scale to reduce capital and operational expenses and validate product quality.

# ADO: INTEGRATION AND SCALE-UP PROGRAMMATIC RESPONSE

## INTRODUCTION/OVERVIEW

BETO thanks the Peer Review Panel for their time and active participation in the ADO: Integration and Scale-Up session, as well as the panelists and steering committee for providing their feedback during the Project Peer Review meeting in March 2019 and the Program Management Review meeting in July 2019. We appreciate the panel's insightful and engaged review of the ADO: Integration and Scale-Up projects. The reviewers provided in-depth and constructive recommendations that can be used to inform the path forward for ADO: Integration and Scale-Up Technology Area in the coming years.

The 2019 Peer Review Panel commented that the ADO team, through its structured project management practices, has generally done a very good job. One instance specifically is that the projects awarded under the PD2B3 FOA underwent a very structured stage-gate review. BETO appreciates this feedback and continuously works to improve project and portfolio management to ensure that the proper controls are incorporated into the award documents and project management interactions. Conversely, the panel noted that it was not clear how much support ADO and BETO provided to the project participants in technology transfer, stating that researchers are heavily focused on solving technical problems without much understanding of business aspects and industry relevance. To clarify, ADO is emphasizing industry collaboration with national laboratory-operated process development units as well as other programs such as Energy I-Corps, which pairs teams of researchers with industry mentors where the researchers define technology value propositions, conduct customer discovery interviews, and develop viable market pathways for their technologies.

The panel also commented on innovation, stating that major technology innovations through the projects are not expected at higher TRLs, which is the general focus of the ADO Technology Area. But the panel does recognize the importance of the higher TRL work, especially work that emphasizes the use of real materials under relevant conditions. The panel also suggested that ongoing modeling work is providing insights into solving operational problems and improving process designs and that the production of coproducts will enhance the attractiveness of bioenergy technologies. ADO strives to strike a balance between innovation and technology readiness. Best practices from the BETO portfolio and elsewhere in industry support the use of industrially relevant conditions and materials, and ADO emphasizes this in its projects. Leveraging computational power by closely coupling with experimental efforts is becoming more widely used in the BETO and ADO portfolio.

The panel was asked to examine possible synergies between projects within ADO: Integration and Scale-Up Technology Area. The panel noted that enabling and crosscutting technologies such as corrosion testing,

analytical methods development, feedstock handling, and other technologies funded by ADO: Integration and Scale-Up have many synergies across ADO and are critical for the success of the entire portfolio. Additional synergies observed by the panel include ADO's efforts to manage the BETO process development units (PDUs) and encouraging teamwork to advance the technologies funded by BETO from the laboratory/bench scale to the pilot scale, which can be leveraged by other BETO projects. Last, the panel mentioned that risk management associated with the development and deployment of new bioenergy technologies through technology verification and validation is one of ADO's primary roles in BETO. DOE agrees, and ADO continues to emphasize total system development, including feedback to prior scale and upstream/downstream operations. For example, during FY 2019, ADO established the PDU working group with key personnel from each national laboratory PDU facility. The intent of this effort is to provide a forum for the various facilities to share best practices on technology, safety, project management, and other topics. In contrast, the panel found potential synergies in the TEAs and LCAs. Specifically, the panel suggested that ADO (and BETO as a whole) should develop uniform guidelines for conducting TEA and LCA studies for all projects. With that said, ADO projects all include a TEA element. ADO and BETO will continue to develop normalized TEA and LCA tools for industry use.

The panel was asked to discuss the focus of ADO: Integration and Scale-Up. The panel stated that some of the laboratory projects funded through the BETO AOPs need industry context. For example, process models must be validated with relevant experimental data, and the catalyst scale-up projects should include a commercial catalyst manufacturer to share industry practices. The panel noted that this type of work at national laboratories will significantly benefit from strong industry partnerships from an early stage and that process modeling is not a substitute for industry input. Additionally, the panel communicated that it was not clear how learnings from individual projects (both successes and failures) were shared with the wider community and other project performers. There are industry best-practice guidelines to share these findings. ADO agrees that industry involvement is critical for developing projects. Many AOP projects have industry advisory boards (IABs) or other industry involvement. BETO will encourage a higher degree of integration into project execution. ADO also notes that the dissemination of data is a core objective of publicly funded projects. ADO will continue to encourage collaboration and other forms of communication.

In addition to program-specific feedback, the Peer Review Panel provided project-specific feedback. The PIs and their project teams will work to incorporate this feedback as they continue with their projects.

As stated, the overall assessment of the Peer Review Panel was that ADO: Integration and Scale-Up is doing a good job of demonstrating and validating integrated biorefinery technologies by focusing on the evaluation of performance at the pilot, demonstration, and pioneer scale to reduce capital expenses and operational expenses and validate product quality. To conclude its review, the panel provided three overall recommendations for the ADO: Integration and Scale-Up Technology Area that, if implemented, would have the greatest impact on the portfolio and its ability to achieve its goals.

# Recommendation 1: ADO/BETO should develop guidelines for a uniform basis for conducting TEA studies for all the projects using a Systems Approach.

ADO has consistently requested a TEA task in its projects; however, the feedback suggesting normalization for this process is fair. BETO has developed quick TEA methods to a certain extent, and ADO will collaborate with other BETO programs to determine how best to disseminate these tools and methodologies.

# Recommendation 2: Project validations using independent engineers should be continued, but with clearer directions provided to project performers.

ADO and BETO have used many different forms of validation for different applications. This is a continuously evolving process seeking to ensure project readiness before proceeding. ADO has initiated discussions internally and with the independent engineer team to develop materials for applicants and recipients to better describe the expectations of these reviews.

# Recommendation 3: Projects at the pilot scale must include a value chain analysis from raw material procurement to offtake agreements for the final product(s).

Although not all projects will address all elements in the value chain, ADO generally always requests target metric or key performance parameter information from projects at the time of application and during key project reviews. The sensitivity of these values might require additional review; ADO will reconsider how best to do this.

As mentioned in previous sections, BETO will consider the panel's recommendations and incorporate them, as appropriate, in program elements and future funding opportunities. The ADO team will also continue to coordinate with other areas of BETO to assess the potential for implementing some of the panel's recommendations for increased synergy among projects.

BETO, the ADO program manager, and the ADO technology managers thank the Peer Review Panel for their time and their engaged review of the BETO's ADO: Integration and Scale-Up Technology Area. The panel's comments were largely positive and provided the program with the type of actionable feedback that can help promote progress toward the development of commercially viable bioenergy technologies.

# **BIOMASS – FEEDSTOCK USER FACILITY**

# Idaho National Laboratory

## **PROJECT DESCRIPTION**

BETO has recognized an INL core competency in scale-up and integration of biomass preprocessing technologies and process design. The foundation of this core competency is INL's biomass feedstock PDU, which is an integrated pilot-scale preprocessing system. This core competency is further supported by DOE's Office of Energy Efficiency and Renewable Energy (EERE) designation as a National User Facility in FY 2013. The Biomass Feedstock National User Facility (BFNUF) designation has expanded the use of the PDU in supporting collaborative projects with industry, universities, and other federal agencies. During the past six years, the PDU has been used extensively for preprocessing research, demonstration, and development;

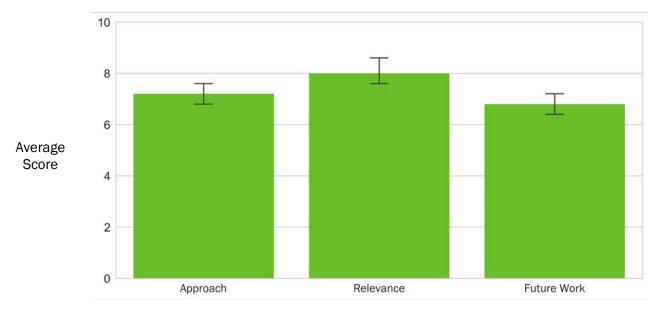
| WBS:                      | 1.2.3.3             |
|---------------------------|---------------------|
| CID:                      | NL0018159           |
| Principal Investigator:   | Mr. Neal Yancey     |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$5,900,000         |
| DOE Funding FY16:         | \$1,700,000         |
| DOE Funding FY17:         | \$1,700,000         |
| DOE Funding FY18:         | \$2,000,000         |
| DOE Funding FY19:         | \$500,000           |
| Project Status:           | New                 |
|                           |                     |

process development; toll processing (for feedstock supply) for both BETO- and industry-funded projects; third-party testing; and validation. The project is intended to transform the PDU to new and innovative uses in system-level research that enable and inform early-stage R&D in biomass preprocessing and handling.

This project has both technical and programmatic objectives. The primary technical objective is to eliminate the slugging caused by the Stage 1 grinder that is perpetuated through the preprocessing of baled biomass, resulting in inconsistent flow of biomass during the size-reduction process. This will be achieved by decoupling the first-stage grinding and bale deconstruction. The project will be replacing the high-speed, energy-intense bale grinder with a low-speed bale processor designed to use low speed and high torque to

# Weighted Project Score: 7.2

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

convert baled biomass into a flowable loose feedstock. The system will be able to process both round and square bales.

A secondary technical objective of this project is to equip the PDU with visualization tools and real-time measurement capabilities that allow in-depth characterization of the interaction of material and machine. The use and benefit of these tools will be demonstrated with a specific study of the mechanics of deconstruction and conveyance of biomass materials. Process visualization and in-line sensor applications will inform early-stage R&D and define operational boundaries. The data generated will be collected and stored in a data collection system that is consistent with and accessible by other DOE laboratories.

The programmatic objective is to increase PDU use. PDU use during the last six years has ranged from 30%–40% (the ratio of the number of days the PDU was in use to the number of days the PDU was available for use). PDU use is a combination of internal use, support of national laboratory AOP projects, and external industry collaborations. The end-of-project goal for the programmatic objective is to increase user facility use from the current baseline of 30%–40% to 60%, with tactical upgrades and improvements along with demonstrated examples and successful use of the PDU and associated capabilities for system-level R&D.

Accomplishing the technical (segmented bale deconstruction) and programmatic (increase BFNUF use) objectives will involve an approach that combines (1) testing new bale deconstruction methods that use low-speed deliberate bale deconstruction methods specifically developed for square or round bales; (2) developing and implementing in-line sensors and visualization tools that will enable the study of basic material and airflow properties within equipment (grinders and mills, conveyors, and other processing equipment) that will lead to more even flow, reduce equipment wear, and enhance separation capabilities; (3) developing data management tools that will increase access of PDU data to FCIC, other labs, and industry; (4) continuing to adapt the PDU to include improvements identified through FCIC, INL, and industry research and interactions; and (5) applying the system-level research capabilities (developed in 1–4) to study the biomass deconstruction and conveyance process in the PDU.



Photo courtesy of Idaho National Laboratory

- The BFNUF offers industry a huge advantage when it comes to the preparation of and dissemination of knowledge related to handling and preprocessing cellulosic feedstocks. This project very much needs to remember that dissemination of this knowledge—especially to equipment manufacturers—is going to have the greatest impact on industry.
- This project focuses on feedstocks that can be economically baled, which likely pertains to feedstocks sourced in the rural arena. The program seems to be focused on making incremental improvements to existing equipment, but ultimately it will result in increased capital expenditures (CapEx) and operating expenditures (OpEx) for feedstock processing. It is aspirational that something new and disruptive will result from this approach.
- There is clearly a need to marry the "smarts" of the national laboratories with the practical considerations of operating biomass preprocessing. Although biomass testing has been performed in the past, it seems we did not always know what we should be looking for. Making this new and improved capability open to industry testing, combined with the expertise of the laboratory personnel, could help industry take leaps forward.
- The facility is a great resource for generating valuable material handling data that are key to biorefinery scale-up. The technical work is well planned and executed, with a good upfront strategy. It is unclear how well integrated the testing is with bale manufactures and equipment vendors to produce a feedback loop.

• This project is aimed at decoupling bale deconstruction from grinding to develop sensing and visualization modeling capabilities with the goal of creating a uniform flow from heterogeneous nonuniform feedstocks. Further, INL wants to achieve greater than 60% use for this facility.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- This is a very good point. We will continue to share data and knowledge gained with industry and equipment manufacturers.
- We have shown that a large portion of the variability observed in grinding and milling can be controlled through proper equipment and controls. This will lead to great control over particle size and potentially other quality parameters.
- We agree.
- This is a good comment, and we will work at better engagement with industry and equipment manufacturers.
- Correct.

# HYDROTHERMAL PROCESSING OF BIOMASS

# **Pacific Northwest National Laboratory**

## **PROJECT DESCRIPTION**

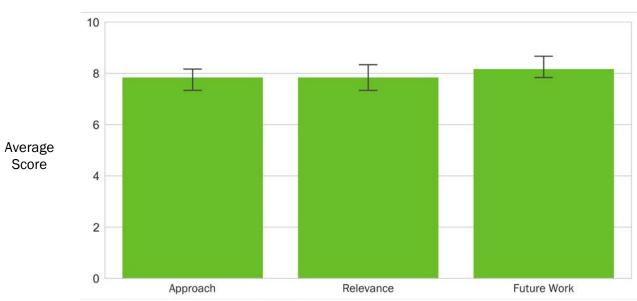
Scaling up conversion processes results in changes to proportions, such as surface area to volume or mass, and to flow regimes, and hence fluid mechanics and even reaction kinetics. Scale-up also affects the control of unit operation parameters, such as temperature and pressure, which can impact the management and efficiency of separations. Designing, building, operating, and maintaining PDUs is essential for de-risking the scale-up of conversion process technologies.

The PNNL PDU program currently focuses on adapting and applying hydrothermal PDU capabilities to produce biofuels and coproducts from wet-waste feedstocks. The

| WBS:                      | 2.2.2.301           |
|---------------------------|---------------------|
| CID:                      | NL0026720           |
| Principal Investigator:   | Mr. Dan Anderson    |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$7,285,613         |
| DOE Funding FY16:         | \$2,200,000         |
| DOE Funding FY17:         | \$2,050,000         |
| DOE Funding FY18:         | \$1,866,105         |
| DOE Funding FY19:         | \$1,169,508         |
| Project Status:           | New                 |
|                           |                     |

project has four major objectives: (1) conduct enabling R&D for hydrothermal processing, (2) performance testing and scale-up using wet-waste feedstocks, (3) support system modifications and capability management, and (4) support collaborative R&D projects.

The PNNL PDU program is addressing engineering scale-up challenges that must be resolved to move forward with later-stage integrated pilot and demonstration testing. Collaborative R&D projects hosted by the PNNL PDU program will produce the data and transfer of technology required for investment and commercialization.



#### Weighted Project Score: 8.0

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 ${f I}$  One standard deviation of reviewers' scores



Photo courtesy of Pacific Northwest National Laboratory

- This project is conducting process development research to evaluate the feedstock impact on HTL yields, valorization of waste streams, PDU operations, and scale-up challenges. In order to produce directly blendable dissels, hydrotreating is required due to the presence of heteroatoms (oxygen, nitrogen, and sulfur). Catalytic hydrothermal gasification has been applied to other streams, and this project is trying to apply it to HTL streams. The block flow diagram shows lots of issues to resolve.
- This project is aimed at the development and commercialization of PNNL's hydrothermal processing to convert wet feedstocks into transportation fuels. This PDU capability has been developed during the last 30 years, and its use is now extended to process wet solids.
- Overall, this project appears to be well thought through, targeting a less-developed process with the unique skills and equipment available or to be available to the national laboratories.
- The discussion of using a centrifuge to separate similar-density liquids did not make sense, and this equipment would not be used in industry for such a task. It seems there must be better equipment to address this separation, even going after the last bit.
- This is a clear and well-organized presentation. The team did a good job describing the technology and plans for continued hydrothermal processing technology development. The approach and planned work are well thought out and focused on value-added areas. The system design focuses on skidding, and the mobile units adds value and flexibility.
- This is a laudable anticipated and continuing use of existing facilities.
- The development of a pilot/demonstration facility for a technology with such potential impact is a critical activity and clearly an important mission for a national laboratory. The impact and support to the industry at large cannot be underestimated. Of relevance is the effort to make this facility flexible and capable to provide engineering data of immediate use for scale-up activities. The only area of concern is the reliance on catalytic technologies that might be of limited scalability and questionable economics. Nonetheless, this is a good platform for a variety of hydrothermal processing R&D activities.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The greatly appreciates the input. Many of the comments affirm the value of the project to BETO and reinforce our R&D and project management approach. Two important areas included a number of comments that will be briefly discussed here: (1) our approach to industrial engagement and (2) what we are doing differently versus our focus in previous years.
- From the onset, this project has heavily relied on industry to provide candidate feedstocks, and generally, the feed suppliers have a vested interest in the application of HTL to their wet waste. Through our collaborative work with the Water Research Foundation, member municipalities (more than 15) are tracking the progress of our work at PNNL and the work on the Hydrothermal Processing of WastewatER Solids (HYPOWERS) HTL demonstration project (a FOA) in Contra Costa County, California. As a result, municipalities are reaching out to us along with about a half-dozen entities working with venture capitalists. Additionally, BETO has set aside funds and is working to put out a broad solicitation for industry engagement with the PDUs.
- With respect to the new focus, as we advance HTL and test at larger scales, the project has identified a number of techno-economic and engineering challenges and uncertainties from feedstock assessment and formatting to HTL scale-up (pumping, heat exchanger evaluation, continuous oil/water separation) through water treatment and upgrading (metal removal, catalyst life, and throughput). Although we have improved in many of these areas during the past five years, the TEA along with interactions with architecture, engineering, and construction professionals (AECs) are helping us establish priorities on the R&D for further improvements.

# **PILOT-SCALE INTEGRATION**

# National Renewable Energy Laboratory

## **PROJECT DESCRIPTION**

The goal of this project is to support BETO's and industry's mission to develop cost-effective biofuels and bioproducts by providing a well-maintained and processrelevant, engineering-scale pilot plant for process development and technology verification. BETO national laboratory projects and consortiums, as well as industry, use the pilot plant to test and develop new technologies supporting ADO's goals to reduce commercialization risk and solve scale-up problems. The plant also produces process-relevant materials for bench-scale research as well as byproducts for testing and market development.

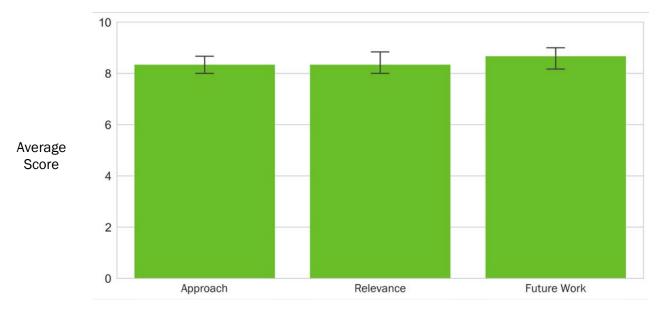
| WBS:                      | 2.4.1.102           |
|---------------------------|---------------------|
| CID:                      | NL0010773           |
| Principal Investigator:   | Mr. Dan Schell      |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$5,604,000         |
| DOE Funding FY16:         | \$2,000,000         |
| DOE Funding FY17:         | \$2,000,000         |
| DOE Funding FY18:         | \$1,604,000         |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | New                 |
|                           |                     |

The 27,000-ft<sup>2</sup> pilot plant has two high bays housing feed

handling through bioconversion and downstream separation equipment with approximately 1,500 analog and digital signals for process monitoring and control using a sophisticated process control system. The project has two tasks: (1) pilot plant upkeep and process material production and (2) development of new capabilities. The former work (Task 1) is organized effort to maintain the pilot plant (equipment maintenance and repair), generate and update plant documentation (Process and Instrumentation Diagrams [P&IDs], operating and lockout procedures, etc.), upgrade and maintain instrument and control systems (calibration, software and hardware changes, etc.), adhere to safety programs (process hazard analysis, change management, permits, etc.), and produce materials (pretreated biomass, enzymatic hydrolysis-derived sugars, soluble and insoluble lignin) for bench-scale research efforts. The goal of the second task is to find new capabilities—in







 ${f I}$  One standard deviation of reviewers' scores

collaboration with other BETO projects and industry partners—that enhance the pilot plant's ability to support future R&D work. At a minimum, yearly brainstorming sessions with BETO project leaders as well as our informal interactions with industry partners are used to identify needed equipment and capabilities. Then we define and implement milestone key decision points (go-no-go) to manage acquisition and installation activities using the available resources.

Future work in Task 1 includes ongoing efforts to maintain, repair, and upgrade existing equipment and instrument systems, update and maintain plant documents, and observe safety programs. Last year, we supplied seven BETO projects with research materials, and we expect to supply 18 projects with materials in FY 2019. We will also complete an update of the control system operator screens using a cheaper, versatile, modern, and more user-friendly software by the end of FY 2019, and we will complete the implementation of a new pilot-plant data-management system by mid-FY 2020. Future Task 2 work will continue efforts to find and acquire new capabilities. One current effort is to assess and modify the pilot plant's existing crossflow filter unit to perform ultrafiltration. Finally, we are beginning the procurement and installation of an advanced pretreatment process known as deacetylation and mechanical refining (DMR), two-stage refining of deacetylated biomass. We have purchased the first-stage 22-in. disk refiner (the delivery date is midsummer 2019), and we are beginning the design of a pilot-scale DMR system with installation targeted to occur in FY 2020 (we still need funds for additional equipment acquisition and installation). Prior to performing biochemical 2022 process verification in this facility, it will be necessary to begin planning in FY 2020 by defining the scope of the effort and needed capabilities to complete the work.

- Pilot-scale operations are critical to any scale-up. Many startup companies cannot afford to move directly to the pilot scale without additional validation or demonstration at scale; this PDU offers that opportunity. Other startups might need to focus on realistic feedstocks to demonstrate the viability of their processes or technology, and again, this PDU offers that. Support of industry at this scale is critical, and this project continues to be highly valuable to the portfolio.
- This project supports a worthy and demonstrated pilot plant.
- Considerable thought and planning have gone into the development of this project, which were supported by this presentation.
- The presentation did not address whether the refiner had been modified for this specific work. Typical pulp and paper refiners are used at a much lower solids ratio than this application. Hopefully the equipment was tested in a manner prior to purchase to confirm that it did what was needed for this application.
- The facility provides key scale-up data for biochemical processes. The project is being refunded and appears to be meeting its stated goals. The asset has proven performance and is a critical resource for the scale-up of biotechnologies.
- This is a national resource for developing and improving biochemical conversion technologies to produce cellulosic fuels and other products. This facility has served well to help scale up technologies, produce relevant product samples, and reduce commercialization risks. This facility has been well maintained.
- A flexible and agile pilot infrastructure open to the industry can considerably speed up the delivery of new ideas to market. Nothing specifically objectionable has been presented. It would be desirable to have a bit more clarity on the mechanism for accessing the capabilities of the facility and on the rationale for specific decisions regarding new capabilities and/or upgrades. The lack of gas fermentation capabilities and the inability to handle hazmat materials might limit use in emerging areas. The decrease

of industrial usage is concerning, and it would be valuable to understand why and if it is a significant, sustained trend. Lastly, it would be good to know what the use statistics are, in particular average use time and average uptime, the latter being the time that the facility—or a specific section—is available for use regardless of whether it is being used or not.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We appreciate the reviewers' comments and their efforts reviewing this work. This project's primary goal is to maintain a safe and process-relevant pilot plant for BETO and industry research needs that produces quality data. We continue to assess new capabilities to enhance the plant's ability to support R&D, and then we will prioritize and acquire equipment considering safety, future BETO R&D directions, and potential needs of industrial clients. As technology development continues and other process options for pilot-scale verification are found, we will continue to increase our collaborations with other BETO projects in the biochemical conversion area. Although the building housing the pilot plant has some limitations for hazardous operations, there are many options for facility modifications and new equipment siting (indoors and outdoors) that would support the investigation and development of new technologies.

# **INTEGRATION AND SCALE-UP**

# National Renewable Energy Laboratory

### **PROJECT DESCRIPTION**

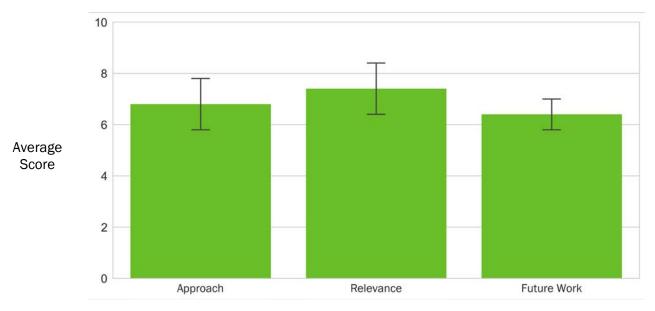
The goal of this project is to verify thermal and catalytic conversion technologies at an industrially relevant pilotscale facility to denote progress over the current state of technology (SOT) for biomass-derived pathways. To achieve this, the Integration and Scale-Up project operates NREL's largest thermochemical pilot facility: The Thermal and Catalytic Process Development Unit (TCPDU). The TCPDU is a highly instrumented, half-ton of biomass per day R&D facility designed to be functionally flexible to adapt to the needs of both BETO and industry partners. Starting a new three-year cycle, the TCPDU will be used to support the FY 2022 catalytic fast pyrolysis verification target by combining technologies

| WBS:                      | 2.4.1.301           |
|---------------------------|---------------------|
| CID:                      | NL0025580           |
| Principal Investigator:   | Dr. Kristin Smith   |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$7,725,000         |
| DOE Funding FY16:         | \$2,500,000         |
| DOE Funding FY17:         | \$2,500,000         |
| DOE Funding FY18:         | \$2,275,000         |
| DOE Funding FY19:         | \$450,000           |
| Project Status:           | New                 |
|                           |                     |

developed in BETO's ChemCatBio, FCIC, and the Consortium for Computational Physics and Chemistry (CCPC). This presentation details our plans for the next three years to prepare for this technology verification, specifically in maintaining consistency with bench-scale SOT and minimizing losses from scaling. This will include installation and commissioning of new capabilities within the TCPDU to meet the catalyst and feedstock requirements set by the bench R&D efforts. To meet the catalyst performance targets, we will install a new packed-bed reactor setup as well as a hydrogen-feeding system. Further, we will work with the core R&D projects (i.e., ChemCatBio, FCIC, and CCPC) to develop scaling relations that link bench and pilot operations. These relations will move beyond traditional, empirically based relations by including a physics-

# Weighted Project Score: 6.8

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 $oxed{I}$  One standard deviation of reviewers' scores

based foundation that will allow the relation to extend beyond the systems found at NREL. Finally, as the largest pilot facility dealing with thermal and catalytic technologies in the BETO portfolio, our dedicated team of operators is ideally placed to identify and develop engineering solutions that mitigate scaling losses from operational challenges that are apparent only when technologies are scaled and integrated. Together, this project reduces the risk to industry by bridging the technology "valley of death," thereby enabling the successful industry adoption of biomass technologies to support the continued growth of the U.S. bioeconomy and the jobs it supports.



Photo courtesy of National Renewable Energy Laboratory

### OVERALL IMPRESSIONS

- As with other national laboratory PDUs, there is tremendous opportunity to have an impact on commercial applications, especially with the ability for industry to use the physical resources available within this project. Key to future performance is decoupling reactor-specific impacts from the kinetic model; the team should focus as many resources as they can on achieving that goal because it will tremendously simplify additional development.
- Continued funding of the PDU is supportive of long-term BETO goals for biofuels cost reduction.
- The project is well defined and clearly directed at supporting BETO's data needs to verify cost production goals. The project team understands the critical nature of the data need and has contingencies in place to mitigate potential issues.
- This project is aimed at developing experimental/modeling approaches to successfully scale up thermochemical biomass conversion technologies from the bench scale to the pilot scale, leading to successful industry adaptation of biomass conversion technologies. The key technology being investigated is biomass pyrolysis.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# BIOMASS GASIFICATION FOR CHEMICALS PRODUCTION USING CHEMICAL LOOPING TECHNIQUES

# The Ohio State University

### **PROJECT DESCRIPTION**

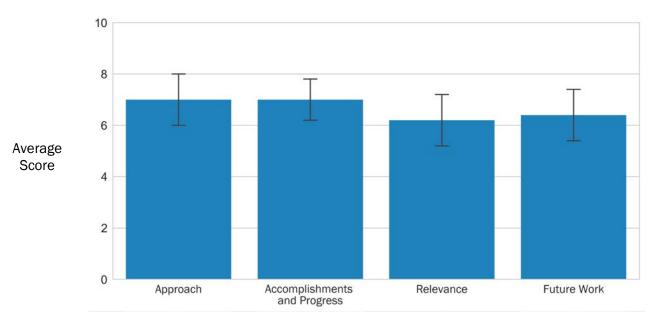
The Ohio State University (OSU) is investigating the biomass-to-syngas (BTS) chemical looping technology to produce syngas for chemical production applications from biomass under DOE Award #DE-EE0007530. The BTS process aligns with the programmatic area of interest of "Conversion, via biological, thermal, catalytic, or chemical means, of acceptable feedstocks into advanced biofuels and/or biobased products including intermediate and end-

| 2.4.1.404           |
|---------------------|
| EE0007530           |
| Mr. Andrew Tong     |
| 10/1/2016-9/30/2019 |
| \$1,500,000         |
| Ongoing             |
|                     |

use products." Compared to conventional biomass gasification processes, the BTS process eliminates the need for air separation units and tar reforming reactors, which leads to energy-efficiency improvement and capitalcost reduction. The overall objective is to ascertain the potential of biomass gasification based on the chemical looping technique through mitigation of the possible techno-economic challenges in the steps of scale-up for commercialization. The scope of work consists of (1) designing, constructing, and operating a 10-kWh commercially scalable sub-pilot BTS system; and (2) completing a comprehensive TEA of the BTS process using methanol production as an example.

# Weighted Project Score: 6.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 $oxed{I}$  One standard deviation of reviewers' scores

#### **OVERALL IMPRESSIONS**

- This project has high potential for success, in no small part because of the approach of building and testing a transparent, cold system first to validate flow performance—an excellent approach.
- The use of chemical looping techniques represents a transformative, and perhaps disruptive, approach to the transformation techniques for biomass so far considered, promising increased conversion efficiency, reduced costs of production, and relative ease of integration into existing fossil-fuel production facilities.
- It will be a big step from the bench scale to the PDU scale for this process because of the difference in design and integration. I look forward to seeing how this process progresses and the results of the studies.
- This project was awarded under the Biomass Research and Development Board in 2016 to develop a chemical looping gasification process for biomass. OSU has been a pioneer in chemical looping reactions for several applications. Theoretically, this concept looks elegant because it can combine gasification, tar reforming, and oxygen separation all in one reactor. Significant operation challenges are associated with this type of system. This project has completed Budget Period 1 and moved on to Budget Period 2, in which a small pilot plant is being assembled for testing. TEA studies are being conducted by Nexant in parallel.
- Gasification of biomass is a key unit operation in converting biomass to fuels and chemicals; however, the presentation did not clearly identify what was new or novel to be demonstrated from this grant. Technical issues such as syngas contaminants and biomass feeds did not appear to be adequately addressed. The project scope should be more clearly defined as gasification alone, not resulting in a methanol product.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# MATERIALS DEGRADATION IN BIOMASS-DERIVED OIL

# **Oak Ridge National Laboratory**

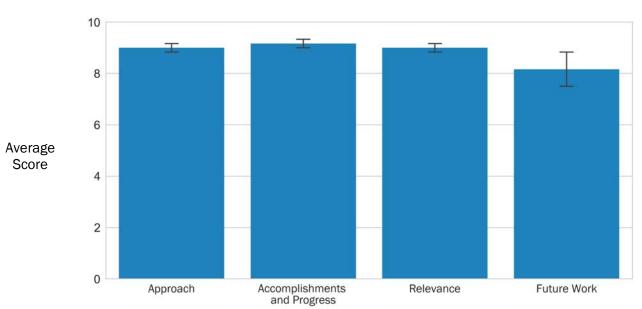
### PROJECT DESCRIPTION

Thermochemical processing of biomass provides a means to convert biomass resources—including trees, grasses, and agricultural waste—into fluids that can serve as liquid fuels or as feedstock for subsequent conversion into more refined liquid fuels or higher-value chemicals. As a result of the significant oxygen content of biomass, the products of biomass liquefaction contain a wide range of oxygencontaining compounds that are components of the biomass-derived oil. Organic (carboxylic) acids are one family of oxygen-containing products, and the presence of these products in bio-oil can make the oils highly acidic (pH often in the 2–3 range). In addition, the bio-oils often contain a significant amount of water as well as

| WBS:                      | 2.4.2.301           |
|---------------------------|---------------------|
| CID:                      | NL0019454           |
| Principal Investigator:   | Dr. Jim Keiser      |
| Period of<br>Performance: | 10/1/2015-9/30/2020 |
| Total DOE Funding:        | \$4,940,000         |
| DOE Funding FY16:         | \$1,600,000         |
| DOE Funding FY17:         | \$1,600,000         |
| DOE Funding FY18:         | \$1,180,000         |
| DOE Funding FY19:         | \$560,000           |
| Project Status:           | Ongoing             |
|                           |                     |

contaminants such as sulfur, chlorine, and nitrogen. Because of the acidic nature of these liquids as well as the presence of other potentially damaging organic compounds and certain contaminants, it has been shown that degradation of metallic containment materials and nonmetallic components is a serious concern and has been identified in industry as an issue.

There is not a good understanding of the role in the corrosion of various oxygen-containing organic compounds, nor is there an accepted test to measure the corrosivity of bio-oils. This project is intended to identify and increase our understanding of corrosive organic compounds in bio-oils as well as the degradation



### Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

mechanisms of metallic and nonmetallic structural materials. Our previously reported studies have demonstrated that in some cases a low-nickel, high-manganese stainless steel appears to perform better in some, but not all, of the processing environments, but considerably more work is needed to determine if this alloy offers a good alternative to 300-series stainless steels. Other studies have suggested that ketones and possibly aldehydes might be responsible for the degradation of some nonmetallic materials. Again, further studies are needed to confirm the causes of degradation and which alternate materials have enough corrosion resistance.

There is also a significant lack of fundamental knowledge regarding the interactions occurring on the surface of corroding materials, so we have added tasks to help us develop a more fundamental understanding. This could lead to the identification of degradation mechanisms occurring on both metallic and nonmetallic materials.

The overall objective of this project is to identify the components of bio-oils that cause degradation of metallic and nonmetallic materials, identify the degradation mechanisms, and then acquire enough information so that materials with acceptable corrosion resistance can be identified. By achieving these goals, materials issues should not prevent the successful commercialization of any biomass liquefaction technology.

#### OVERALL IMPRESSIONS

- This is an excellent project that clearly focuses on an industry-specific need. Dissemination of knowledge acquired during the project will be critical to the successful implementation of lessons learned.
- The project has largely met its objectives. The information produced is valuable for selecting materials of construction, both metallic and nonmetallic.
- The work overall is impressive. At first glance, I felt the scope was too broad, but the team was able to meet its objectives. I look forward to more work of this kind.
- The project supports wide commercial usage of biofuel/oils in existing fuel storage and delivery systems.
- This is a good example of core research to enable bioprocess commercialization. Materials of construction are a significant decision, and on new processes, necessary data often do not exist. This work is valuable to provide data necessary to mitigate project risk.
- During the pyrolysis process, a significant amount of oxygen in biomass manifests into bio-oils containing compounds extremely corrosive to many structural materials, both metallic and nonmetallic. This project is aimed at identifying suitable materials of construction for biomass conversion systems that handle bio-oils. Mechanistic studies are being conducted to understand corrosion mechanisms and eventually identify suitable materials that are corrosion resistant.
- This is an excellent project. An industry is built by creating standards and shared knowledge, which is essential to translating process ideas into operating plants. The selection of material is one area of shared knowledge that DOE can effectively foster. There is nothing to add or remove to the project as it stands today other than inviting its continuation and hope for more like this.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We appreciate the positive comments, and we will work to disseminate the information to a broader audience.

# STRATEGIES FOR COPROCESSING IN REFINERIES

# National Renewable Energy Laboratory

### **PROJECT DESCRIPTION**

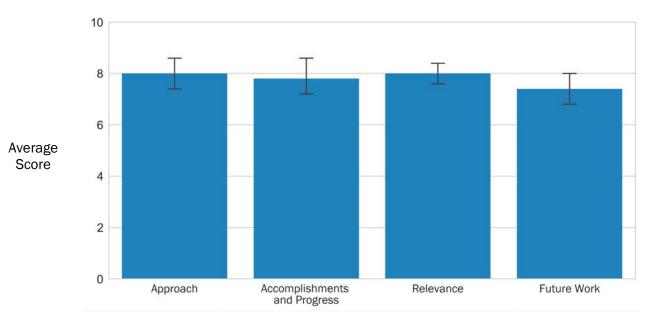
The objective of this project is to accelerate the adoption of coprocessing biomass-derived feedstocks with petroleum feedstocks in current refineries by (1) identifying blend levels for fast pyrolysis, catalytic fast pyrolysis (CFP), and HTL bio-oils and biocrudes that achieve  $\geq$ 5 wt % biogenic carbon incorporation into coprocessed fuels via fluid catalytic cracking (FCC) and hydrotreating/hydrocracking; and (2) advancing catalysts used in existing FCC and hydrotreating refinery processes to increase biogenic carbon incorporation into finished fuels while maintaining catalyst lifetime to be consistent with current industrial operation. Coprocessed fuels will be comprehensively analyzed for hydrocrarbon and oxygenate composition and

| WBS:                      | 2.4.2.304          |
|---------------------------|--------------------|
| CID:                      | NL0032422          |
| Principal Investigator:   | Dr. Robert Baldwin |
| Period of<br>Performance: | 8/1/2017-9/30/2020 |
| Total DOE Funding:        | \$3,300,000        |
| DOE Funding FY16:         | \$0                |
| DOE Funding FY17:         | \$1,000,000        |
| DOE Funding FY18:         | \$1,200,000        |
| DOE Funding FY19:         | \$1,100,000        |
| Project Status:           | Ongoing            |
|                           |                    |

biogenic carbon content. Additionally, tracking isotope-labeled biomass throughout coprocessing will provide detailed chemical information on conversion and upgrading that does not currently exist. FCC catalyst performance will be measured by producing hydrocarbon fuels of  $\geq 5$  wt % biogenic carbon incorporation, a factor of two improvement compared with the 2 wt % incorporation recently achieved with fast pyrolysis oil coprocessed at Petrobras. Hydrotreating catalyst performance will be measured by a 50% improvement of activity (heteroatom removal rate per catalyst volume) for coprocessing at least 10 wt % bio-oil biocrude blending in the feed compared to a commercial NiMo/Al<sub>2</sub>O<sub>3</sub> baseline catalyst. Catalyst lifetime will be assessed by measuring and mitigating coprocessing coking rates and/or degradation rate. FCC and

# Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



One standard deviation of reviewers' scores

hydrotreating/hydrocracking operations are the first industry coprocessing options to be developed as pilotscale equipment, and industrial catalysts are available at both laboratories, with NREL focusing on FCC coprocessing and PNNL focusing on hydrotreating/hydrocracking coprocessing. Alkylation units are also an option if biogenic carbon can be directed to C2–C5 olefins.

Increasing biogenic carbon incorporation into conventional fuels is a critical step in biofuels development and adoption. Coprocessing petroleum feedstocks with biomass-derived feedstocks leverages the existing petroleum-refining infrastructure, which significantly reduces CapEx. The coprocessing opportunity is significant because 106 of 136 U.S. refineries have conversion capabilities using FCC and/or hydrotreating. Research to date has explored only FCC coprocessing of raw pyrolysis bio-oil with vacuum gas oil at low blend levels (less than 10 vol % with 2 wt % biogenic carbon incorporation) and hydrotreating coprocessing of vegetable and animal fat oils. Many data gaps still exist, and this ongoing project is establishing the baseline and filling in the data gaps across different oil types, blend levels, and coprocessing strategies. Additionally, the performance challenges associated with coprocessing requires catalyst development targeting bio-oil crude conversion. Catalyst improvement will focus on (1) catalyst modification (using industrially available catalysts) to improve biogenic carbon incorporation efficiency into fuels and (2) understanding the impact of coprocessing on catalyst lifetime and developing deactivation mitigation strategies.

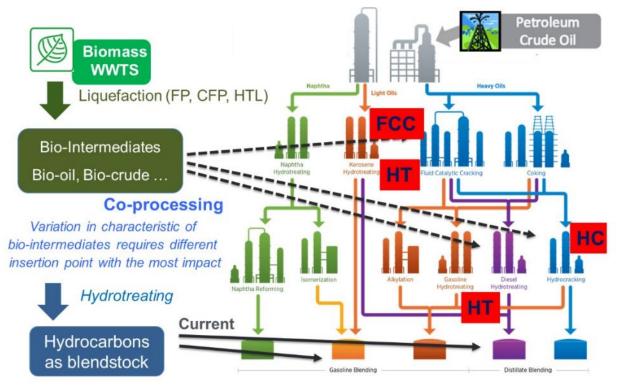


Photo courtesy of National Renewable Energy Laboratory

### OVERALL IMPRESSIONS

• This project has tremendous potential to shortcut the financing and commercial-scale construction required for many biofuel projects. The key concern is whether there will be enough de-risking the use of biofeedstocks within petrochemical facilities to actually convince those facilities to essentially upset the balance they have developed throughout decades.

- This project is aimed at coprocessing biocrude (produced from biomass pyrolysis) into an existing refinery infrastructure by understanding fundamental chemistry and process-engineering issues. Two main insertion points in the refinery have been identified: FCC and hydrotreating/hydrocracking units.
- The petroleum industry needs to see biofuel production as part of their portfolio rather than a competitor for the biofuel industry to be a success, so finding a way to make the "marriage" work is important. This project could certainly help incorporate the synergies, but I do not see petroleum industry involvement in this project. The presenter did an excellent job of showing the complexity of what was being/will be accomplished.
- Coprocessing of bio-oils can provide a robust pathway to increasing biobased fuel production and distribution by using existing assets. The project has good representation of industry insight, but it had limited information on performance to date.
- This is a much-needed project whose success will significantly advance the displacement of fossil carbon with biogenic carbon.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• Reviewer comments focused on three primary areas: scalability, catalyst development, and refinery involvement. We are addressing scalability by developing FCC and hydrotreating/hydrocracking coprocessing at the laboratory, in small and large pilot scales with enough generated operating data provided to refiners to assess adoption potential. FCC catalyst development is being conducted with Johnson Matthey, a major industrial supplier of FCC catalysts. Refinery involvement is accomplished with biannual project review of progress with our industry steering committee, which provides guidance on the future direction of interest to the petroleum industry.

# DEVELOPMENT AND STANDARDIZATION OF TECHNIQUES FOR BIO-OIL CHARACTERIZATION

# National Renewable Energy Laboratory

# **PROJECT DESCRIPTION**

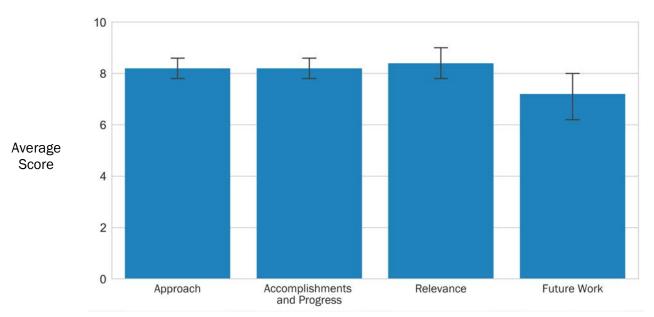
This project began in FY 2014 to address the lack of standard chemical characterization analytical methods for bio-oils. Bio-oils are very complex and present numerous analytical challenges, yet reliable chemical information (quantification of both individual compounds and chemical functional groups) is needed to inform upgrading research and refinery coprocessing. In this project, analysis needs are first determined from engaging the bioenergy community; we ask different entities about the biggest analytical challenges they face. Next, standard methods are developed to meet these needs, and then they are subsequently validated via interlaboratory studies with external partners. Methods that are successfully validated

| WBS:                      | 2.5.2.301           |
|---------------------------|---------------------|
| CID:                      | NL0026690           |
| Principal Investigator:   | Dr. Jack Ferrell    |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$2,812,000         |
| DOE Funding FY16:         | \$1,000,000         |
| DOE Funding FY17:         | \$1,000,000         |
| DOE Funding FY18:         | \$512,000           |
| DOE Funding FY19:         | \$300,000           |
| Project Status:           | Ongoing             |
|                           |                     |

(greater than 10% variability) are then shared as laboratory analytical procedures (LAPs), which are free and publicly available. We have been tracking LAP use for several years and have seen sustained usage, as evidenced by an average of 500 page views and 100 downloads per quarter, demonstrating the value of these methods to the bioenergy community. LAP methods that are particularly useful and reliable will be chosen for the next level of standardization through ASTM. ASTM standardization is being pursued to facilitate worldwide adoption of methods standardized in this project. Additionally, standard methods from an agency

# Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

such as ASTM are required to enable commerce with bio-oils. During the past two years, we have engaged with ASTM and successfully achieved approval by ASTM for our carbonyl titration method. This method (ASTM E3146) is now available and is the first example of an ASTM standard solely focused on the chemical characterization of bio-oils. This method has a broad scope (applying to bio-oils with a carbonyl content between 0.5–8 mol/kg) and is intended to help reliably describe bio-oils as intermediates that will undergo further upgrading. Work in this project is meeting the analysis needs of the bioenergy community and will ultimately help enable the commoditization of bio-oils.

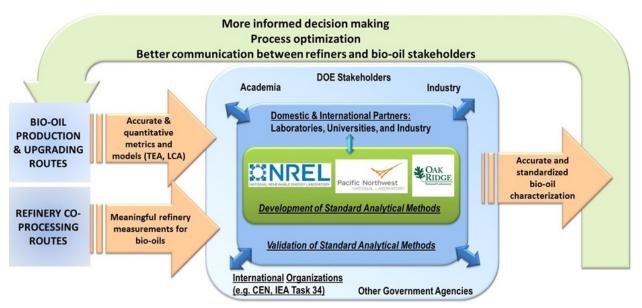


Photo courtesy of National Renewable Energy Laboratory

### OVERALL IMPRESSIONS

- This project clearly meets an industry need, and the described approach offers a high likelihood of success. Dissemination of the knowledge should help drive acceptance and use of the standards and methodologies developed.
- This project is targeted toward the development of analytical methods to characterize the bio-oils produced in pyrolysis processes (fast pyrolysis [FP], CFP, HTL). Chemical compositions of these bio-oils vary widely, and there are no standard methods to measure the chemical composition. Several very useful analytical methods were developed and disseminated to various participants to validate them.
- This project is a perfect example of work that should be done by national laboratories to promote biofuel understanding and specifications.
- This is valuable R&D work supportive of industry needs. It is aspirational to think that national laboratories could be a repository of standards—the collaboration with ASTM is key to this work for global dissemination.
- Standardization of analytical procedures is a key and valuable goal. The project generated positive results, including publication of an ASTM procedure. More information on milestones and project management criteria would have been valuable.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewer for the comment, and we agree that engagement with ASTM is essential for global dissemination (and use) of our methods. In addition, we believe the publication of LAPs is very

useful for the research community, and it is also a good first step before approaching ASTM with a specific analytical method.

• We thank the reviewer for the comment. In the future, we will aim to clearly provide more information on milestones and specifics on project management.

# IMPROVED HYDROGEN UTILIZATION AND CARBON RECOVERY FOR HIGHER-EFFICIENCY THERMOCHEMICAL BIO-OIL PATHWAYS

# **Research Triangle Institute**

### **PROJECT DESCRIPTION**

The objective of this project is to evaluate the potential for improved hydrogen use and carbon recovery in a novel, direct biomass liquefaction process. The primary aspect of this concept is to use hydrogen during *in situ* catalytic biomass pyrolysis to maximize the biomass carbon and energy recovery in a low-oxygen-content, thermally stable biocrude intermediate that can be efficiently upgraded into a finished biofuel. The secondary aspect of this concept is

| WBS:                      | 2.5.4.405          |
|---------------------------|--------------------|
| CID:                      | EE0006636          |
| Principal Investigator:   | Dr. David Dayton   |
| Period of<br>Performance: | 9/1/2014-8/31/2019 |
| Total DOE Funding:        | \$3,140,526        |
| Project Status:           | Sunsetting         |
|                           |                    |

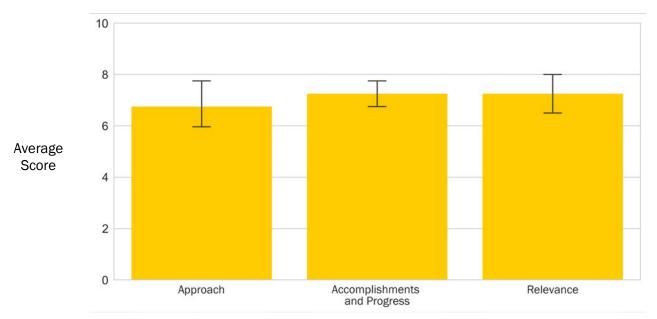
to improve the carbon efficiency of the integrated process by (1) converting the carbon in the various aqueous streams to methane for hydrogen production, (2) recovering oxygenated hydrocarbons for hydroprocessing, or (3) upgrading aqueous-phase carbon to value-added byproducts.

New and novel catalysts are being developed to improve hydrodeoxygenation during catalytic biomass pyrolysis to reduce biocrude oxygen content. Hydrogen in the pyrolysis reactor improves biocrude yield and quality while reducing char and coke formation.

Anaerobic digestion (AD) is being evaluated for aqueous-phase carbon conversion to methane that can be reformed for hydrogen production. Carbon recovery from the aqueous phase maximizes the renewable carbon efficiency, provides a renewable hydrogen source for the process, and improves water quality so freshwater consumption is reduced.

# Weighted Project Score: 7.1

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 ${f I}$  One standard deviation of reviewers' scores

Experimental results inform the TEA and LCA to determine the technical and economic feasibility and environmental sustainability of the integrated process. The overall hydrogen demand is comparable to other integrated thermochemical conversion processes, and the potential to reduce biofuels production cost with this novel, low-severity *in situ* CFP process to convert lignocellulosic biomass to hydrocarbon fuels has been validated. This proposed project supports the DOE BETO goal of producing hydrocarbon transportation at less than \$3/GGE with greater than 50% greenhouse gas (GHG) emission reduction potential compared to fossil fuels.



Photo courtesy of Research Triangle Institute

### OVERALL IMPRESSIONS

- This is a worthy project with the long-term potential for success.
- The modifications to the scope required during the project could likely have been foreseen at the start.
- The team ran out of biocrude during the project because of significant losses. Given the length of the trial, it would seem prudent to have significant biocrude on hand.
- This is a well-organized presentation with strong project management. Representative materials were produced and sent to industry partners for conversion testing. Significant data were presented supporting the achievement of goals, which provides credibility to the project.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• This project was selected in FY 2014 in response to the FOA on "Carbon, Hydrogen, and Separation Efficiencies in Bio-Oil Conversion Pathways." At that time, our approach was to improve both carbon efficiency and hydrogen use by leveraging two complementary technologies in an integrated direct biomass liquefaction process called reactive catalytic fast pyrolysis (RCFP). Hydrogen is added during the *in situ* catalytic pyrolysis to improve yield and the quality of the biocrude intermediate and reduce

char and coke formation. Liquid products separate into an organic biocrude and an aqueous phase. Under optimized reaction conditions, the RCFP biocrude contains as low as 6 wt % oxygen, compared to 20–30 wt % for a conventional CFP process. The improved quality of the RCFP biocrude is expected to be more readily integrated with downstream hydroprocessing to produce drop-in blendstocks or finished biofuels for transportation. RCFP upgrading studies to be completed by the end of the project will verify process improvements. Recovering carbon from the aqueous phase with AD was a new concept at the time this project began. Clearly, AD as an alternative to wastewater treatment provides a solution for improving carbon efficiency in the integrated process by producing renewable methane that can be converted to hydrogen for RCFP. The efficiency of methane production has been improved 150-fold with microbial population adaption such that 70% of the aqueous phase carbon is converted into methane. TEAs and LCAs to be completed by the end of the project will demonstrate that carbon and energy recovery from the aqueous phase has the potential to reduce the hydrogen demand and overall GHG emission for the integrated direct biomass liquefaction process to meet the BETO goal of producing transportation fuels for \$3/GGE with greater than 50% GHG emission reduction potential compared to fossil fuels.

# BUILDING BLOCKS FROM BIOCRUDE: HIGH-VALUE METHOXYPHENOLS

### **Research Triangle Institute**

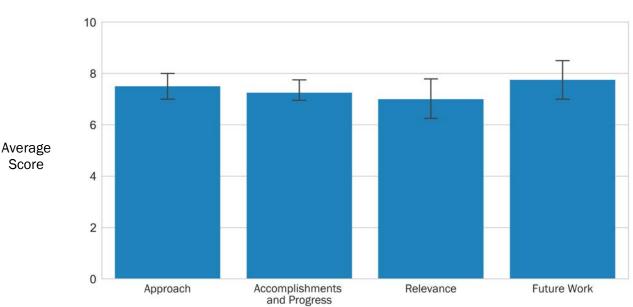
# **PROJECT DESCRIPTION**

Integrating biofuels production with bioproducts presents an opportunity to explore options for recovering highvalue chemicals as additional revenue-generating products from biofuel conversion pathways. Also, the inherent functionalized nature of biomass offers a unique opportunity for producing oxygenated chemicals that are not easily synthesized from petroleum; however, efficient separation approaches are required to recover the oxygenated species as marketable value-added products.

| WBS:                      | 2.5.5.406           |
|---------------------------|---------------------|
| CID:                      | EE0007730           |
| Principal Investigator:   | Dr. Ofei Mante      |
| Period of<br>Performance: | 10/1/2016-9/30/2019 |
| Total DOE Funding:        | \$1,987,148         |
| Project Status:           | Ongoing             |
|                           |                     |

RTI, Arkema, and AECOM are investigating the technical feasibility and economic potential as well as the environmental and sustainability benefit of recovering mixed methoxyphenols (eugenols and guaiacols) from biocrude as building-block chemicals alongside the production of biofuels. The optimization of a comprehensive separation strategy to recover the target methoxyphenols as a bioproduct is at the heart of this project.

Successful completion of this research will result in a process design, TEA, and LCA of an integrated biorefinery (IBR) for biofuel production and coproduct recovery. A product development assessment will also be conducted. Achieving technical success in recovering high-value methoxyphenols from biocrude prior to



### Weighted Project Score: 7.4

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

upgrading to biofuels could provide a significant source of revenue to improve overall process economics and help meet the \$3/GGE modeled production cost target for advanced biofuels technologies by 2022.



Photo courtesy of Research Triangle Institute

### OVERALL IMPRESSIONS

- It is good to see projects focusing strongly on the generation of valuable coproducts to offset biofuels production costs and achieve market-reasonable sales prices. Much of the current research focuses strongly on the primary product or a specific production technology, whereas this project looks at developing a separations technology that has the potential to be applied more broadly.
- This is a potentially useful line of R&D that could result in the supply of valuable methoxyphenols to industry. This is a great presentation with good justification for the project going forward.
- Although there appears to be an improvement to the cost of fuel production by adding value-added coproducts, I wonder if a biorefinery could be financed with the added complexity of additional new technology risk.
- Fractionation of biocrude to high-value products has the potential to improve overall pathway performance. Compounds in bio-oil have high value if they can be economically isolated. The large number of unit operations outlined in the proposed process flow generates concerns of unacceptable recovery yield; however, initial results appear favorable.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• A hybrid separation strategy has been developed and optimized to recover high-value methoxyphenols from biocrude to improve the process economics and environmental impact of advanced biofuels production via catalytic pyrolysis integrated with hydroprocessing. Seventy-five percent efficiency can be achieved for recovering a bioproduct with more than 90 wt % purity and no residual losses. The integrated strategy consists of permutations of three techniques: distillation, extraction, and adsorption chromatography to achieve different bioproduct purity levels depending on the end-use application. A 7gallon-per-day laboratory-scale separation unit has been designed, fabricated, and installed to demonstrate the scalability of the separation strategy. Market prices and market demand for recovered methoxyphenols has been evaluated to identify specific product-development pathways. Productdevelopment activities include the identification and evaluation of chemical pathways for vanillin synthesis, flame-retardant additives, biocidal products, caprolactone synthesis, and bisguaiacol F production. The results demonstrate the use of the mixed-methoxyphenols bioproduct as a feedstock for other applications, showing the potential of matching the bioproduct volume with market demand. Preliminary TEA based on a 2,000-bone-dry-ton/day plant with a separation unit for bioproduct recovery suggests that the methoxyphenols could help reduce the cost of fuel production. Cost estimation was based on factoring/parametric estimation and vendor quotes. The analysis indicates that the minimum fuel selling price (MFSP) decreases by 20% if the methoxyphenol bioproduct sells for \$2/kg and by 40% if the methoxyphenol bioproduct sells for \$3/kg. Preliminary capital costs increase by 5% or less if a separation unit operation is added to the base biofuel process for methoxyphenol recovery. Preliminary sensitivity analysis shows that the initial mass concentration of the methoxyphenols in the biocrude and the market price of the recovered methoxyphenols bioproduct has the largest impact on the MFSP.

# ADVANCED BIOFUELS AND BIOPRODUCTS PROCESS DEVELOPMENT UNIT (ABPDU) SUPPORT

# Lawrence Berkeley National Laboratory

### **PROJECT DESCRIPTION**

The ABPDU was established nearly 10 years ago to provide process optimization, scale-up, verification, and feasibility analysis services to the biofuels and bioproducts community, including industry, academia, and the national laboratories. This AOP project covers expenses related to facility readiness, process benchmarking, PDU teaming, and partnering and project development. The base operations budget is required to maintain the ABPDU in a not-for-profit collaboration facility model. In addition, the ABPDU's sponsors and collaborators fund full cost recovery for their specific statements of work and the team's actual expenses associated with the work at this facility. The partnerships enabled by this BETO-supported

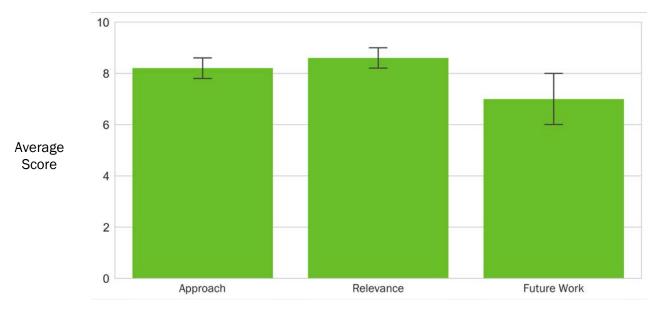
| WBS:                      | 2.6.1.101           |
|---------------------------|---------------------|
| CID:                      | NL0022407           |
| Principal Investigator:   | Dr. Todd Pray       |
| Period of<br>Performance: | 10/1/2015-9/30/2021 |
| Total DOE Funding:        | \$10,750,008        |
| DOE Funding FY16:         | \$2,750,000         |
| DOE Funding FY17:         | \$2,500,000         |
| DOE Funding FY18:         | \$3,000,008         |
| DOE Funding FY19:         | \$2,500,000         |
| Project Status:           | New                 |

model allow for the advancement of key technologies from the early stages to deployment in industry, bringing value to the entire biofuels and bioproducts community and providing high-visibility examples relevant to the BETO mission.

To provide cutting-edge technical services and process development expertise, the ABPDU will repeatedly baseline its processes to ensure team training and robust performance across all unit operations, from deconstruction through fermentation, separations, chemical catalysis, purification, and analytics. The ABPDU

# Weighted Project Score: 7.7

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f ar I}$  One standard deviation of reviewers' scores

will also maintain and upgrade its equipment and physical plant to offer access to technologies, processes, and analytics in demand by its clients, whether using small-scale process optimization capabilities or scaling up to the 300-L fermentation suite and biomass deconstruction and chemical catalysis capacity.

To date, the ABPDU team has worked with more than 40 industry partners in either company-sponsored or federally funded, competitively awarded projects. Industry projects at the ABPDU have spanned several sectors and product types: biomass and waste-stream use; biofuels production; biobased chemicals and biomaterials production and characterization; more sustainable food and protein production process development; and microbiome production and characterization for the waste remediation, agriculture, and health care industries. To date, three ABPDU partners have launched products that are commercially based, at least in part, on processes developed in working with the ABPDU team.

The ABPDU group and facility participate very broadly across several DOE project areas, also in a full-cost recovery model where these projects fund incremental work. BETO consortium projects that the ABPDU plays key roles in include the Agile BioFoundry, the Bioprocessing Separations Consortium, Co-Optima, and the FCIC. The ABPDU team also recently was asked to join the Fuel Cell Technologies Office (FCTO) BioH2 Consortium. The ABPDU capability is also leveraged by Office of Science programs such as the Bioenergy Research Centers, and the ABPDU group is also actively involved in BETO new consortium development and in a recently formed PDU working group. The goals of this working group are to share best practices in industry engagement, team training, and process safety, development, and scaling.

Another key activity supported by the ABPDU is workforce development and education. The team usually has at least one, and very often several, interns each academic semester. These students can get hands-on experience in all the unit operations at the facility and emerge as well-qualified candidates for industry employment or to pursue higher degrees at top academic institutions.

This combined set of activities, prioritized in close consultation with BETO management as well as LBNL stakeholders, continue to maintain the ABPDU as a critical resource and key shared capability to enable the bioeconomy's growth into more products, processes, and sustainable feedstocks.



Photo courtesy of Lawrence Berkeley National Laboratory

#### OVERALL IMPRESSIONS

• This is a tremendous resource to industry, and the model that has been used for the past several years (industry collaboration via essentially "rental" of resources and expertise) is clearly successful. Future work should focus on expanding this role and working to identify areas in which industry is lacking in both expertise *and* equipment for testing of novel technologies, such as gas fermentation with flammable

gases. The application of federal funds to support this type of work will have a significant impact on startup and small companies working to commercialize expensive but potentially lucrative biotechnologies.

- This is a good programmatic approach to operation and maintenance of a critical resource that supports BETO goals.
- This project has a strong and clear mission with good performance and a history of success. The facility is impressive, with significant equipment and qualified staff.
- This project is aimed at enabling biofuels and bioproduct commercialization, verification, and scaling in a DOE-funded facility that acts as an incubator/accelerator for bioprocess research. This has attracted industry and startups in multiple sectors: biofuels, materials/chemicals, food, health, environment, and agriculture.

#### **RECIPIENT RESPONSE TO REVIEWER COMMENTS**

We thank the reviewers for their time and thoroughness of their reviews. We look forward to implementing their constructive feedback. A reviewer identified a focus area with which we are in complete agreement: gas fermentation. We made a strategic hire three years ago who was awarded internal LBNL laboratory-directed R&D funds to ensure that gas fermentation capabilities are established at the ABPDU. We are pursuing other funding sources for the purchase of pressurizable bench-scale bioreactors. Also, as a part of the Bioprocessing Separations Consortium, we are developing technologies to continuously recover high-vapor-pressure molecules from the gas phase of bioreactors. Not having to perturb the liquid phase in fermentation and thereby prolonging biocatalysis can provide economic incentives. Further, we collaborate with NREL on a biological production of hydrogen project funded by the FCTO. The ABPDU will continue to prioritize this area of using gaseous feedstocks and generating and recovering gaseous products. A reviewer opined that ABPDU is a critical resource supporting BETO goals. The ABPDU and LBNL management work closely with BETO's technology managers to ensure that the ABPDU continues to add value to the BETO portfolio. This aspect is given very high emphasis at the ABPDU by its core team members. Our equipment and staff were referred to as "impressive." We are rigorous in our approach of maintaining state-of-the-art scale-up equipment and expertise. ABPDU researchers routinely participate in I-Corps programs to identify industry-wide issues and develop technologies and services that will be widely adopted. We will continue to be an empathetic listener to industry needs. One key aspect to the ABPDU's culture is maintaining an agile environment and adapting to our collaborators' needs. For example, our engineering and facilities teams customize equipment as desired by our collaborators. This approach opens us to multiple sectors, as identified by the reviewer.

# THE ENGINEERING OF CATALYST SCALE-UP

# National Renewable Energy Laboratory

### **PROJECT DESCRIPTION**

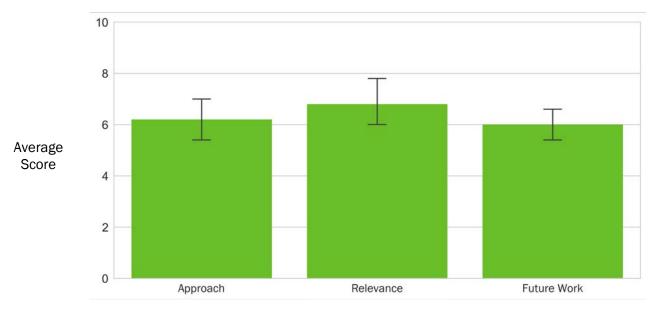
The goal of the Engineering of Catalyst Scale-Up (EOS) project is to create a flexible, engineering-scale catalyst synthesis capability within BETO to develop the critical scientific basis of catalyst scale-up required to translate emerging biomass conversion materials from the laboratory to commercial relevance by supporting engineering-scale performance evaluation of novel catalytic materials. The use and performance verification of next-generation catalyst materials at the engineering scale requires the development of strategies for preparing complex technical bodies (i.e., active phase, support, binder, modifiers, filler, porogen) suitable for operation in pilot reactors. Moreover, the impact of translating the

| WBS:                      | 3.2.1.1             |
|---------------------------|---------------------|
| CID:                      | NL0034842           |
| Principal Investigator:   | Dr. Fred Baddour    |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$400,000           |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$400,000           |
| Project Status:           | New                 |
|                           |                     |

syntheses of these catalysts from the laboratory scale to the engineering scale on the key catalyst physical properties (e.g., ionic speciation, colocation of active sites, active site ratios, particle size) is nontrivial and remains largely unexplored for research catalysts being developed in BETO's conversion portfolio. This development of methodologies to prepare engineering-scale quantities of technical catalysts based on the products of the robust catalyst development cycle that operate at the core of the ChemCatBio is critical to enabling the evaluation of advanced catalytic materials within DOE's pilot plant PDU and reducing the risk associated with the commercial adoption of these technologies. Further, the five-year biomass conversion pathway verification cycle employed by BETO has demonstrated that the consistent year-over-year

# Weighted Project Score: 6.2

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



 ${f I}$  One standard deviation of reviewers' scores

performance improvements yielded by fundamental catalyst design and synthesis at the laboratory scale does not trivially translate to larger scales, largely limiting the types of catalysts that can be tested in BETO's PDUs to commercial materials. Previous biomass conversion pathway verification efforts of internally developed catalysts have encountered significant scale-up challenges that have impacted catalytic performance.

The EOS project will address the needs of the catalyst development projects within BETO by decoupling fundamental (TRL 1–3) catalyst research from the scale-up of promising catalyst materials (TRL 4–6). The project's initial focus is on scaling up the catalyst candidates selected for the FY 2022 CFP verification while concurrently developing a capability that is broadly applicable to the catalysts developed across BETO's portfolio. These goals will be achieved through a multistep collaborative approach between NREL and Argonne National Laboratory (ANL) and will leverage existing scale-up technologies within ANL's Materials Engineering Research Facility, which include the Applied Materials Process R&D and Scale-Up and Advanced Materials Synthesis programs. This presentation highlights the unique set of capabilities and scale-up methodologies being developed by this partnership that are specifically tailored to the demands of preparing engineering-scale quantities of catalysts for bioenergy.

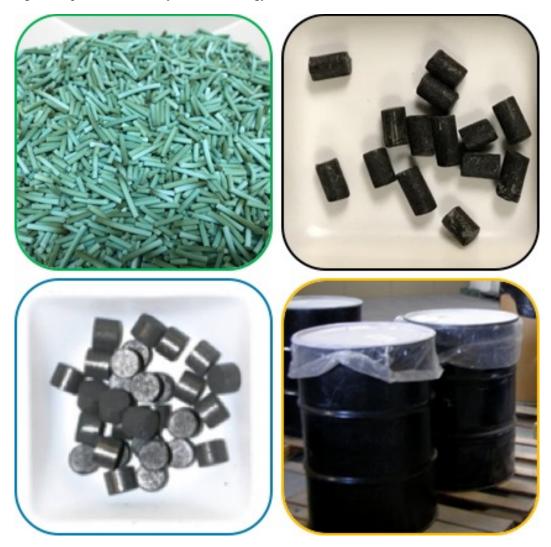


Photo courtesy of National Renewable Energy Laboratory

#### OVERALL IMPRESSIONS

- This project appears to have significant value to the industry inasmuch as commercial-scale production of novel catalysts is a clear bottleneck to rapid technology transfer to scale. Continued focus on adaptation/use of existing commercial production technologies will provide the fastest path to scale-up of novel catalyst production.
- NREL and ANL are developing a flexible, engineering-scale catalyst test facility to scale up catalysts used in biomass conversion. This is a very ambitious project because most of the catalyst scale-up knowhow is essentially a "black art."
- This project has newly started.
- The goals and objectives appear to be clearly defined.
- The go-no-go is outlined as part of future work. An IAB has been established.
- The project clearly meets DOE catalyst and technical needs for advancing the bio-industry through its PDU work.
- The project reduces risks for smaller/new businesses by providing testing at the pilot scale for catalystspecific needs.
- The project clearly identifies current obstacles that need to be overcome to more efficiently scale up solid catalysts, but the presentation discussed the work at a high level with generic terms and did not provide adequate detail to evaluate the value. Future work should include a better definition of how the end work product will be used to advance BETO goals.
- This project nominally supports BETO goals and objectives by providing a de-risking step in catalyst manufacturing that should translate well to traditional manufacturers.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer's feedback and agree that focusing efforts on reducing the bottleneck of commercial-scale production of novel catalysts is of potential value to the industry.
- We thank the reviewer for their comments and through this effort hope to address some components of the "black art" nature of catalyst scale-up.
- We appreciate the comments of the reviewer and will strive to achieve the outlined goals and enable engineering-scale evaluation of novel materials.
- We appreciate the insight of the reviewer and apologize if the presentation did not sufficiently highlight the value of the planned work. We see the value of this project being threefold:
  - 1. To prepare quantities suitable for operation in DOE PDUs that enable the evaluation of promising catalysts developed within the DOE national laboratory complex and directly support BETO technology verification efforts
  - 2. To reduce risks for smaller/new businesses by assisting with scale-up efforts, thus enabling pilot-scale evaluation
  - 3. To evaluate nontraditional manufacturing techniques for the preparation of catalytic materials.
- We agree with the reviewer that the EOS project provides an important de-risking step in catalyst manufacturing that should translate well to traditional manufacturers and that this effort supports the BETO MYP goals.

# IMPROVED FEEDING AND RESIDUAL SOLIDS RECOVERY SYSTEM FOR IBR

# ThermoChem Recovery International, Inc.

# PROJECT DESCRIPTION

This project aims to enhance the versatility and economic viability of IBR technologies. Specifically, this project will enable IBRs to employ a greater variety of non-pristine feedstocks that differ in geographic source, age, composition, size, energy content, and moisture content. It also incorporates improved solids-handling systems to selectively remove inert solids and discharge residual fine solids (ash) from the reactor more reliably, efficiently, and

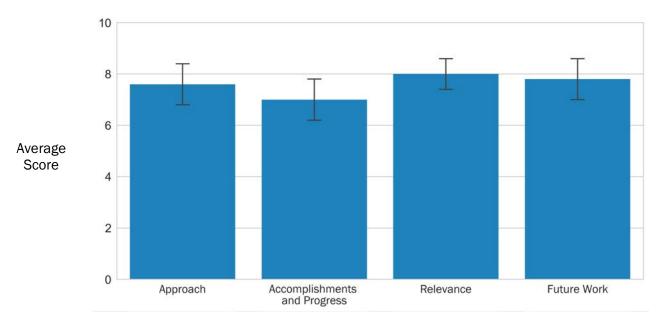
| WBS:                      | 3.4.1.10             |
|---------------------------|----------------------|
| CID:                      | EE0008249            |
| Principal Investigator:   | Dr. Ravi Chandran    |
| Period of<br>Performance: | 10/1/2017-11/30/2021 |
| Total DOE Funding:        | \$1,578,776          |
| Project Status:           | Ongoing              |
|                           |                      |

safely. These will increase annual feedstock throughput, decrease energy costs, decrease GHG emissions, and accelerate IBR deployment. These improvements could be offered together or individually and will catapult the state-of-the art technology available to all IBRs. These will also help meet BETO objectives to dramatically reduce dependence on imported oil and spur the development of the domestic bio-industry.

This project will leverage the existing commercial, technical, and operational capabilities of TRI to reliably introduce a variety of feedstocks into a reactor and remove process residuals safely and economically. Aligned to accommodate the FOA's intent, the present project will use TRI's existing four-ton-per-day PDU at the TRI Advanced Development Center (ADC) in Durham, North Carolina, with modifications to its first-generation feed system and residual fine solids discharge system and the addition of a classifier system for selective removal of inert solids and agglomerates from the reactor. The project will be validated by performing a continuous, long-duration trial with forest residuals, agricultural waste, and sorted municipal solid waste

# Weighted Project Score: 7.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

(MSW) feedstock in the four-ton-per-day PDU and evaluating the benefits for a reference 500-ton-per-day biomass-to-diesel commercial plant. The anticipated benefits at this scale are:

- Thirty percent increase in feedstock annual throughput per feeder
- Energy savings of 3,500 MWh per year
- Reduction in GHG emissions of 2.5 CO<sub>2</sub> equivalent g/MJ diesel (i.e., 3,000 tons CO<sub>2</sub> equivalent per year).

TRI has completed successful experimental validation of all three unit operations in Budget Period 1A. Budget Period 1B is in progress with mechanical design of the three systems ongoing. Feedstock selection and design of experiments for the PDU trial as well as National Environmental Policy Act (NEPA) documentation have been completed.



Photo courtesy of Thermochemical Recovery International, Inc.

#### **OVERALL IMPRESSIONS**

- TRI is addressing solids-handling issues in their biomass gasification system by improving biomass feeding to the gasifier, enabling more efficient removal of ash particles and the bed material from the gasifier to improve process stability and reduce CapEx and OpEx as well as improve efficiency. Handling of solids is one major issue in any gasification system, and the work done in this project provides a new approach to improve the reliability of the overall system.
- This project is designed to upgrade the feedstock and ash-handling capability of the PDU—goals that are supportive of integrated and long-term operations of the PDU.
- The work done by TRI is exemplary and appears to have addressed a significant gulf in the biomass industry for feeding a pressurized gasifier system. The approach and philosophy to develop scientific methods gives confidence to the work they do.
- The goal of the project is necessary for the success of larger-scale gasification. The use of multiple feedstocks under the testing program is valuable. The project needs a better definition on scope, and how it is integrated with other TRI projects was not clearly defined.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful comments and insights. We agree. We do employ sound scientific- and engineering-based approaches to accomplish the project goals.
- The overall scope is to design, fabricate, test, and validate improvements to feed and solids removal systems to optimize IBR. Although this project is focused on solids feeding and handling, the other project has a different target directed toward the process intensification of biomass conversion and syngas cleanup to decrease the IBR CapEx and OpEx.

# MULTI-STREAM INTEGRATED BIOREFINERY ENABLED BY WASTE PROCESSING

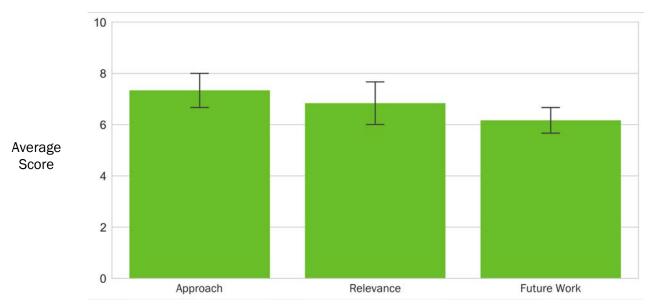
# Texas A&M AgriLife Research

# **PROJECT DESCRIPTION**

This project will integrate recent advances developed by a multidisciplinary academic-industrial coalition to address one of the most challenging issues in lignocellulosic biofuel: the use of biorefinery waste in producing valuable products. The success of a modern biorefinery heavily depends on the creation of diverse and valuable product streams using all fractions of input material. Essentially, all current lignocellulosic bioconversion platforms lead to a

| WBS:                      | 3.4.1.11           |
|---------------------------|--------------------|
| CID:                      | EE0008250          |
| Principal Investigator:   | Dr. Joshua Yuan    |
| Period of<br>Performance: | 5/1/2018-4/30/2021 |
| Total DOE Funding:        | \$2,236,211        |
| Project Status:           | New                |
|                           |                    |

lignin-containing waste stream that needs further processing into valuable products. Although a certain amount of lignin (approximately 30%–40%) is needed for the thermal requirements of biofuel production, a modern cellulosic processing plant will have approximately 60% excess lignin that is mainly burned. Use of lignin-containing biorefinery streams as feedstock for renewable products offers a significant opportunity to improve operational efficiency, reduce costs, reduce carbon emissions, and enhance sustainability of lignocellulosic biofuels. We will uniquely address these challenges by developing technologies for a multi-stream integrated biorefinery (MIBR), where the lignin-containing biorefinery waste will be used for producing high-value products.



#### Weighted Project Score: 6.6

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%

 ${f I}$  One standard deviation of reviewers' scores

This research will pursue three objectives:

- 1. MIBR development by advancing fractionation, conversion, and processing technologies to enable valuable bioproduct streams. Innovative chemical and biological fractionation technologies will be developed and enhanced to generate lignin fractions amenable to different applications in bioconversion, asphalt binder modifiers, and carbon fiber. The processing technologies will be advanced to enable the complementary use of lignin fractions based on their different structural characteristics.
- 2. MIBR optimization through process design, TEA, and LCA. Process design will be used to maximize MIBR profitability and enhance sustainability via the integration of fractionation, conversion, and processing technologies. TEA will be carried out to evaluate profitability, and LCA will be used to evaluate sustainability, with both guiding profitable and sustainable enhancements using process optimization.
- 3. MIBR scale-up to one dry-ton-per-day capacity. This will be done at an ICM, Inc. biorefinery site. Thus far, the project has successfully passed the initial verification and developed integrated processes for lignin-based carbon fiber, asphalt binder modifier, and lipid conversion.

The proposed research will leapfrog current technologies to address one of the most eminent issues in biorefineries and an under-researched topic of scientific and commercial importance. The research uniquely addresses all four priority areas in the FOA and represents a highly innovative solution for biorefinery configuration. The innovative effort has significant scientific merit, and the successful development of an MIBR represents a transformative solution for lignocellulosic fuel production. An MIBR will reduce fuel production cost by creating the means to produce high-value bioproducts, including asphalt binder modifiers and quality carbon fiber, and by mobilizing a valuable way of using all carbon in the feedstock. MIBR development will also promote rural economic development, build energy independence, and enhance U.S. agricultural incomes.

#### **OVERALL IMPRESSIONS**

- This three-year project to develop an MIBR is scientifically sound and well planned. It is highly relevant to the BETO MYP goals. A good team is in place for the project's execution. Successful completion of this effort is likely to lead to serious commercial interest in scaling up and deploying this technology.
- The processing of wastes to generate valuable coproducts is likely the only near-term path to the commercial application of cellulosic biofuels, and projects such as this greatly support the industry moving to this model. Focus on applications using real-world waste streams to achieve the fastest success, and do not spend time working to modify upstream processes to produce "improved" (waste) feedstocks, because the impact on the primary model will likely overwhelm any potential for positive impact.
- Valorization of waste streams is critically important to BETO's goals. This program is supportive in unique ways.
- This project has a specific target of reducing the cost of ethanol (by \$0.50/GGE). Having a target instead of a general objective is more likely to get the team to achieve the target.
- This project has a strong industry partner in ICM. Hopefully the project will use ICM to keep the focus on pragmatic results.
- This project has a reasonable goal of turning waste biomass into asphalt filler that provides enhanced properties. The team is well qualified and organized, although it is very early in the project. The process is complicated, and it was difficult to understand from the presentation.

• This project appears to be a solution in search of a problem. This is a very complex process with too many different pathways. Any of these pathways could require more than 100% of the project resources for a complete investigation. It appears that the team might need to modify the front end, which is existing, thereby greatly increasing the cost of this integration. Overall, the project points to a lot of very interesting opportunities, but it appears to be more of a conceptual study than a real developmental one. There is no shortage of the former, and I think the latter should be preferred. A stronger focus on the fractionation and much less, if any, on the next phase of product development from specific lignin fraction would give this project more practical value and meaningful goals. The TEA is aspirational at best.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the comment and acknowledgement of the potential impact of the project.
- We appreciate the comment and acknowledgment on the interest from industry. We agree with the reviewer that we should focus on real-time cases. The fractionation/pretreatment development focuses on tailoring existing pretreatment conditions without significant changes to biorefinery configurations. We will focus on scenarios close to current biorefinery configurations yet yielding lignin with better processability characteristics.
- We appreciate the comment and acknowledgement of uniqueness.
- We appreciate the comment and the acknowledgement of strong industry relevance and partnership.
- We appreciate the comment and acknowledgement of a strong team. We agree with the reviewer that an MIBR with different products is rather complicated. In fact, some current wet-milling corn ethanol refineries are also rather complicated in terms of different product streams.
- We appreciate the acknowledgement of interesting solutions and we agree that the project has three different product paths, which makes this project more complicated than a traditional project. In fact, some of the most profitable corn ethanol wet-milling biorefineries also produce multiple products, such as starch, corn oil, and syrup. The multiple-product approach is critical to avoiding market saturation and maximizing the economic return. The project actually focuses more on developing each product processing, instead of the fractionation. The pretreatment and fractionation technologies will be based on a modification of current pretreatment without change in infrastructure, which will allow us to quickly scale up the project within three years. We very much agree with the limited budget and resources available to the project; however, as discussed in the question-and-answer session, the project is based on an extensive preliminary study, a previous DOE project (DE-EE0006112), and internal support. The project is at the beginning stage, and the TEA has just begun.

# UPGRADING OF STILLAGE SYRUP INTO SINGLE-CELL PROTEIN FOR AQUACULTURE FEED

# White Dog Labs

### **PROJECT DESCRIPTION**

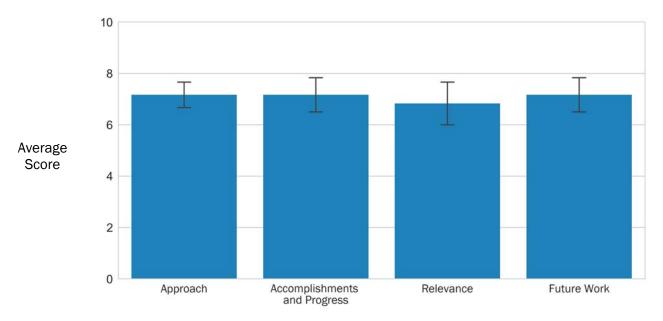
In this project, the undervalued stillage filtrate from a cellulosic ethanol plant will be upgraded into a single-cell protein (SCP) product for aquaculture feed applications. Currently, the stillage stream is sent to an anaerobic digester for conversion into biogas; however, residual cellulosic carbon is still within this stream and can be converted into a higher-value product. White Dog Labs (WDL) proposes using this stillage stream to generate an

| WBS:                      | 3.4.1.12           |
|---------------------------|--------------------|
| CID:                      | EE0008251          |
| Principal Investigator:   | Dr. Shawn Jones    |
| Period of<br>Performance: | 1/1/2018-10/1/2020 |
| Total DOE Funding:        | \$2,233,290        |
| Project Status:           | Ongoing            |
|                           |                    |

SCP as a higher-value product than biogas. The generated SCP is a good alternative to fish meal in aquaculture applications because of its comparable protein content (greater than 60%) and amino acid profile (particularly in lysine, threonine, and methionine). For SCP generation, WDL will use its proprietary fermentation technology, called MixoFerm, which enables significantly higher cell yields than conventional fermentation. In the proposed project, led by WDL Vice President of Microbiology Shawn Jones, we will produce SCP from cellulosic stillage and undertake a salmon-feeding study to validate the nutritional value of the SCP. Inclusion of the proposed SCP process in an IBR will provide another high-value coproduct and help improve plant economics.

# Weighted Project Score: 7.1

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${f I}$  One standard deviation of reviewers' scores

#### **OVERALL IMPRESSIONS**

- SCP has been a coproduct goal for many years, and it is laudable when the concept is applied to coproducts for improved financial viability of larger projects; however, all these projects—including this one—need a more detailed assessment of the existing market and what the competition will be for commercial acceptance of the final product. Realistically, there is no path to \$2/kg SCP from cellulosic feedstocks, so production costs *must* be kept to a minimum while maximizing proximate analysis/SCP value.
- This project is very supportive of overall BETO goals.
- This project is well focused at converting a low-value waste stream from cellulosic ethanol facilities and upgrading it to a protein product. The target of protein makes sense, and the basic technical plan is sound. The team is using real-world material from a commercial cellulosic facility. The team would benefit from integrating a better understanding of the target market into directing development efforts.
- The production of SCP from a biorefinery waste stream is highly relevant to the BETO MYP goals. The proposed technology appears to be scientifically sound. There were challenges with the filtrate materials received from POET. Identifying a suitable waste stream should be a project priority.
- The production of SCP is in theory scalable—as long as the market develops as promised—and the technology could have application in the conventional corn ethanol industry. It does not appear that the complexity of purifying the product has been considered—currently, there is very limited commercial SCP production using clean dextrose as a feedstock—nor the regulatory complexity. Last, the project overestimated the value of their SCP product using fish meal as a proxy. The lack of omega-3 fatty acid is likely to make soy meal a much more likely and less valuable proxy.

### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# PILOT-SCALE BIOCHEMICAL AND HYDROTHERMAL INTEGRATED BIOREFINERY FOR COST-EFFECTIVE PRODUCTION OF FUELS AND VALUE-ADDED PRODUCTS

# South Dakota School of Mines and Technology

### **PROJECT DESCRIPTION**

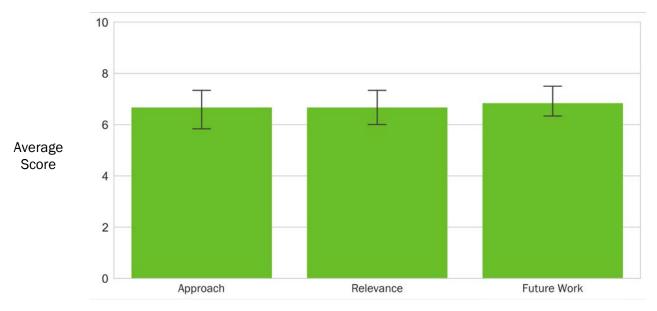
The major goal of this project is to demonstrate the production of value-added products from the waste streams generated during conventional biochemical processing of lignocellulosic biomass. These waste streams include unhydrolyzed solids (solid waste-I) and aqueous waste streams (I). Unhydrolyzed solids will be processed via catalytic hydrothermal treatment, which will produce biochar (solid waste-II) and aqueous waste streams (II).

| WBS:                      | 3.4.1.13            |
|---------------------------|---------------------|
| CID:                      | EE0008252           |
| Principal Investigator:   | Dr. Rajesh Shende   |
| Period of<br>Performance: | 2/15/2018-2/14/2021 |
| Total DOE Funding:        | \$1,926,160         |
| Project Status:           | New                 |

Typically, the proposed technology platform produces two aqueous waste streams and two solid waste residues, which will be converted into high-value products (lactic acid, phenols, biocarbon, and nanofibers). The solid waste lignin residue derived from corn stover will be treated hydrothermally to produce biochar, which will be converted into graphitic battery-grade biocarbon (product-1) and carbon nanofibers (product-2) as final products. Because biochar is commercially available, the production of marketable high-value carbon materials (biocarbon and carbon nanofibers) from biochar will have tremendous economic impact on reducing the fuel cost. Additionally, from the aqueous waste stream, coproduct lactic acid/polylactide (product-3) will be enriched. During hydrothermal processing of solid waste lignin residue, phenol (product-4) will be selectively produced and recovered as a coproduct. While generating these products, bio-oil is also generated, which can be upgraded to fuel quality. In our preliminary TEA/LCA, the products/coproducts derived from the

# Weighted Project Score: 6.8

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 5 0%



 ${f I}$  One standard deviation of reviewers' scores

waste streams have been shown to reduce the fuel cost and reduce GHGs. The three major objectives to advance the technology include (1) demonstrate bioproducts from waste streams at the pilot scale with a minimum of one ton per day via integrated biochemical and hydrothermal pathways to validate the cost-effective production of the fuel, (2) document the final product yields and estimate the revenues that can be generated based on current market price and provide profit summary, and (3) perform detailed TEA and LCA using standard tools to understand the economic and environmental impacts of the proposed activities.

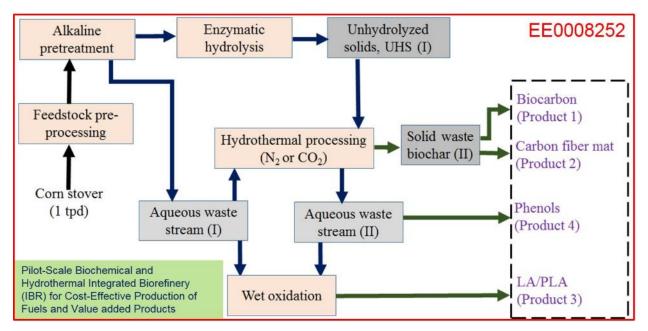


Photo courtesy of South Dakota School of Mines and Technology

### OVERALL IMPRESSIONS

- Although it is always interesting to hear about methods of making a "silk purse out of sow's ear," the use of waste biogenic carbon streams to produce carbon fiber and powder to support new industry is intriguing.
- The project brings forward an interesting approach and range of products, with most of the work still pending. If proven successful, it has the potential to add great value; however, the large number of unit operations and wide range of products bring concern about reaching economic viability for the process.
- This is an important project to advance the BETO MYP goals to use waste streams to produce valuable coproducts. This project provides a holistic approach to use both solids and aqueous wastes to produce industrially relevant products.
- In process schemes designed to be attached on the back end of existing processes to improve the value of current low-value or waste streams, is not uncommon to see the process becoming more complex and expansive than the original process it integrates. It behooves the developer to prove that this is justified economically and that the process is indeed scalable. I look at this with some skepticism because (1) it appears to be tailored around the alkaline pretreatment of biomass, which is not a widely accepted process technology; and (2) it proposes a complex slate of coproducts whose economics and further processing complexity are only marginally investigated. This project would benefit from a stronger focus.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We truly value this viewpoint because both carbon fibers and biocarbon generated from waste carbon will support new industries.
- We understand the concern raised by the reviewer about the economic viability of the process. A specific task on TEA has been included in our proposed work.
- We appreciate the reviewers' comments.
- We believe that alkaline pretreatment-derived unhydrolyzed solids will be more suitable for the generation of coproducts with superior characteristics. Higher liquefaction or bio-oil yields were realized with the HTL of the solids derived from the alkaline pretreatment than with the dilute acid pretreatment. For the former, the char was found to have a higher specific surface area than the latter. Prior to the pilotscale trials, we plan to optimize the alkaline treatment with the characteristics of the derived coproducts. We agree with the reviewer that the economics of the coproducts have not yet been fully investigated. Note that the processing complexity and economics of the coproducts will be fully investigated under specific tasks. The TEA will lead us to a stronger focus on certain project aspects. If the pretreatment method is only hydrothermal, the pH of the aqueous phase can drop to less than 3. The low pH (<3) of the medium causes the precipitation of solubilized lignin and catalyzes the degradation of hemicelluloses. To avoid the formation of inhibitors, the pH should be controlled between 4 and 7 during the pretreatment. This pH range minimizes the formation of monosaccharides and therefore the formation of degradation products that can further catalyze the hydrolysis of the cellulosic material during pretreatment. Maintaining the pH near neutral helps avoid the formation of fermentation inhibitors during the pretreatment. Therefore, we proposed the alkali-assisted pretreatment method, where potassium carbonate ( $K_2CO_3$ ) is added in a small fraction to maintain the aqueous-phase pH near neutral. The approach is clearly different from the conventional alkaline, where pH is 8 or more by the addition of alkali.

# SMALL-SCALE DECENTRALIZED FUEL PRODUCTION FACILITIES VIA ADVANCED HEAT EXCHANGER-ENABLED BIOREFINERIES

# ThermoChem Recovery International, Inc.

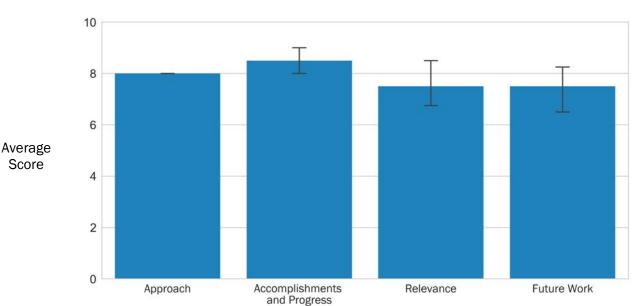
# **PROJECT DESCRIPTION**

The steep CapEx and OpEx levels required by the firstgeneration IBR technologies have forced project developers to focus on very large-scale projects and negatively priced (i.e., MSW, hazardous waste) feedstocks, driving market pull forces away from the ample feedstocks that comprise the industry-defining DOE's *Billion-Ton Study* (2005), the 2011 follow-up report, and the expanded 2016 report. The resultant mass migration of project

| WBS:                      | 3.4.1.21            |
|---------------------------|---------------------|
| CID:                      | EE0007964           |
| Principal Investigator:   | Dr. Ravi Chandran   |
| Period of<br>Performance: | 1/15/2017-3/31/2019 |
| Total DOE Funding:        | \$807,984           |
| Project Status:           | Ongoing             |
|                           |                     |

interest away from smaller-scale wood and agricultural waste projects represents an overreaction to existing market forces. Project developers' and owners' answers should not be to abandon otherwise solid projects because feedstock collection and transportation logistics unavoidably increase average delivered costs as catchment area radii increase, but rather to meet the market where it is (i.e., at significantly smaller scales than what has been pursued to date). This is where technologists such as Velocys, RTI International, and TRI, by openly working together, can help move the fulcrum just enough to usher in countless smaller biomass projects, thereby breaking the megaproject mindset.

Considering this decade-plus underperforming context, we believe that we need to go small to go big. It is a market-validated fact that the current thermochemical-to-fuels process configurations will simply not scale down to the circa 150-dry-ton-per-day size, a feedstock-supply size that is widely understood to be one that



# Weighted Project Score: 7.9

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

could be met in countless locales, with multiple feedstock sources. Although these current "first-generation" configurations benefit from years of development and some demonstration, the team of TRI, Velocys, and RTI International have configured an advanced biorefinery to go small based on a key technical breakthrough, coupled with best-in-class gas cleanup, Fischer-Tropsch synthesis (via a modular, microchannel unit), and system-wide process intensification.

This project will leverage the existing commercial, technical, and operational capabilities of both TRI and Velocys to demonstrate this in a four-ton-per-day IBR PDU at the TRI ADC in Durham, North Carolina, which includes both TRI and Velocys systems. The modifications will include the addition of an advanced heater and changes to the gas cleanup system. The project will be validated by performing a continuous, long-duration integrated trial to produce diesel and naphtha and estimating the benefits for a reference 150-dry-ton-per-day biomass-to-diesel commercial plant. The anticipated benefits at this scale are:

- A 25% increase in usable syngas (hydrogen + carbon monoxide [H<sub>2</sub>+CO]) per unit mass of dry feedstock
- A 35% decrease in overall CapEx of the IBR
- A decrease in IBR OpEx so as not to exceed \$2/GGE.

The team has completed successful experimental validation of all the relevant unit operations in Budget Period 1. This included a 31% increase in syngas ( $H_2$ +CO) per unit of biomass, which surpassed the 25% target. Budget Period 2 is in process with the mechanical design of the advanced heater, CO<sub>2</sub> capture unit design, computational fluid dynamics and computational particle fluid dynamics modeling, and simulations and validation of data from Budget Period 1. The simulations indicate a 28% improvement in syngas ( $H_2$ +CO) yield per unit mass of biomass over that for the first-generation gasification system; this, again, surpasses the 25% target. NEPA documentation and permitting are nearing completion.



Photo courtesy of ThermoChem Recovery International, Inc.

#### OVERALL IMPRESSIONS

- This project continues to advance the promise of microchannel reactor development, which promises costs reductions in CapEx and OpEx when compared to traditional technology deployment for Fischer-Tropsch liquids products.
- This is a well-managed project focused on targeted improvements in gasification to address obstacles identified in first-generation technologies. Initial results showed strong validation of modeling with pilot operations.
- This project is trying to leverage process intensification to increase syngas yields per unit of biomass feed by the integration of an advanced heater, novel processes for the removal of CO<sub>2</sub> and syngas contaminants, and a novel microchannel Fischer-Tropsch reactor from Velocys. Budget Period 1 validation has been successfully completed, and now all the process components are being demonstrated to complete the remainder of the project.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their thoughtful comments and insights. We agree.

# PILOT-SCALE ALGAL OIL PRODUCTION

# **Global Algae Innovations**

## **PROJECT DESCRIPTION**

This project will scale up the advanced open raceway algae cultivation and processing technology developed by Global Algae Innovations (GAI) to design a pilot-scale algal biofuel facility for construction in the Imperial Valley of California. The project team includes the California Center for Algal Biotechnology at the University of California, San Diego and TSD Management Associates.

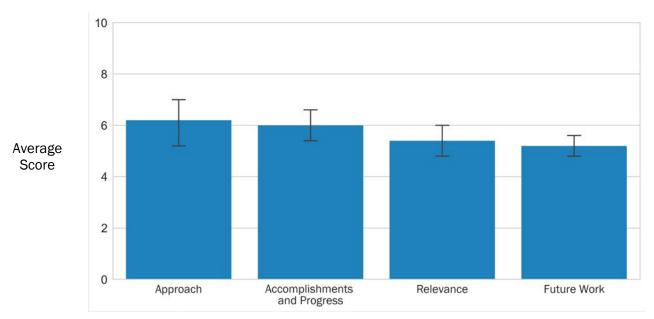
| WBS:                      | 3.4.1.22            |
|---------------------------|---------------------|
| CID:                      | EE0007965           |
| Principal Investigator:   | Dr. David Hazlebeck |
| Period of<br>Performance: | 1/15/2017-6/30/2019 |
| Total DOE Funding:        | \$1,235,790         |
| Project Status:           | Ongoing             |
|                           |                     |

GAI has developed and demonstrated novel technologies

to improve every process step in the algae production process. The technology includes massively scalable open raceways with cultivation innovations that attain triple the productivity of conventional raceways; the Zobi harvest system that achieves 100% harvest efficiency with  $1/100^{th}$  the energy use of centrifuges; a suite of contamination control innovations that enable stable, large-scale open raceway cultivation; and a CO<sub>2</sub> supply system using power-plant flue gas. All these technologies have been validated at the acre scale, and this project will provide the opportunity to validate them at the pilot scale for algal biofuel production.

## Weighted Project Score: 5.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



I One standard deviation of reviewers' scores

#### OVERALL IMPRESSIONS

- It is not clear that this project advances the state of the art.
- This project needs a backup financing plan.
- This project is in the early stage and appears to be based on historic technologies that did not prove to be economically viable. It was unclear from the presentation and questioning of the presenter what will be different about this process. The goal of being profitable is overly aggressive and unlikely to be achieved.
- Although this project shows potential, the focus on building and operating a self-sustaining ("profitable") pilot plant has tremendous potential to distract from completing the necessary work. Pilot plants by their nature are too small to yield commercially viable cost of goods sold (COGS). Even if the goal is to charge research or access fees to achieve the self-sustaining pilot goal, it appears that the focus will be more on how to engineer and construct something ancillary to the R&D goals here rather than be supportive of them.
- This project is aimed at planning and designing an open raceway algae production facility to produce about 10 tons per day of algae, which could be commercially viable. Good effort has been made to identify the right technologies and equipment to reduce the technology risks. It appears that without significant government investment (>50%), it is unlikely that this technology will become commercially viable.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The technology suite being scaled includes dozens of radical advances resulting in at least an order-ofmagnitude cost reduction every process step. This project is the first scale-up effort for such an innovative process that is projected to be economically viable for algal-based commodities; thus, developing a pilot-scale design for these innovative technologies will greatly advance the state of the art for algal biofuel production.
- Financing is very important; thus, a business assessment and preparation of a business plan are a significant part of the project, and the design basis includes versatility in the selection of products to provide greater flexibility in options for backup financing plans.
- This project includes multiple advances that lead to order-of-magnitude cost reductions in each area of algae production. A few examples include (1) a 99% reduction in the inoculum size through open raceway contamination control; (2) a 90% cost reduction and 14-fold increase in flue gas carbon capture and use; (3) a raceway design that increases productivity threefold, reduces energy use by 90%, and enables a 100-fold larger raceway area; (4) harvesting technology that reduces the energy use by 98% and cost by 93% while attaining 100% capture efficiency and returning crystal-clear recycled media; and (5) an extraction system that reduces the cost by 91% and the energy use by 78%.
- The design objective is a self-sustaining pilot-scale facility to generate the long-term, large-scale data needed to drive investment in a commercial algal biofuel industry. The algal oil produced by the pilot-scale facility will be sold to cover the operating costs. The pilot-scale facility for biofuels will be larger than any of the current high-value algal farms and have much better technology, so the production of moderate-value algal oil products to cover the operating cost is reasonable.
- Full-scale algae production facilities are projected to be commercially viable without government investment. A pilot-scale facility is not economically viable for commodity production, so government investment is needed at this scale. This project includes the preparation of a TEA based on the pilot facility design that demonstrates that full-scale production facilities will be commercially viable.

# HYDROTHERMAL PROCESSING OF WASTEWATER SOLIDS (HYPOWERS)

# Water Research Foundation

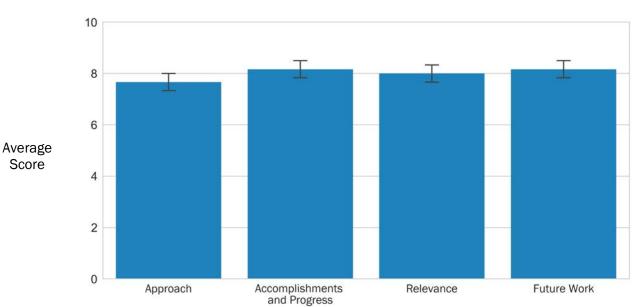
# **PROJECT DESCRIPTION**

The purpose of the HYPOWERS project is to design, build, and operate a hydrothermal processing system to convert wastewater solids into renewable oil and natural gas at an operating wastewater treatment plant. The process has already been demonstrated at smaller scales, but a larger system running continuously in an industrial environment is needed to support full commercialization. The project has attracted intense interest from the

| WBS:                      | 3.4.1.23            |
|---------------------------|---------------------|
| CID:                      | EE0007969           |
| Principal Investigator:   | Mr. Jeff Moeller    |
| Period of<br>Performance: | 1/15/2017-3/31/2019 |
| Total DOE Funding:        | \$803,632           |
| Project Status:           | Ongoing             |
|                           |                     |

wastewater industry because the technology addresses critical problems with specific advantages not provided by other processes. The HYPOWERS project will be located at the Central Contra Costa Sanitary District near San Francisco and will serve a portion of the district's wastewater flow equivalent to a population of approximately 45,000 people. The project is a critical step in the BETO goal to spur creation of a domestic industry for advanced and cellulosic biofuels.

Hydrothermal Processing (HTP) uses temperature (350°C), pressure (200 bar), and water in a continuous process that converts organic material into biocrude oil and natural gas. Typically, between 40%–50% of the dry equivalent mass of feedstock is converted to oil, with another 20%–30% converted to methane. HYPOWERS will produce both oil and gas, with oil output of approximately seven barrels of biocrude oil per day. The biocrude oil can be converted to finished fuels by a conventional upgrading step followed by



## Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

coprocessing with petroleum in an existing refinery. The methane gas can be inserted into a natural gas pipeline after a proven commercial process to remove a small amount of  $CO_2$  from the methane. The overall TRL of HTP is 6, with a goal of achieving 7–8.

The project is structured in two phases. The goal of Phase 1 (the current phase) is to develop a project and business plan with enough confidence and detail to support immediate contracting for construction and operation of the system in Phase 2. Phase 1 will conclude on March 31, 2019. DOE will then evaluate the plan, and if approved, DOE will award funds for Phase 2, concluding in September 2023. The budget for Phase 1 is \$2.4 million, and for Phase 2 it is \$22 million, with the DOE expenditure limited to half of these figures. Phase 1 has 10 team members, and Phase 2 will have the same team members plus two new additions.

HYPOWERS is targeted for wastewater treatment plants (WWTPs), with more than 16,000 WWTPs in the United States alone. The potential world market for HTP systems is approximately \$350 billion. Other organic feedstocks have also been tested and represent large additional potential, including wood, algae, agricultural waste, animal waste, food processing waste, chemical waste, and others. If fully exploited, HTP could produce renewable fuels to replace significantly more than 5% of total U.S. use of petroleum and natural gas for transportation, with corresponding reductions in GHG emissions. The nearest competitor to HTP is anaerobic digestion (AD), but compared to AD, the life-cycle cost of HTP is approximately 50% less while eliminating feedstock solids, which AD cannot do. Government incentives further improve the economics of HTP.

#### **OVERALL IMPRESSIONS**

- Processing biosolids from a WWTP using HTL to produce diesel and methane is being demonstrated in this project at a WWTP. Most process steps have been demonstrated at smaller scale at PNNL and other places. A key technology risk is process integration to obtain cost-effective production of diesel and methane.
- This is an excellent project with considerable opportunity for application and outstanding public (utility) partnership for knowledge and technology transfer.
- This is a valuable project with potential for commercial success and economic viability in regions where suitability incentives exist for favorable economics.
- This project has been well executed both technically and from a project management standpoint. The demonstration-scale unit will still have issues to work out, as noted in the presentation, which is often the case. Financing for the next phase is the main question left. Overall, this is well done.
- This is a well-defined and organized project, following industry best practices for design and scale-up. The size of the team and number of members is a concern, but they appear to be making it work and achieving positive results.
- Although this is still a pilot effort, bringing hydrothermal process technology to a real industrial setting is of extremely high value, and this is a very important project. Actual and forecast economics are not clear from this presentation. Also, some process technology solutions—such as catalytic hydrothermal gasification—might not be amenable to distributed deployment at a relatively small scale. The key question to address is whether the economics of bio-oils—and the potential supply—are such to make the delivery to refiners for centralized processing. This is currently largely unresolved.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# LOW-CARBON HYDROCARBON FUELS FROM INDUSTRIAL OFF-GAS

# LanzaTech, Inc.

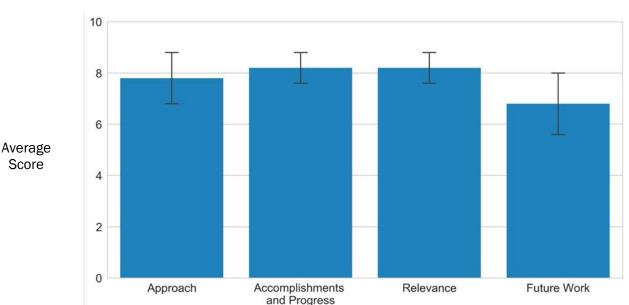
# PROJECT DESCRIPTION

| WBS:                      | 3.4.2.5             |
|---------------------------|---------------------|
| CID:                      | EE0007966           |
| Principal Investigator:   | Dr. Laurel Harmon   |
| Period of<br>Performance: | 1/15/2017-3/31/2019 |
| Total DOE Funding:        | \$3,644,107         |
| Project Status:           | Ongoing             |
|                           |                     |

the International Civil Aviation Organization's Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA), which will require significant volumes of SAF to meet international commitments. Because jet fuel has accounted for as much as 40% of an airline's operating costs in 2013, and 20% today, reducing price fluctuations associated with petroleum is another significant driver.

This will be the first demonstration-scale project on the production of low-carbon jet and diesel fuels from ethanol. The project will demonstrate an entirely new pathway to low-carbon fuels from industrial waste and biomass, with the potential to create significant jobs and revenues in both agriculture and manufacturing.

Since the proposal, LanzaTech has commercialized its gas fermentation technology to produce an ethanol intermediate ("Lanzanol") from industrial off-gas. Therefore, the project is now focused on demonstrating the alcohol-to-jet (ATJ) process developed by LanzaTech and PNNL to convert ethanol to jet and diesel. The synthetic paraffinic kerosene from this pathway is now qualified for use in commercial aviation at blends of up



## Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

to 50% with conventional jet fuel. The facility will be located at LanzaTech's Freedom Pines Biorefinery in Soperton, Georgia. The demonstration will model commercial ATJ production, in which ethanol from multiple sources is processed in a larger, centralized ATJ unit.

An engineering-procurement-construction company is providing the design and engineering services, and other partners are providing catalyst and technology services. Michigan Technological University will conduct LCA of the integrated process. Engine manufacturers will support the project by evaluating fuel properties and advising on fuel registration and logistics requirements. To demonstrate process versatility, Aemetis, Inc. will supply cellulosic ethanol from a unit under development to produce ethanol via fermentation of biomass syngas, and qualifying ethanol feedstocks will be sourced from other suppliers. The primary fuel product will be sustainable aviation fuel, with some diesel production. Preliminary LCA shows more than 60% reduction in GHG emissions from this new fuel compared to fossil jet fuel with competitive costs of production.

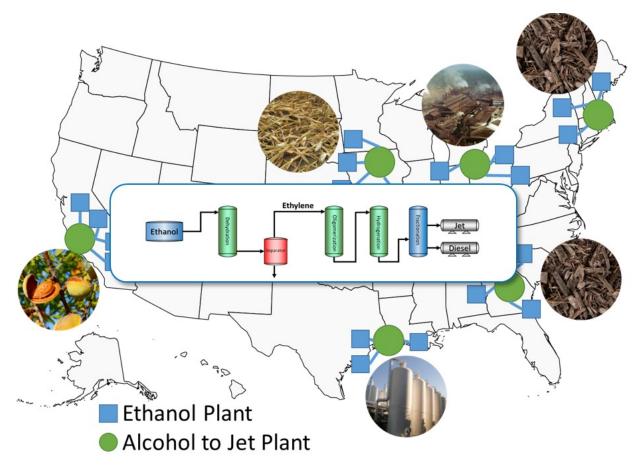


Photo courtesy of LanzaTech, Inc.

## OVERALL IMPRESSIONS

- This is a worthwhile project with a high likelihood of success that will result in the further penetration of biofuels into the transportation sector.
- Many steps toward commercialization have been or are being approached as part of this project. One key element, besides financing, will be securing the appropriate ethanol feedstock to feed the plant, and it was not clear this is near or "on its way."

- This is a well-managed and technically sound project that has used industry best practices for the frontend loading to develop a project that can be financed from a technical perspective. The feedstock is based on the limited resource of cellulosic ethanol, which generates concern about the economic viability of the project.
- Most unit operations (ethanol to ethylene, fractionation, gas fermentation, etc.) for this process are already commercially proven, so a focus on the core oligomerization process is key here. Identifying a green source of hydrogen is going to be critical for any commercial scale.
- LanzaTech is developing a production facility to produce 10 million gallons per year of jet and diesel fuel. This project is aimed at planning and designing this facility. Significant progress was made in selecting a production site, obtaining environmental permits, and negotiating ethanol supply and product offtake agreements. Most technology risk was mitigated by having an operating plant in China, which started in May 2018.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the positive feedback.
- LanzaTech is interacting with its own network of contacts with suppliers as well as with producers that are developing projects to produce qualifying ethanol.
- We appreciate the evaluation, and we certainly recognize that existing supplies of ethanol produced via enzymatic hydrolysis are limited. In 2018, 8.16 million gallons of cellulosic ethanol were available in the United States, 1.62 million of which were imported. That said, there are multiple indications that supplies of cellulosic ethanol are increasing: (1) multiple companies are commercializing corn kernel fiber ethanol technology, which can be integrated with existing corn ethanol facilities to produce cellulosic ethanol with a total U.S. potential of 450 million gallons; (2) Aemetis is building a commercial-scale gas fermentation facility to produce 12 million gallons of cellulosic ethanol per year from the gasification of residual biomass; (3) LanzaTech is working with other customers to develop additional cellulosic ethanol projects based on gasification and fermentation; and, finally, (4) LanzaTech is working with industry partners to develop regional supply chains of advanced (i.e., nonfood) ethanol from novel resources. The combination of these existing and potential sources will be enough to supply this project.
- The hydrogen requirements for ATJ pathways are significantly less than the requirement for other sustainable aviation fuel pathways. Although "green" hydrogen would further reduce the life-cycle GHG emissions of the final jet and diesel products, favorable emissions reductions have been calculated using merchant hydrogen or dedicated hydrogen production via steam methane reforming or electrolysis.

# ADVANCED BIOFUELS AND BIOPRODUCTS WITH AMERICAN VALUE-ADDED PULPING

# AVAPCO, LLC

## **PROJECT DESCRIPTION**

The project Advanced Biofuels and Bioproducts with American Value-Added Pulping (ABBA) involves upscaling the patented American Value-Added Pulping (AVAP) pretreatment technology from AVAPCO, coupled with innovative sugar fermentation to mixed alcohols, which are then converted to full replacement liquid hydrocarbon biofuels at the existing biorefinery site in Thomaston, Georgia. The targeted scale is 50 dry tons per

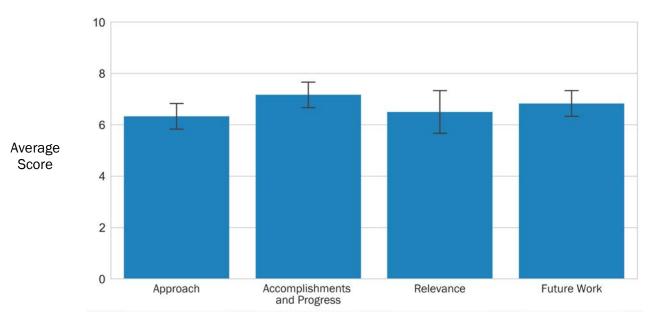
| WBS:3.4.2.6CID:EE0007967Principal Investigator:Dr. Theodora RetsinaPeriod of<br>Performance:1/15/2017-12/31/2019Total DOE Funding:\$3,670,329Project Status:Ongoing |                         |                      |
|---|-------------------------|----------------------|
| Principal Investigator:Dr. Theodora RetsinaPeriod of<br>Performance:1/15/2017-12/31/2019Total DOE Funding:\$3,670,329   | WBS:                    | 3.4.2.6              |
| Period of<br>Performance:         1/15/2017-12/31/2019           Total DOE Funding:         \$3,670,329   | CID:                    | EE0007967            |
| Performance:         1/15/2017-12/31/2019           Total DOE Funding:         \$3,670,329  | Principal Investigator: | Dr. Theodora Retsina |
| <b>.</b>  |                         | 1/15/2017-12/31/2019 |
| Project Status: Ongoing   | Total DOE Funding:      | \$3,670,329          |
|   | Project Status:         | Ongoing              |

day of woody biomass from neighboring sawmill residues and harvesting operations. The coproducts include revolutionary API BioPlus nanocellulose and biobased 1,4-butanediol (Bio-BDO) with project partner Genomatica. Both the nanocellulose and Bio-BDO production will use much of the existing pilot plant.

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 for one hour at 150°C. These conditions dissolve nearly all lignin and hemicellulose without creating unwanted side products. The chemicals are recovered via washing and stripping and 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 one ton per day of dried nanocellulose material. The rest of the cellulose is enzymatically saccharified at a low-enzyme dose to achieve 90% hydrolysis to C6 sugars. One ton per day of C6 sugars are directed to Bio-BDO fermentation and a

# Weighted Project Score: 6.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



One standard deviation of reviewers' scores

purification skid provided by Genomatica. Genomatica's direct fermentation to Bio-BDO is cost-advantaged to the petrochemical route.

The remaining 18 tons per day of cellulosic sugars and 10 tons of hemicellulosic sugars are fermented to produce a mixture of alcohols—namely, ethanol, propanol, and butanol. Remaining lignin and fermentation residuals are burned for process energy. In the hydrocarbon plant, these alcohols are converted to full-replacement liquid hydrocarbons using a catalytic synthesis process that produces petroleum distillate equivalents with overall LCA reduction of more than 60%. Alcohols are dehydrated over catalyst to produce alkenes using the technology from project partner Petron Scientech Inc. Using the technology from project partner Petron Scientech Inc. Using the technology from project partner Byogy, the resulting alkenes are then oligomerized to mixed olefins, which are then further molecularly adjusted to a variety of distilled biofuels, such as jet fuel, diesel, and gasoline. 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 four companies out of 90 under the Federal Aviation Administration's Continuous Lower Energy, Emissions, and Noise Program, in which rigorous engine testing was performed by Rolls Royce that demonstrated Byogy's fuel characteristics showing a premium full-replacement renewable aviation fuel. Byogy's technology is a direct, chemically and thermally efficient route to convert ethanol to jet fuel.

The ABBA process producing cellulosic liquid transportation biofuels with value-added products such as Bio-BDO and nanocellulose is expected to reach the goal of \$3/GGE in commercial applications. The demonstration plant proposed herein is an essential step toward reaching this goal.

The ABBA process is innovative because of the unique integration of the process steps. The AVAP biorefinery can use any feedstock, especially abundant U.S. softwood. Because these sugars have high purity, conversion to ethanol, butanol, and propanol is done fast with high yields. The hydrocarbon plan is unique starting from alcohols.



Photo courtesy of AVAPCO, LLC

#### OVERALL IMPRESSIONS

- This project reflects the development of the biorefinery concept using high-value coproducts to reduce the overall cost of the production of a target biofuel.
- Overall, this project looks promising, and the coproduct clearly looks like a potential means to support the BETO \$3/GGE MFSP. The reasoning for producing a biojet intermediate instead of sticking with cellulosic ethanol is not clear though, and the financial viability of the process is uncertain.
- Time needed for ASTM certification should not be underestimated and needs to be completed on the actual product that is produced in an integrated manner. A "raw jet equivalent" is not proof of a drop-in fuel until it meets certification.
- A sensitivity analysis should be done for the nanocellulose and other coproduct pricing because increased production could reduce the price.
- The project needs verification that the AVAPCO ethanol produced does not have bad actors that affect all the downstream processing.
- Loosening the ethylene production specification seems like it would be best considered when there is a plant that works, rather than beforehand.
- I am unsure how much of the facility is covered under the Front-End Loading Phase 3. Does this include feedstock processing and handling? Feedstock is changing form hardwood to softwood, but no information was given about why the change was made or the expected results with this process.
- This project is well organized and managed with clear goals. The inclusion of key process data performance against key performance indicators was very valuable and showed great progress. Multiple technology vendors combined with multiple changes in project management increases risk, but to date the project appears well managed.
- This is an IBR project to convert cellulosic biomass into ethanol through biochemical conversion and the conversion of ethanol into jet fuel via dehydration and oligomerization and nanocellulose as an additional product. The technical approach is sound and well established. The goal is to do project planning and engineering design of a biorefinery plant processing approximately 50 tons per day of biomass. The project has made good progress and has passed the DOE validation. It is now moving into Budget Period 2.
- The project is built on an excellent technology foundation but is also marred by being shoehorned inside the BETO requirements and the investigators' poor understanding of catalytic upgrading of ethanol and fuel fraction. The authors are misleading by mentioning the drop-in fuels or using terms such as "raw jet" that have no meaning in industry. In reality, they are producing a bioderived aliphatic middle-distillate stream that needs to be upgraded via hydrogenation to fuel specifications. That upgrade—which is technically very doable but economically burdensome—is ignored in all considerations. The conversion of ethanol to jet fuel is a particularly troublesome idea to begin with because one needs to lose considerable mass. In general, producing a highly reduced molecule from an oxygenated compound is likely to be economically unattractive. Further, losses in the oligomerization and the need to have highly refined ethanol make this even less attractive. The economics of this process are driven by nanocellulose, and under these conditions, ethanol is a coproduct that could be sold in the regular ethanol market. This process could bring to the market enough nanocellulose at a price that finally drives the adoption, and in that it is meritorious, but this is outside the scope of BETO.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Producing fuel-grade cellulosic ethanol rather than U.S. pharmacopeia-grade ethanol for biojet fuel is a scenario that can be evaluated in the Budget Period 2 economic analysis.
- The certification of the biojet fuel is a Budget Period 2 activity as noted in the presentation. The production of the raw jet was a Budget Period 1 activity (Milestone 1.5) and should not be confused with the certification of the drop-in biojet fuel final product (Milestone 10.2).
- The AVAPCO ethanol produced from hardwood sources has not contained bad actors that could not be removed in the ethanol purification process. In Budget Period 2, AVAPCO ethanol will be produced from softwood to determine if there are any difficult-to-separate bad actors associated with that feedstock. The need for ethanol purification prior to dehydration was identified at the outset of the project, and it has been incorporated into the process. The purification operation was executed in the validation work of Budget Period 1, and it will be part of the final design.
- The feedstock for the project will be selected based on an economic analysis of the cost of both producing and purifying the ethanol from these two feedstocks.
- The Front-End Loading Phase 3 will cover the entire facility, including feedstock handling.
- The certification of the biojet fuel is a Budget Period 2 activity as noted in the presentation. The production of the raw jet was a Budget Period 1 activity (Milestone 1.5) and should not be confused with the certification of the drop-in biojet fuel final product (Milestone 10.2).
- Hydrogenation is part of the outlined process. It will be demonstrated in Budget Period 2 during the biojet fuel final product production and included in the economic analysis.
- Nanocellulose is indeed a very good coproduct, and it is a major driver in the overall process economics. A scenario of selling ethanol in the fuel ethanol market can be included in the economic analysis of Budget Period 2.

# RIALTO ADVANCED PYROLYSIS INTEGRATED BIOREFINERY

# **Rialto Bioenergy Facility, LLC**

#### PROJECT DESCRIPTION

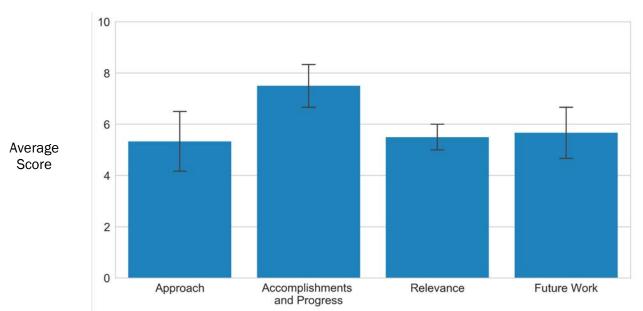
Rialto Bioenergy Facility, LLC, a wholly owned subsidiary of Anaergia, proposes leveraging more than \$150 million in prior investments at its project site to design, build, and operate an advanced, precommercial IBR system that will cost-effectively convert post-AD biosolids from regional wastewater treatment facilities and post-AD food waste residuals provided by Anaheim Energy, LLC into 6.4 MW of low-carbon, renewable

| WBS:                      | 3.4.2.7             |
|---------------------------|---------------------|
| CID:                      | EE0007968           |
| Principal Investigator:   | Dr. Yaniv Scherson  |
| Period of<br>Performance: | 1/15/2017-3/31/2019 |
| Total DOE Funding:        | \$1,999,096         |
| Project Status:           | Ongoing             |
|                           |                     |

biopower. The project will rely on self-generated waste heat to drive an advanced, low-temperature thermal conditioning process that will convert post-AD biosolids and food waste into a digestible substrate for enhanced biogas production. Subsequent AD will produce biogas for combined heat and biopower production. When fully operational, the proposed facility will consume 140 tons per day of post-AD food waste, which is currently landfilled, and 160 tons per day of post-AD municipal wastewater biosolids, which is currently landfilled. The project will use Anaergia's precommercial advanced thermal conditioning processes while demonstrating a novel option for the management of biosolids and residual digester solids. Thus, the project will address a critical need for biosolid mass reduction and ultimate reuse through the production of quality soil amendments (Class A biosolids or better) while producing renewable bioenergy. Through offsetting fossil-based power generation, the project will strongly reduce reliance on fossil fuels while reducing GHG emissions.

## Weighted Project Score: 6.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

# **OVERALL IMPRESSIONS**

- This is a phoenix rising from the ashes of the EnerTech SlurryCarb project. This is an interesting combination of biogas production and pyrolysis for biochar production. The inclusion of the pyrolyzer is a significant advancement in the development of an integrated approach to biosolids processing as represented in this process flow diagram. It feels like there should be an available funding mechanism at the federal level for the integration of TRL 9 unit operations for the sake of demonstrating an optimized system (technologically and/or economically).
- This project is essentially a fully functional AD plant with a pyrolysis back end; given that the entire front end of the plant is a mature, well-proven technology, if financial viability is not proven to be achievable without government assistance then the project has a very slim chance of *ever* achieving commercial success. An evaluation of the issues and dissemination of lessons learned would go a long way toward helping similar future projects.
- The novel nature of the technology was not clear. The removal of pyrolysis from the project leaves a facility that uses proven technologies.
- This project was aimed at designing a facility to process food and other wastes and included a pyrolysis system for biosolids. Basic engineering design was completed, and various permits were obtained. BETO decided not to fund the pyrolysis, so the project went ahead with getting commercial financing without the pyrolyzer. The project is almost complete.
- From a commercial prospective, this is an interesting project, but when limited to the AD component, it is one that can be carried out without DOE support because it is a completely traditional mixed-waste AD project. DOE supports the demonstration and implementation of the pyrolysis of the digestate and subsequent use of the bio-oils inside the digester as an additional carbon source. The authors have demonstrated that bio-oils can be used in digesters—despite their intrinsic toxicity—without ill effect. Although interesting, this is not a completely surprising result because dilution always has a mitigating effect on toxicity. The relevant but unproven statement is about the increase in biogas production and the increase in the value of the residual biochar compared to the original digestate. The authors do not provide any indication to support this fact and whether those benefits are enough to pay the addition of the pyrolytic step. The information is also scant on the proposed implementation of this step.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# LAUNCH OF AN INTEGRATED BIOREFINERY WITH ECO-SUSTAINABLE AND RENEWABLE TECHNOLOGIES IN Y2009 (LIBERTY)

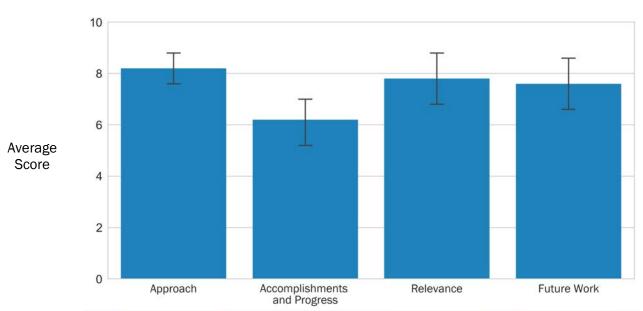
# **POET Project LIBERTY, LLC**

# **PROJECT DESCRIPTION**

Project LIBERTY is dedicated to the development and operation of a commercial-scale cellulosic ethanol biorefinery. The plant is co-located with POET Biorefining-Emmetsburg, an existing corn-based ethanol biorefinery in Emmetsburg, Iowa. The corn-based biorefinery currently has a nameplate capacity of 50 million gallons per year and is one of 27 POET biorefineries. At full capacity, Project LIBERTY will

| WBS:                      | 3.4.3.3              |
|---------------------------|----------------------|
| CID:                      | G018121              |
| Principal Investigator:   | Mr. Mike Dishman     |
| Period of<br>Performance: | 10/1/2008-12/31/2019 |
| Total DOE Funding:        | \$87,844,240         |
| Project Status:           | Ongoing              |
|                           |                      |

produce an additional 25 million gallons per year of ethanol from a feedstock of lignocellulosic material (i.e., corncobs and high-cut material from the corn plant). Corn farmers from the surrounding area supply the feedstock to the biorefinery. The Project LIBERTY business model will enable the rapid deployment of the cellulosic ethanol process across an expansive corn ethanol industry. The rollout of LIBERTY technologies will help the nation rapidly advance toward its biofuels mandates as well as reduce its dependence on foreign oil.



# Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${f I}$  One standard deviation of reviewers' scores



Photo courtesy of POET Project LIBERTY, LLC

#### **OVERALL IMPRESSIONS**

- This project has accomplished a lot in the 11 years it has been underway and deserves significant praise for its achievements since startup. The lack of transparency and clear performance metrics limit the evaluation of success and commercial viability of the technology.
- Project LIBERTY is a showpiece of what DOE/BETO can do with industry participation.
- POET has made significant strides since the last BETO review in terms of uptime and production. Although this meets the BETO requirements from the year granted, it is still disappointing that the knowledge gained might only help POET with the advancement of cellulosic ethanol. POET has done the hard work and likely spent countless extra dollars on this project than was originally planned. What is most impressive is their commitment to this process/project. It is that kind of commitment that brings the technology forward.
- This is an impressive project that is well aligned with BETO program goals. POET-DSM has shown commitment to work through obstacles that have been identified. The project execution appears well organized and managed. Limited technical information was provided supporting reaching the technical goals, and this would have been valuable.
- POET Project LIBERTY is a flagship project to build a plant producing 20 million gallons per year of cellulosic ethanol using 700 metric tons per day of corn stover via a biochemical conversion route. This project started in 2007 and has resumed commercial operation—albeit it still does not meet the availability (uptime) and product yield targets. Continuous improvements are being made to reach the design targets.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# AN AFFORDABLE ADVANCED BIOMASS COOKSTOVE WITH THIN-FILM THERMOELECTRIC GENERATOR

# Lawrence Berkeley National Laboratory

# **PROJECT DESCRIPTION**

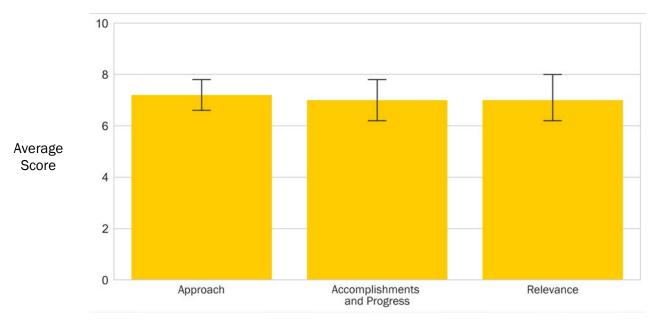
This project aimed at and achieved a technological breakthrough in major emission reductions and performance improvements in natural-draft air-assisted biomass cookstoves. These breakthroughs aligned with DOE goals of helping to reduce emissions from biomass cooking by 90% and fuel usage by 50%. Additionally, knowledge gained during the design, development, and testing was transferred to the cookstove community, by means of conferences and training, to spur innovation, a key component of BETO's mandate. Additional effort was invested to support the standardization of laboratory testing protocols via participation in the International Organization for Standardization and in creating a library of free web-based video tutorials.

| WBS:                      | 5.2.0.1             |
|---------------------------|---------------------|
| CID:                      | NL0026667           |
| Principal Investigator:   | Dr. Vi Rapp         |
| Period of<br>Performance: | 10/1/2015-9/30/2019 |
| Total DOE Funding:        | \$3,000,000         |
| DOE Funding FY16:         | \$0                 |
| DOE Funding FY17:         | \$0                 |
| DOE Funding FY18:         | \$0                 |
| DOE Funding FY19:         | \$0                 |
| Project Status:           | Sunsetting          |
|                           |                     |

Our technical approach for developing the Berkeley Advanced Stove was driven by (1) a design that is economically and aesthetically attractive, safe, and culturally appropriate; (2) an assessment of the current status of advanced technology for thermoelectric generators (TEGs) to produce electrical power with waste heat from the cookstove to drive a fan; and (3) innovative application of advanced combustion concepts of

# Weighted Project Score: 7.0

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



 ${f ar J}$  One standard deviation of reviewers' scores

turbulent and swirl diffusion flames to reduce emissions—all while meeting the constraints of user-centered design within the limits of economically feasible electrical power for the fan (less than 10 W).

We aimed to apply our improvements to the Berkeley-Darfur Stove; which is already a success story of DOE's Technology Commercialization Fund applied to LBNL research. The Berkley-Darfur Stove offers an ideal scaffold for applying these breakthrough technologies because every aspect of its current design is fully understood, and its performance has been thoroughly characterized; therefore, breakthrough technologies or design changes are easily identified. This project has paved the way for novel designs, as well as subsequent manufacture and large-scale sales, of ultraclean self-powered biomass stoves by addressing the key cost and user-acceptance challenges faced by current unsuccessful fan stoves.



Photo courtesy of Lawrence Berkeley National Laboratory

#### **OVERALL IMPRESSIONS**

- This project has shown significant progress and offers value not only to the three billion people who could use the cookstove but also to other organizations doing similar work. The laboratory and test standards developed should be shared to further the overall SOT.
- This project appears to have been executed in a manner that reflects scientific and technical best practices and is well run from a project management perspective. Although the project is clearly a need, it will only reduce emissions and improve health to the level adopted.
- This is a project of questionable value to BETO, given indications that the produced intellectual property is worse in performance than the identified technology baseline, the three-stone fire (TSF), but certainly other funding programs should be interested.
- This is an interesting technology, and the loss of the TEG vendor limited its impact. The team appeared to do their best to meet the intent of the initial goals. End results were unclear and would have benefitted from the team focusing more on process technology and how to overcome them.
- This LBNL project started in 2013 and went through several scope changes. It is essentially finished and now wrapping up later in 2019. The goal was to design an improved cookstove that had 90% reduction in particulate matter. Several designs were evaluated, and significant reduction in the particulate matter emissions was achieved. The knowledge gained was widely disseminated. A state-of-the-art test facility was built at LBNL to test cookstoves.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the feedback, and we agree that the laboratory and test standards developed should be shared. We have initiated this process through peer-reviewed journal publications, reports, and training videos, all of which are available on the website https://cookstoves.lbl.gov/.
- We agree with the reviewer that improvements in health will be realized only if the stove is adopted.
- We respectfully disagree with the reviewer's comment. This project added great value to BETO by identifying scientific underpinnings to reduce harmful emissions from biomass cookstoves and could inform design improvements to wood-heating stoves used in the United States. Additionally, the reviewer is factually incorrect because the produced final product presented demonstrated a 90% *reduction* in particle emissions and nearly *double* the efficiency (approximately 40% thermal efficiency) compared to the baseline TSF, as noted by a comment from another reviewer.
- We agree that the loss of the TEG vendor forced us to pivot from our original plans. The pivot, undertaken in consultation with a DOE funding manager, was successful. We respectfully disagree that "end results were unclear." In fact, the end results have led to major breakthroughs and insights in biomass combustion and ways to reduce emissions from such combustion, which were published in peer-reviewed top journals in the field.
- Thank you. We agree with this accurate and concise summary.

# CONVERTING MSW INTO LOW-COST, RENEWABLE JET FUEL

# Fulcrum BioEnergy

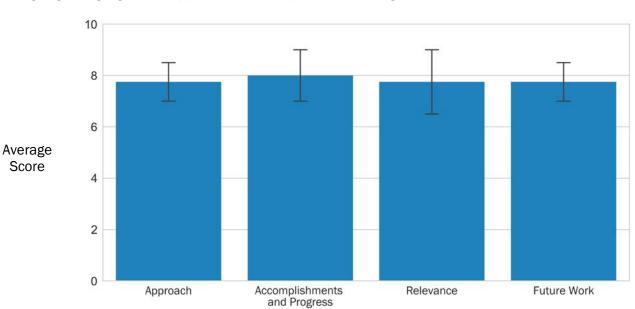
## **PROJECT DESCRIPTION**

The project is currently constructing the Sierra Biorefinery, where a prepared municipal solid waste (MSW) feedstock produced at the adjacent Sierra Feedstock Processing Facility (FPF) will be converted into a low-carbon syncrude. The syncrude product will then be transported to a Marathon Petroleum refinery to be further processed into transportation fuel. The biorefinery, currently under construction, is expected to begin operation in 2020.

| WBS:                      | DPA.1              |
|---------------------------|--------------------|
| CID:                      | EE000DPA1          |
| Principal Investigator:   | Mr. Pete Tiverios  |
| Period of<br>Performance: | 5/1/2013-6/30/2021 |
| Total DOE Funding:        | \$76,600,000       |
| Project Status:           | Ongoing            |

#### **OVERALL IMPRESSIONS**

- It is nice to see commercial-scale projects coming out of the extensive portfolio that BETO has been working on for many years. This project has a lot of potential, but it also made clear that there are issues to be resolved without discussing the plan or path to resolve these issues. The focus going forward should be a clear risk assessment and path to commercial success that is realistic and forward looking.
- This project, long overdue, makes use of a neglected feedstock and is worthy of BETO support.
- This is a well-managed and executed project with key approaches to mitigate risk. The design, based on 120 performance tests combined with bringing the MSW facility online in advance, improves likelihood of the project's success.



## Weighted Project Score: 8.0

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

 ${\mathbb T}$  One standard deviation of reviewers' scores

• This project is a demonstration project to convert 500 tons per day of MSW into Fischer-Tropsch products using a TRI gasifier and a commercial Fischer-Tropsch synthesis technology. This project was started in 2013 and is expected to produce Fischer-Tropsch fuels in 2020. This involves a major scale-up of the TRI gasifier, from the pilot scale to a commercial scale, along with all associated feed systems and downstream ash and syngas handling equipment. Successful demonstration of this project will pave the way for processing MSW into renewable transportation fuels.

## RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# WOODY BIOMASS BIOREFINERY CAPABILITY DEVELOPMENT

# **Red Rock Biofuels**

#### **PROJECT DESCRIPTION**

| RRB was founded in 2011 and is positioned to be the        |
|--|
| leading producer of drop-in, renewable, low-carbon jet and |
| diesel fuels. With broad international agreement in the    |
| aviation industry for carbon-free growth beyond 2020       |
| under CORSIA, airlines are actively seeking low-carbon     |
| jet fuel to reduce their GHG emissions. The civil aviation |
| industry alone will require approximately 1.5 billion      |
| gallons per year of new renewable jet fuel production      |
|  |

| WBS:                      | DPA.2              |
|---------------------------|--------------------|
| CID:                      | EE000DPA2          |
| Principal Investigator:   | Mr. Terry Kulesa   |
| Period of<br>Performance: | 5/1/2013-6/30/2021 |
| Total DOE Funding:        | \$76,600,000       |
| Project Status:           | Ongoing            |
|                           |                    |

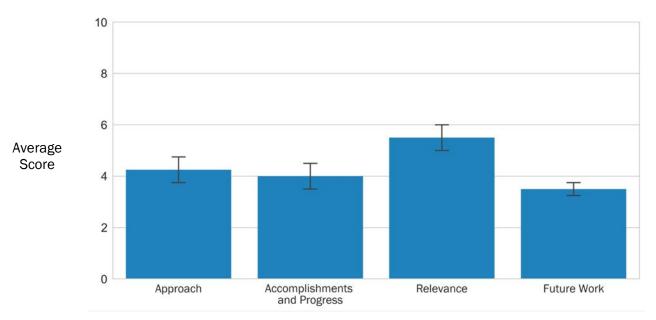
capacity to meet this commitment. The U.S. military has also emerged as a major driver in the renewable jet and diesel fuel markets. To meet these high demands for low-carbon renewable fuels, RRB will build a global portfolio of biorefineries to convert waste woody biomass into renewable jet and diesel fuels.

## **OVERALL IMPRESSIONS**

- This project has great potential, but the presentation gave much less information than expected for a project of this size. Commercial application of these technologies clearly requires the input of government funding, but discussion of the challenges and risks that have prevented industry application and self-financing were neither mentioned nor discussed. Success with this technology is not guaranteed, and the funding recipient needs to focus future efforts on risk assessment and a risk management plan.
- This is probably a project worthy of BETO support, but it is not apparent from the supplied presentation, which was more suitable for marketing and fundraising.

## Weighted Project Score: 4.3

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



 ${\mathbb T}$  One standard deviation of reviewers' scores

- There is no real way to judge on the necessary BETO criteria.
- The project did not follow the required template and provided little technical information to be able to evaluate it. The majority of the presentation was on unrelated wildfire topics. The funding of the project would indicate that major risk items and economics are covered, but without any information provided, it is not possible for a reviewer to provide an informed opinion with any credibility. Verbal discussions indicated that demonstration testing did not meet industry best practices.
- RRB is demonstrating the scale-up of a thermochemical conversion technology to produce 15 million gallons per year of Fischer-Tropsch products in Lakeview, Oregon, using forest residue. The plant construction started in July 2018 and is expected to be completed by the end of 2019. This project will demonstrate the first-time scale-up of TCG's biomass gasifier technology.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

The recipients choose not to respond to the reviewers' overall impressions of their project.

# **CO-OPTIMIZATION OF FUELS & ENGINES**



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# INTRODUCTION

The Co-Optimization of Fuels & Engines (Co-Optima) initiative (or "consortium") is one of 14 sessions reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review. Co-Optima was initiated in 2016 and was previously reviewed at 2017 BETO Project Peer Review. While it is part of the Advanced Development and Optimization (ADO) portfolio, Co-Optima was reviewed in a separate session due to the scope and crosscutting nature of the initiative. In the Co-Optima session, six external experts reviewed nine presentations.

This review addressed a total U.S. Department of Energy (DOE) investment of approximately \$59,000,000 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 6.8% of BETO's portfolio reviewed during the 2019 Peer Review. The principle investigators (PIs) for the FY 2018 Co-Optima DE-FOA-0001919 were invited to present posters at the 2019 Peer Review and reviews are not included in this report. Co-Optima was also reviewed at the 2019 Vehicle Technologies Office (VTO) Annual Merit Review.<sup>1</sup> That review focused on the VTO-funded tasks and projects.

The review panel evaluated and scored projects based on their approach, technical progress, and accomplishments from FY2017 to FY 2019, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the Co-Optima initiative, full scoring results and analysis, the Review Panel Summary Report, and BETO's Programmatic Response are also included in this section.

BETO designated Alicia Lindauer as the Co-Optima Technology Area Review Lead with contractor support from Mr. Robert Natelson (Allegheny Science & Technology). In this capacity, Ms. Lindauer was responsible for all aspects of review planning and implementation.

# **CO-OPTIMA OVERVIEW**

The Co-Optima initiative aims to advance the underlying science needed to develop fuel and engine technologies that will work in tandem to achieve significant efficiency and emissions benefits. This research and development (R&D) collaboration between VTO, BETO, nine national laboratories, and over 20 university and industry partners is a first-of-its kind effort to combine biofuels and combustion R&D, building on decades of advances in fuels and engines.

Co-Optima research is focused on identifying blendstocks that offer efficiency and performance benefits for the entire on-road vehicle fleet, from light-duty passenger cars to heavy-duty freight trucks. The initiative takes a three-pronged, integrated approach to identifying and developing:

- Engines designed to run more efficiently on affordable, scalable, and sustainable fuels
- Fuels designed to work in high-efficiency, low-emissions engines
- Strategies that can shape the success of new fuels and vehicle technologies with industry and consumers.

## CO-OPTIMA SUPPORT OF OFFICE STRATEGIC GOALS

Co-Optima's main goal is to identify the combinations of fuel properties and engine characteristics that maximize efficiency, independent of fuel composition or production pathway, to allow the market to define the best way to blend and provide these fuels. The initiative is pursuing a systematic study of fuel blendstocks

<sup>&</sup>lt;sup>1</sup> U.S. Department of Energy. 2019. "Vehicle Technologies Office Annual Merit Review." https://www.energy.gov/eere/vehicles/vehicle-technologies-annual-merit-review.

(represented as classes of molecular families) to identify a broad range of feasible options. The objectives are to identify blendstocks that can provide target ranges of key fuel properties, identify trade-offs on a consistent and comprehensive basis, and share information with stakeholders.

Co-Optima activities develop the knowledge, data, and tools to expand the blendstock options available to achieve desirable fuel properties. Co-Optima seeks to identify technology options for commercial liquid fuels and high-performance engines powering the entire on-road vehicle fleet (i.e., passenger to light truck to heavy-duty commercial vehicles, including hybrid-electric-vehicle architectures). The aggressive research timeline is structured around researching fuel and engine technologies to the point that industry can consider product development with confidence, setting the stage for commercial introduction of better fuels and engines sooner than otherwise possible without federal support. This will provide an opportunity to create market demand for up to 25 billion gallons of advanced bio-derived blendstocks estimated in a billion-ton biomass economy,<sup>2</sup> diversifying our resource base and providing valuable flexibility to refiners to respond to significant evolving global trends in transportation fuel demand.

While the Co-Optima initiative is jointly funded by the Office of Energy Efficiency and Renewable Energy's (EERE's) BETO and VTO, this review focused on the BETO-funded work. The national lab consortium work was reviewed in a series of five presentations. Four projects selected from the FY 2016 Co-Optima Funding Opportunity Announcement (FOA) DE-FOA-0001461 were reviewed in the session.

| Name                 | Affiliation                                      |
|----------------------|--|
| Harry Baumes*        | Retired, U.S. Department of Agriculture          |
| Charles Abbas        | iBiocat  |
| Cory Phillips        | Phillips 66                                      |
| Kristin Lewis        | U.S. Department of Transportation – Volpe Center |
| Bhupendra Khandelwal | University of Sheffield                          |
| Steven Przesmitzki   | Aramco   |

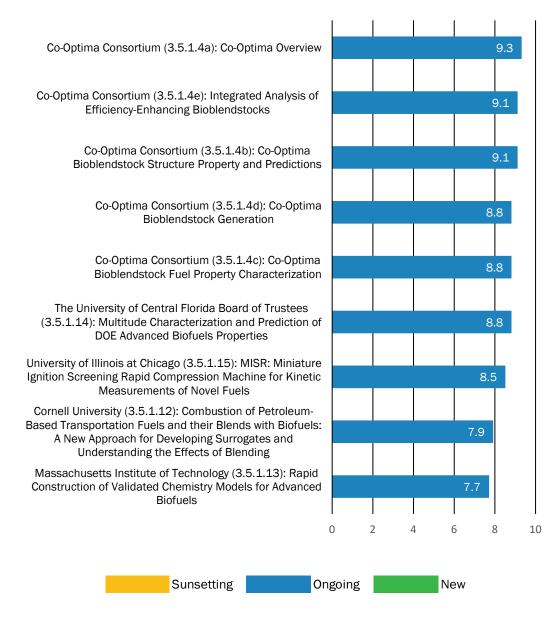
# **CO-OPTIMA REVIEW PANEL**

\* Lead Reviewer

<sup>&</sup>lt;sup>2</sup> Rogers, J. N., B. Stokes, J. Dunn, H. Cai, M. Wu, Z. Haq, H. Baumes. 2016. "An Assessment of the Potential Products and Economic and Environmental Impacts Resulting from a Billion Ton Bioeconomy." *Biofuels, Bioproducts & Biorefining* 11:110-128 (2017). http://doi.org/10.1002/bbb.1728.

# TECHNOLOGY AREA SCORE RESULTS

# Average Weighted Scores by Project



# **CO-OPTIMA REVIEW PANEL SUMMARY REPORT**

#### Prepared by the Co-Optima Review Panel

The Co-Optima portfolio is an important area of work within DOE. The program of work is co-led by BETO and VTO. The program objective is to advance the underlying science needed to develop and match new fuel and engine combinations for greater efficiency and lower emissions. BETO funds a large body of work focusing on biomass-derived fuels and the specific properties required for optimal performance including environmental and economic goals. Specific goals are (1) to identify low carbon fuel/engine combinations that increase fuel economy by 35% (light-duty) or 4% (heavy-duty) over a 2015 baseline, and (2) to achieve environmental performance benefits, particularly by lowering carbon intensity.

The peer review for the BETO-funded portfolio was held on March 7, 2019. The peer review panel was diverse and consisted of six members. The panel heard a total of nine presentations discussing the work; five of the presentations focused on BETO/VTO national lab co-led work: an overview; bioblendstock structure property relationships and property predictions; bioblendstock generation; bioblendstock fuel property characterization; and integrated analysis of efficiency enhancing bioblendstocks. In addition, there were four university research efforts led by PIs from Cornell University (combustion); University of Central Florida (UCF) (characterization and prediction of advanced biofuels properties); Massachusetts Institute of Technology (MIT) (rapid construction of valid chemistry); and University of Illinois–Chicago (UIC) (miniature ignition screening – rapid compression machine). The panel would like to thank the PIs for their innovative approaches, valuable contributions, and presentations. Based on the overall relatively high scoring of the projects, the panel members valued this work.

The national lab co-led projects by BETO/VTO had a strong team with crosscutting technical expertise and frequent team interaction, clear identified goals, and a desire to make work available/accessible to the public sector. Information sharing across labs and with BETO leadership was emphasized. While coordination is a key strength of these five projects, the university led projects do not seem to be as well integrated and linked into the experience and expertise of the national labs.

#### IMPACT

The Co-Optima initiative is working to develop new high-performance fuels, including biomass-derived fuels (identify and characterize fuel properties) that can boost engine efficiency and overall performance and cut emissions when combined with advanced combustion approaches. The 2019 Peer Review is the second peer review for Co-Optima, but the first that work has been conducted over a two-year period, and much has been accomplished. The entire portfolio has the potential to be significantly impactful to the biofuels industry and the bioeconomy in the process of providing/identifying efficiency enhancing bioblendstocks/fuels to technologically advanced engines design and control strategies. As evidenced by the Co-Optima overview and the individual presentations, the eight projects that were reviewed are unique and complementary. Therefore, it is difficult to identify any one project as being more impactful than another. Crosscutting goals are identified, including those that stimulate the domestic economy, create new bioeconomy jobs, and generate clean fuel options.

The Co-Optima portfolio comprehensively addresses identification of candidate bioblendstock molecules, the prediction and confirmation of candidate chemical performance, generation of candidate molecules from biological pathways, and potential for integration as viable and sustainable fuel options that should be further investigated. The approach adopted by BETO/VTO has been designed to execute on unique program areas, and to simultaneously share research results and accomplishments so they can be integrated with the other projects.

For example, the structure-property relationships and property prediction project focuses on chemical structure/property relationships (what is the molecular structure of advanced single-component biofuel

candidates and how are the property characteristics of these single compounds related to this molecular structure). These properties are used to extrapolate or predict the suitability of these multicomponent blendstocks using a broader mixture of individual biomass-derived molecules or molecular families.

This work feeds into the blendstock fuel generation and pathways work by selecting the most appropriate bioprocess to generate the larger volumes required to feed into the fuel property characterization work. Data and databases, models, and other tools have been and will continue to be developed and refined/expanded during the life of the program and made available to other Co-Optima team members, the national labs, and other stakeholders to facilitate and advance future research. Collectively, the work leads to integrated analyses/evaluation of co-optimized bioblendstock and engine technologies from environmental and economic perspectives while conducting R&D guiding analyses (techno-economic analysis [TEA], life cycle assessment [LCA], bioeconomy jobs, economic growth, etc.). Select impactful results are identified below.

The Co-Optima team has developed an approach to the bioblendstock candidate selection process that reduces costs and time to evaluate and assess suitability of blendstocks, enhances likelihood of developing a successful biofuel, and accelerates the time required to bring a bio-blend fuel to market. The Co-Optima team, through a defined filtering approach (tier fuel/desired performance/merit), started with 400 blendstock samples for boosted spark ignition and down-selected to 10 blendstocks for evaluation. This was further reduced to six blendstocks based on merit function scores (and fewest barriers to market).

The blendstock structure/property relationships and predictions and project approach is clearly defined and focused on chemical molecular structure/fuel property relationships to enhance the team's capability to identify potential blendstocks. The team utilizes machine learning and computational chemistry at the quantum level to correlate against a significant number of performance and operability parameters clustered within molecular classes. The approach of property/structure relationship for the fuel blend selection is an important step forward.

The merit objective function for light-duty engine efficiency was developed and is considered to be the most critically advanced engine tuning parameters from a multivariate standpoint allowing objective evaluation and optimization of fuel candidates for boosted spark ignition (BSI), multimode spark ignition (MMSI), and mixing-controlled compression ignition (MCCI) combustion modes. For light-duty engines, BSI and multimode (MM) engine modes, factor such as research and motor octane numbers, sensitivity, charge cooling, burn rate, and emissions are included in the measure. For medium-duty (MD) and heavy-duty (HD) MCCI engine modes, a different set of factors based primarily on fuel properties (e.g. cetane number, flash point, heating value) are weighed.

In the case of BSI, six blendstocks with the highest merit function scores (out of 24 screened candidates) were selected as having the fewest barriers to market specifically with technical readiness, economics, supply logistics, and environmental impact. The merit function has potential to become an industry standard metric in the future, not for fuel specifications but rather for biofuels R&D.

The Fuel Properties Database work has made very important progress. It has been expanded and now includes over 800 compounds and mixtures. The concept of the Fuel Properties Database will be essential for the success of Co-Optima and BETO's Chemical Catalysis for Bioenergy Consortium (ChemCatBio). A fully searchable database with fuel property candidates supplied from multiple labs and researchers has been developed and was used extensively for BSI and MCCI candidate screening. A significant number of analyses have been performed, including on toxicity, levels of partitioning, and biodegradability. The latter two lead to a greater differentiation of the blendstocks than toxicity. The team was able to identify that synergistic effects of blending on spark-ignition (SI) performance are not just due to pure component octane numbers but also due to the ability to shut down the formation of low research octane number (RON) products in combustion. These data are forming the basis of multiple Co-Optima projects doing further investigation of blendstock candidates. The work helps to develop ASTM standards based on interactions identified between fuel effects and

combustion modes. This is critical for deployment and acceptance of fuels by the wider stakeholder community of biofuel manufacturers, distributers, auto original equipment manufacturers (OEMs), and regulators. The team has created the fully searchable Fuel Properties Database that is updated regularly and available online, with over 8,000 users in the last three years. The Co-Optima team will utilize the database for future screening.

The integrated analysis team has completed blendstock review and identified alcohols, olefins, and furans as the molecular families with the most likely high-efficiency candidates. Next, the team reviewed 23 bioblendstocks based on initial screening through the use of the Analysis of Sustainability, Scale, Economics, Risk and Trade (ASSERT) model. The critical challenge of matching diesel energy density is harder than achieving efficiency. One of the most valuable elements of this project is the development and dissemination of many models and tools for the public that are being disseminated on GitHub.

All projects received relatively high scores from the panel members. The projects reviewed by the panel indicate the Co-Optima team is working toward its overall objective by conducting basic research on fuel properties and engines and by developing models, tools, accessible databases, and instruments. The Co-Optima program should have significant impact from dissemination and reporting of research results from the approximate 125 journal articles published and/or accepted for publication, approximate 50 technical reports, and the more than 90 presentations given to multiple venues by team members.

The overview and four national laboratory-led DOE projects tended to be scored higher than the four university-led projects. The range of the average panel ranking between the highest and lowest was 0.55 for the lab-led projects and 1.0 for the university-led projects. Further, no university-led project was ranked higher than any lab-led program. This should not be misconstrued to suggest that the university-led projects are any less valuable or important to the Co-Optima initiative. The lab-led projects are well coordinated and integrated, and this is an area in which the university-led projects could be improved, as identified in the recommendations.

Both the UCF and UIC presented impactful work on the effect of biofuels on engine-parameter-tuning uncertainty as well as, the miniature ignition screening rapid compression machine (MISR) instrument respectively. Both of these projects generate significant, sizeable quantities of relevant data quickly and efficiently while providing statistical analysis on traditional combustion kinetic parameters (e.g., laminar flame speed, soot volume fraction-shock tubes, rate constants, coking volume fraction). This work will be important for hardware design implications with MM, MCCI, and kinetically controlled combustion modes.

#### **INNOVATION**

This Co-Optima portfolio itself is innovative in a sense that the initiative is looking at many fuels, including biofuels (design, synthesis pathways, properties) and engines simultaneously and is focusing on what developing fuels (bio-based) are desired to optimize the advanced engines. This offers a unique opportunity to identify and generate novel bio-based blendstocks that meet chemical, economic, and sustainability criteria. As such, multidisciplinary efforts and resources are required, which calls for a great deal of management oversight and a high degree of integration and coordination among and between the individual projects. The Co-Optima portfolio overall uses an innovative approach to generate new opportunities for biofuel/engine advancement. The component elements are comprehensive and the national lab led projects are well integrated and coordinated. The four university-led projects appear to function independently of the others, but the work is valuable and contributing to the ultimate objectives of the Co-Optima program. The data, tools, and models being developed through the initiative will be valued across the portfolio, by other public and private sector researchers, and by bioeconomy stakeholders.

Many of the projects are utilizing state of the art analytical, informational science, and big data techniques, algorithms, and software to advance the project work and ultimately the Co-Optima portfolio. Computer learning techniques, predictive modeling, and data-mining techniques are examples of tools/software being

utilized and developed. They are using machine learning and computational chemistry at the quantum level to correlate against a significant number of performance and operability parameters clustered in molecular classes. The approach of the property/structure relationship for blend selection is an important step forward. Computational, experimental, chemical kinetics, and machine learning approaches are being used to deliver results. This will eventually help select the right blends.

The blendstock generation project has presented an impressive and clearly laid out approach of combining predictive modeling with retrosynthetic analysis to identify the method of production, then validate the production method. The team is also generating blendstocks for characterization (if unavailable from industry). This is one of the most innovative approaches in the consortium, because it ties the synthesis pathway into the evaluation activities, which is a more holistic approach.

The structure/property and prediction component of the Co-Optima project is crucial to the successful development of novel biofuel options in that it:

- Provides the predictive modeling and validation of blendstock characteristics
- Isolates the effects of specific functional chemical families or groups on fuel properties
- Provides a method for high-throughput screening level analyses of blendstock candidates
- Identifies unexpected structure/property relationships.

The data and models from this project will be extremely useful across the Co-Optima team but also for industry and other researchers. Computational, experimental, chemical kinetics, and machine learning approaches are being used to deliver results. This would eventually help in speeding up the process of biofuels and engines for better efficiency. This is also assisting in taking steps forward for achieving BETO objectives and technology area goals.

The MIT project is developing combustion chemical kinetics models for advanced biofuels to assess and predict potential performance. The approach combines computer modeling generalization to enable new compound analysis combined with real experimental data on fuels/chemistry. For combustion modeling, the key is to identify the most important reactions to include and capture in the modeling framework. The MIT project is world leading because it focuses on creating a machine-learning program to generate reduced chemical kinetics models in batches, rather than the traditional method of developing them one at a time by hand. This would be a breakthrough in the field once successful and widely deployed.

The UIC project is similar in motivation to the MIT project in that it seeks to automate an extremely expensive and time-consuming process, namely running a rapid compression machine. The project has the potential to generate more data in months than the previous body of research in this field did in years, if successful. Combining the results of the UIC and MIT projects could completely change the nature of fuel chemical kinetics modeling and make the current methods look antiquated by generating an order of magnitude more data in the same amount of time.

There are many innovative aspects to the Co-Optima initiative in addition to those technical items identified above. A strong management team is in place. The inclusion of an external advisory board (EAB) provides guidance and insights from various stakeholder perspectives. There is a strong effort to make methodologies, tools, models, and databases available and accessible to the public. The Co-Optima team actively engages with its stakeholders.

#### SYNERGIES

The Co-Optima Overview presentation identified the initiative's objective as, "Advancing the underlying science needed to develop biomass-derived fuel and engine technologies that will work in tandem to achieve efficiency, environmental, and economic goals." As such the individual projects, particularly the five projects led by the national labs, have a great deal of synergies between them. The management structure of each project is similar: team expertise in cross-cutting areas (fuels, vehicle, infrastructure, etc.) for the specific projects, participation by multiple national labs, monthly and quarterly meetings focusing on progress, issues, and reporting to senior leadership (BETO/VTO). In many instances, individual project management members may participate in more than one project. The coordinated design of the Co-Optima projects (see figure to the right, titled "Approach of the Four Co-Optima National Laboratory Research Projects" is highly integrated, with results and accomplishments and feedback flowing from one project to



Approach of the Four Co-Optima National Laboratory Research Projects

another. There is a high degree of synergy; projects rely on similar inputs and tools. What is not clear is if these groups interact sufficiently to ensure good communication and streamlining of efforts to avoid redundancy.

The four university-led projects are more distinct and do not exhibit the same degree of integration with the national labs or each other. There needs to be a better flow of information, results, and accomplishments from the four university-led projects to the other Co-Optima projects, especially information that could be added to databases and modeling.

The review panel supports the national lab-led projects to make data, databases, models, and tools available to and accessible by stakeholders and the public.

#### FOCUS

The Co-Optima program remains compositionally neutral on recommending future fuels. This approach needs to reconcile with BETO's need to satisfy the market with commercially viable fuels. There should be an effort to identify a deliberate driver to seek a natural overlap from both sides, or the overall approach will be inefficient and work will continue to move forward in silos rather than in a community approach.

The structure property relationships and property predictions and the fuel property characterization projects provide a tiered approach to the initial blendstock assessment, the results of which feed into most, if not all, of the other Co-Optima projects. The team has successfully narrowed a large field of candidates to a key set of highly likely candidates, incorporating not only chemical characteristics but also certain environmental performance criteria. Given the importance of biodegradability and low toxicity for these blendstocks for which sustainability and improved environmental performance will be critical, it makes sense to evaluate these blendstock elements as an early screening; these should be part of the Tier 1 screening rather than waiting until Tier 3.

Validation work should continue along with benchmarking against traditional hydrocarbons currently being produced in the refinery to establish precision and accuracy metrics. The structure property relationships and property prediction team has demonstrated the ability to predict synergistic non-linear combustion behavior which is an extremely important capability. The team should continue to provide fundamental insights on such counter-intuitive fuel blending properties or behavior.

The Bioblendstock Generation project team should keep expanding their fuel generation scope within the targeted viable biomass-derived fuel candidate classes by considering blends made up of alcohols, alkanes, and ethers together along with commercial hydrocarbons to form a true fuel matrix. Pure component data are only good to an extent for extrapolation to the blending values, which is what really matters.

Many of the surrogate fuel blends identified will require decades to enter the market, if ever. At least one panelist suggests the program consider having at least one track focused on engines specifically for hybridelectric vehicles (HEVs), since hybrids will be likely the most common internal combustion engine by 2050. For example, a high-compression, lean Atkinson cycle engine running in a very small operation window can exceed the fuel efficiency of an MCCI engine operating over a wide range of speed-load points (per a reviewer's internal analysis from their company). Developing a new fuel for a narrow engine operating range of an HEV may significantly lessen the operating robustness requirements, making the fuel commercialization easier.

The potential barriers to introduce the new fuels (requiring new infrastructure) appear to have been somewhat trivialized. While not really an R&D issue, it should be considered somehow, perhaps as part of the integrative analysis component. This would require more interactions between the ChemCatBio and Co-Optima consortia. Analytical results presented infer a short time is required to bring a fuel to market, whereas it takes several years for approval and development of infrastructure (in some cases). Perhaps some ranking of the difficulty of introducing the fuel nationwide and worldwide could be added to the merit function, i.e., methanol would rank lower than ethanol on market introduction.

#### COMMERCIALIZATION POTENTIAL

The objective (per the Co-Optima overview presentation) of the Co-Optima initiative is to "Advance the underlying science needed to develop biomass-derived fuel and engine technologies that will work in tandem to achieve efficiency, environmental, and economic goals" by identifying low carbon fuel/engine combinations that increase fuel economy by 35% (light-duty) or 4% (heavy-duty) over a 2015 baseline, with reduced emissions. This is a long-term project and although there has been a great deal accomplished over the initial three years of the work, the target date to meet the object is 2030.

The project's value provides foundational knowledge of underlying science to understand and predict fuel properties to stakeholders to improve the value proposition for biofuels. The work that has been accomplished to date, such as the Fuel Properties Database, the merit function, and the retrosynthetic analysis tool, is laying a foundation for the future development of commercially available bioblendstock fuels for advanced light, medium-, and heavy-duty engines that provide efficiency, environmental, and economic benefits.

#### RECOMMENDATIONS

The review panel makes the following recommendations to BETO leadership.

- 1. Better leverage the industry, environmental, and technical expertise of the EAB.
  - A. Review the composition of the EAB to ensure relevant stakeholder industries and sciences are represented.
  - B. Add at least one environmental scientist, biochemist, and explicit fuel and vehicle OEM representative. Appropriate science expertise on the EAB would recognize and improve sustainability criteria (toxicity, biodegradability, miscibility) which need to be moved from Tier 3 to Tier 1 in the review of viable fuels. If a fuel is detrimental to the environment, then it should not be considered as viable.
  - C. EAB should provide guidance on the review and analysis of complex blends.

- i. Explore if the results can feed back to the catalytic conversion work and reduce conversion selectivity concerns.
- 2. Increase engagement with the fuel additive manufacturers (Afton Chemical, Innospec Inc., NALCO Champion, etc.) and other relevant stakeholders (such as potential biofuel producers beyond the existing supply chain of fossil fuels and blenders) for the purposes of resources, perspective, and risk mitigation:
  - A. To study fuel impact on lubricants, ignition improvers, etc.
  - B. Use the additives' engine dynamometer facilities
  - C. Engage commodity processors and leverage new and evolving federal programs.<sup>3</sup>
- 3. Make a Co-Optima landing page with all models and data ready for the public.

# **CO-OPTIMA PROGRAMMATIC RESPONSE**

# INTRODUCTION/OVERVIEW

BETO sincerely thanks the review panel for its time, active engagement, and constructive review of the Co-Optima portfolio. In putting together the panel, it was our hope to welcome a wide range of perspectives, and thus we invited reviewers from the Analysis and Sustainability, Catalysis, and Biochemical Conversion review panels. The value of the diverse panel members' feedback was clear in the thorough comments and recommendations. The praise of the potential value and impact of the Co-Optima work is appreciated. The panel's recommendations will be used to enhance the effectiveness of Co-Optima activities and contribute to BETO's goals.

This was the first peer review where Co-Optima's university (competitive/2016 FOA) projects were presented. It was refreshing to see generally positive scores and comments for the university projects. The issue raised by the panel about an apparent limited engagement between the university projects and the national labs will be considered. Recurring stakeholder calls continue, and the arrangement of the recurring calls has been reorganized to facilitate more direct communication between specific stakeholders. Additionally, the new competitive university projects under the FY 2018 FOA (which, as mentioned, did not present at peer review) each have a specific liaison at the national labs to streamline Co-Optima stakeholder communication.

Reviewers provided feedback on the national lab and university activities. The Co-Optima Leadership Team is working with PIs to address this feedback to strengthen future work plans. The reviewers also provided feedback to the overall Co-Optima initiative, which was organized into three general recommendations. We greatly appreciate these recommendations and are working to incorporate these suggestions into FY 2020 priorities and beyond.

<sup>&</sup>lt;sup>3</sup> One panelist felt BETO's Co-Optima efforts could be enhanced by reaching out to commodity processors of wood products and wood residues, citing that there is an opportunity to tie in with a new presidential initiative for a healthy forest that the Technical Advisory Committee (TAC) is now trying to tackle. With the great abundance of trees in the west and southeast regions (healthy and otherwise) there is a potential there to having significant volumes of feedstocks. With the right incentives, these feedstocks can be tapped into by the Co-Optima team.

# Recommendation 1: Better leverage the industry, environmental, and technical expertise of the EAB.

BETO agrees that the EAB is a critical part of the Co-Optima organization. BETO will work with the VTO and the Co-Optima leadership team to review the EAB composition. Recent additions to the EAB include two new members representing the biofuels industry.

# Recommendation 2: Increase engagement with fuel additive manufacturers and other relevant stakeholders.

BETO will continue working with VTO and the Co-Optima leadership team to prioritize stakeholder engagement, including with fuel additive manufacturers and OEMs.

# Recommendation 3: Create a Co-Optima landing page with all models and data accessible for the public.

BETO agrees with the recommendation and is actively working to make models and data accessible to the public. A revised website was launched in August 2019 that features a searchable and sortable publications database that includes over 150 technical reports, journal articles, conference papers, and presentations produced under the Co-Optima initiative. Additional web content is being developed to highlight models, tools, and data as well as consortium capabilities.

# COMBUSTION OF PETROLEUM-BASED TRANSPORTATION FUELS AND THEIR BLENDS WITH BIOFUELS: A NEW APPROACH FOR DEVELOPING SURROGATES AND UNDERSTANDING THE EFFECTS OF BLENDING

# **Cornell University**

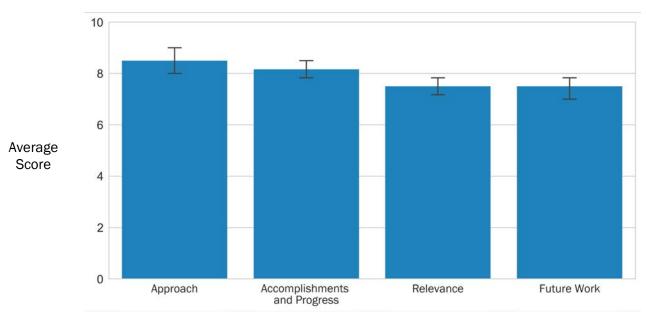
# **PROJECT DESCRIPTION**

The objective of this project is to develop surrogates for petroleum-based transportation fuels and their mixtures with bioblendstocks that are relevant to the Co-Optima initiative, and to determine the combustion kinetic mechanisms of the surrogates to enable numerical tools to predict performance of combustion engines. The project is aligned with MYP barrier ADO-E (Co-Development of Fuels and Engines) by its focus on a generalized

| WBS:                      | 3.5.1.12                |
|---------------------------|-------------------------|
| CID:                      | EE0007978               |
| Principal Investigator:   | Dr. C. Thomas Avedisian |
| Period of<br>Performance: | 1/15/2017-9/30/2020     |
| Total DOE Funding:        | \$1,131,791             |
| Project Status:           | Ongoing                 |

simulation capability that can accommodate co-development of fuels and engines. The project is developed in two parts. The first examines a model biofuel binary blend comprised of heptane and isobutanol. The second part will examine more complex gasoline biofuel blends with the biofuels selected for their relevance to Co-Optima. A binary is the lowest order multicomponent system for a surrogate and is useful to assess the ability to predict mixture effects without complications of developing a surrogate or a kinetic mechanism for the mixture. These latter aspects will be addressed in the second period. The focus is on experiments and simulations with ostensibly known inputs in the first period. The burning configuration is that of an isolated droplet burning with spherical symmetry. This canonical liquid fuel burning configuration is among the very

# Weighted Project Score: 7.9



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%

 $oldsymbol{\mathbb{I}}$  One standard deviation of reviewers' scores

few multiphase configurations that are amenable to detailed numerical modeling, yet also with a strong link to spray flames, which set the initial conditions in combustion engines. It is an attractive burning configuration that is devoid of many complexities of a spray flame, yet which nonetheless captures the inherent unsteadiness of liquid, gas and radiative transport, complex combustion chemistry, and moving boundary effects inherent to a spray flame. Heptane is a component of a primary reference fuel for gasoline and its kinetic mechanism is also sometimes used as a surrogate for diesel fuel; iso-butanol is a biofuel with a comparatively high merit function score from Co-Optima. The combustion kinetic mechanism of the binary is known and the ability to simulate burning is evaluated. In the first period of the project, the OpenSMOKE++ computational code was used with a kinetic mechanism consisting of 225 species and 7,645 reactions that also included unsteady gas and liquid transport, variable properties, and radiative transport. The heptane isobutanol mixture provides a simplified platform to assess the ability to predict mixture burning properties and to simulate combustion without the need to develop a surrogate. In the second period, surrogates for gasoline biofuel will be studied. The tasks will require formulating surrogates and new kinetic mechanisms. Selected burning properties of the petroleum fuel biofuel blends will be incorporated into the process of formulating a surrogate and validating its combustion kinetic mechanism. The presentation at the BETO 2019 Project Peer Review meeting summarizes results obtained to date for the first period. It includes experimental measurements of combustion properties and simulations for the model system.

#### OVERALL IMPRESSIONS

- This project will assist BETO and other government agencies and policy makers in addressing the challenges faced by lack of sufficient understanding of the burning characteristics of new biofuels in blends.
- The analysis of spray geometry is critical to modeling flame combustion characteristics, yet a dearth of information exists in literature. This project deals with this gap by providing single-drop flame characteristics that can be used in common engine modeling tools like CONVERGE CFD. The project team should continue to build out the experiments and show a clear connection to advanced engine design assumptions.
- The team is developing combustion kinetic mechanisms for biofuels. In order to do this, they have already developed a few mechanisms. The team is using a 1-D droplet burning configuration to get an understanding of how biofuels burn and prepare mechanisms accordingly. The appropriate combination of experiments and simulations has been presented in future work. Some risk factors have been considered. All the conventional combustion models are based on a pre-vaporized approach, whereas in this case the actual liquid droplet model is being developed. Development of biofuels combustion mechanisms is important to increase biofuels uptake, which aligns with BETO objectives.
- This project has effectively developed a method to test characteristics of fuel blendstocks and multicomponent blends using a single droplet analysis, which will provide useful data for predictive modeling of fuels and blendstocks being tested at the bench scale. It would be helpful to outline how the outcomes of current work and the results of future work would be disseminated throughout the Co-optima team and integrated into the overall project execution.
- The objective of this project is to develop surrogates for petroleum-based transportation fuels and their mixtures with bioblendstocks that are relevant to Co-Optima, and to determine the combustion kinetic mechanisms of the surrogates to enable numerical tools to predict performance of combustion engines.
- Barriers addressed: Co-Development of Fuels and Engines (ADO-E).

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• A range of combustion configurations are used by a national laboratory and some co-Optima team members to provide data for validating kinetic mechanisms of biofuels and their blends with

transportation fuels. These include shock tubes, rapid compression machines, and jet-stirred reactors to name a few. They share a common element that the liquid phase is eliminated by pre-vaporization and the gas transport process is zero or one-dimensional. Ab-initio models then become viable for simulating the experimental data in a process for validating combustion kinetic mechanisms and associated property databases. However, sprays set the initial conditions for combustion in engines but cannot yet be modeled with this level of detail. Droplets represent the sub-grid element of sprays and are amenable to such detailed modeling. In particular, the 1-D droplet flame is an alternative configuration which the work of this project is designed to show and has value for validating kinetic mechanisms required for engine simulations. The kinetic mechanisms and property databases that result from using 1-D droplet flame data can supplement the configurations noted above by folding into the validation process properties with a direct link to liquid fuels and spray flames. A more stringent test of mechanism validation is then possible by eliminating the liquid phase from consideration.

# RAPID CONSTRUCTION OF VALIDATED CHEMISTRY MODELS FOR ADVANCED BIOFUELS

# Massachusetts Institute of Technology

# **PROJECT DESCRIPTION**

One of the main concepts underlying the Co-Optima initiative is that co-optimization of new fuels with new engines can be greatly accelerated using computer power. In order to do this, one needs accurate computer models for the engine chemistry of each fuel of interest, so one can predict how they will perform under various engine conditions. The main objective of this project is to demonstrate the capability to rapidly generate accurate

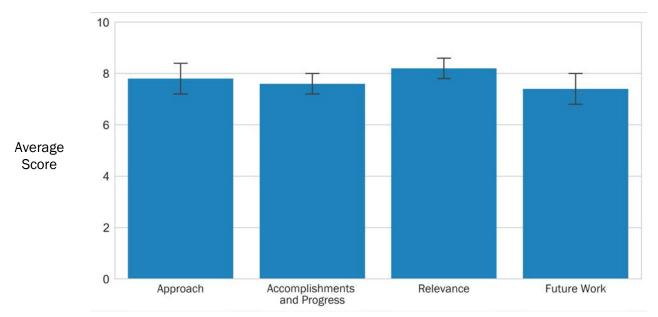
| WBS:                      | 3.5.1.13            |
|---------------------------|---------------------|
| CID:                      | EE0007982           |
| Principal Investigator:   | Dr. William Green   |
| Period of<br>Performance: | 1/15/2017-3/30/2020 |
| Total DOE Funding:        | \$893,427           |
| Project Status:           | Ongoing             |
|                           |                     |

combustion chemistry models for advanced biofuels, using automated mechanism generation approaches and rate parameters derived from quantum mechanical calculations. We validate the new fuel chemistry models by measuring time-histories of combustion intermediates and ignition-delay times in a shock tube, using laser and spectroscopic probes, as well as by comparisons with experimental data measured by others in the Co-Optima team and any other data available. As part of this project, new experimental probes for reaction intermediates and improved biofuel modeling methods are being developed, documented, and disseminated. Some key technical lines of research of this project include:

• Improving the ability to rapidly identify important reaction pathways and intermediates and include them in the computer model, without including unimportant species and reactions that slow engine simulations without improving the accuracy of performance predictions.

# Weighted Project Score: 7.7

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

- Development of suitable laser spectroscopic probe protocols for accurately measuring the time-profiles of low levels of combustion intermediates formed in shock tube experiments. Different approaches are needed at high pressure due to pressure-broadening leading to overlaps and interferences in the spectroscopy.
- Development of methods for accurately accounting for intramolecular hydrogen bond effects on the reaction kinetics of biofuels and biofuel oxidation products. Existing methods for computing rates were developed for simpler molecules which did not have any internal hydrogen bonds.
- Development of combined theoretical and experimental methods for modeling the ignition behavior of fuels which are complex mixtures.

The newly improved and validated capability to rapidly construct accurate computer models for many fuels is being used to develop accurate models for several of the Co-Optima initiative target biofuels. The fuel chemistry models constructed by this project are shared with other members of the Co-Optima program, in particular with those team-members doing engine simulations, making it possible for them to accurately predict fuel effects on engine performance.

Detailed chemical kinetic models will be constructed for several biofuels using an advanced computational approach. The models will be based on mechanism generation algorithms, computation of reaction rates through quantum chemistry, and experimental measurements. The models' predictive ability will be determined by comparisons to additional data.

At the time of this review, about 1.5 years into this ongoing project, we have constructed an apparatus and developed laser techniques to accurately measure the time profiles of the disappearing fuel and the rising reaction intermediates like formaldehyde (HCHO), ethylene (C2H4), and carbon monoxide (CO) even before the fuel ignites. We have also calculated the rates and thermochemistry of many key radicals using high level quantum chemistry. We have also developed new and improved methods for estimating rate coefficients and thermochemistry during automated mechanism construction. We have applied these calculations and methods to construct detailed models for the Co-Optima biofuels cyclopentanone and methyl propyl ether and compared the model predictions with our own experimental measurements and additional data measured by our collaborators.

#### **OVERALL IMPRESSIONS**

- The ability to rapidly construct models predicting characteristics and performance of novel biofuel blend stocks will provide a framework for predictive performance modeling for multiple characteristics that have not been measured experimentally. This project undertakes the model adjustment for characteristics found in biofuel blendstock candidates, such as hydrogen-bonding and complex reactions. If successful, this methodology will save time and resources during the exploration of new chemicals of any kind and should enable more rapid testing of novel fuel blendstocks. A suggested future milestone would be to engage standard-setting bodies (e.g., ASTM) to identify concerns and/or enable use of models to enable new fuel qualification for use. This would be valuable to ensure that novel fuels can be easily adopted.
- The premise of the work seems reasonable to help accelerate the development of accurate kinetic mechanistic combustion schemes with simple, clear objectives like, "pre-ignition species time-profiles are most useful." The work uses a machine learning methodology to help generate kinetic pathways followed by quantum verification in an iterative convergence technique. This really helps simplify and focus the work. The project team provided clear and compelling data describing the way the formaldehyde sensors work. The future engine implications for the experimental early carbon monoxide extinction curves should be stated. The machine learning approach should demonstrate that there are only a number of allowable paths for nature to choose and a systematic way to discriminate between them should be established. The project team should consider Consortium for Computational Chemistry

and Physics resources and other VTO collaborations when exploring the hydrogen bonding issues and effects on the kinetic calculations, as well as, other molecular interactions captured in aggregate constants like activity coefficients to increase the level of rigor. The project team should try to provide a better understanding of flow reactor data as related to internal combustion, real engine dyno-tuning activities and benchmarking with real test blends and primary reference fuels from an OEM perspective. Project lead has a very collaborative approach and ambitious technical approach of modeling first and comparing to experimental data. Several training dataset algorithms should be explored to help tune the models and measure the statistical approach to overfitting, as well as, adjust the hierarchical molecular clusters established for the kinetic pathways.

- The team is doing a good job of coming up with faster mechanisms for biofuel combustion calculations. The project would help make combustion calculations faster for biofuel combustion. Development of biofuels combustion mechanisms is important to increase biofuels uptake, which aligns with BETO objectives.
- The overall objective of the project is commendable; to demonstrate the capability to rapidly generate accurate combustion chemistry models for advanced biofuels and using automated mechanism generation approaches and rate parameters derived from quantum mechanical calculations.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipient chose not to respond to the reviewers' overall impressions of their project.

# MULTITUDE CHARACTERIZATION AND PREDICTION OF DOE **ADVANCED BIOFUELS PROPERTIES**

# The University of Central Florida Board of Trustees

# **PROJECT DESCRIPTION**

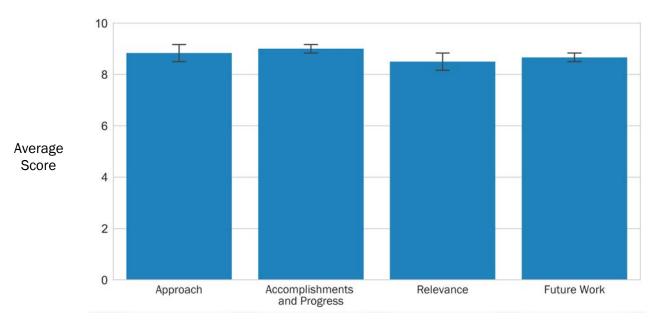
| The goal of this project is to provide a detailed data set of | WBS          |
|---|--------------|
| multiple combustion experiments relevant to the engine        | CID:         |
| combustion of Co-Optima fuels. The data and information       | Prin         |
| for the fuel behavior will mitigate the potential for         |              |
| combustion operability issues due to the particular fuel      | Peri<br>Perf |
| being used. The research project accelerates the              |              |
| introduction of affordable, scalable, and sustainable high    | Tota         |
| performance bio-based fuels for use in high-efficiency, low   | Proj         |
|   |              |

| WBS:                      | 3.5.1.14            |
|---------------------------|---------------------|
| CID:                      | EE0007984           |
| Principal Investigator:   | Dr. Kareem Ahmed    |
| Period of<br>Performance: | 1/15/2017-8/31/2020 |
| Total DOE Funding:        | \$894,336           |
| Project Status:           | Ongoing             |

emission engines thereby achieving the Co-Optima and BETO outcomes.

# Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 ${\mathbb I}$  One standard deviation of reviewers' scores

# **OVERALL IMPRESSIONS**

This project is an important part of the Co-Optima suite of projects by providing the experimental • combustion data and correlation of structural correlation to properties for the Co-Optima blendstock candidates. This project is complementary to the other projects looking at fuel characteristics modeling and prediction. Some of the qualitative characteristics of the fuels (e.g., causticity) are important and should be documented as well.

- This project like several of the others in Co-Optima seeks further understanding through quantitative measurements and development of tools that can used to determine properties of new bio-blends.
- The project lead gave an excellent background on why the experiments are necessary and the approach ties back to OEM engine tuning. Further, this project has important implications on advanced engine design decision thresholds. Essentially this work is trying to solve the classic chicken and egg problem in engine-fuel design optimization by triggering the hardware modification as a result of the degree of approach toward parametric uncertainty thresholds caused by new fuel candidate testing. This is essentially the objective, uncertainty quantification which should involve statistical control charting techniques which is the classic method for measuring uncertainty (laminar flame speed, soot volume fraction-shock tubes, detail kinetics from synchrotron, coking volume fraction). This work will be important for hardware design implications with MM, MCCI and kinetically controlled combustion modes.
- The team is involved in providing a large amount of combustion and fuel systems related experimental data to the Co-Optima members. All the tests which are being done by the team are important for ensuring the compatibility and performance of different fuel blends. Clear plans of future work have been presented with appropriate milestones and these look feasible. Good integration with the national labs. The team has presented that they will test compounds of heavy fuels in the next 18 months.
- The goal of this project is to provide a detailed data set of multiple combustion experiments relevant to engine combustion of Co-Optima fuels. The product that will result from this project is data and information for the fuel behavior that mitigate the sensitivity of the alternative fuels.
- Barriers addressed: Co-Development of Fuels and Engines (ADO-E).

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipient chose not to respond to the reviewers' overall impressions of their project.

# MISR: MINIATURE IGNITION SCREENING RAPID COMPRESSION MACHINE FOR KINETIC MEASUREMENTS OF NOVEL FUELS

# University of Illinois at Chicago

## **PROJECT DESCRIPTION**

This project is a combined experimental and modeling effort with goals of (1) the development of a small-volume high-throughput ignition delay apparatus, (2) the use of that apparatus to measure characteristics of candidate fuels and blends in the Co-Optima program, (3) and the development of mechanistic-based modeling tools to describe and predict ignition characteristics, especially in advanced compression ignition (ACI) engines.

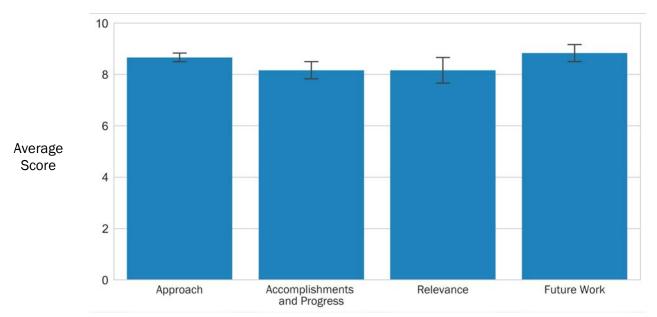
| WBS:                      | 3.5.1.15            |
|---------------------------|---------------------|
| CID:                      | EE0007985           |
| Principal Investigator:   | Dr. Patrick Lynch   |
| Period of<br>Performance: | 1/15/2017-5/14/2020 |
| Total DOE Funding:        | \$518,828           |
| Project Status:           | Ongoing             |
|                           |                     |

In this project, we are building and will use a novel miniature rapid compression machine suitable for highthroughput screening of ignition delay times: the MISR. This device will be used for characterizing properties from very small volumes of low-volatility fuels, less than  $20\mu$ L per experiment. The MISR will operate with high repetition rate (~1 Hz), high repeatability, and can quickly map out a wide range of temperature and pressure conditions.

The modeling effort and analysis tools under development provide kinetic insights from extracting the temperature, pressure, and concentration specific constant-condition ignition delay times (i.e., a chemically based multiparameter map) from the MISR data using an inverse-staged Livengood-Wu integral technique. That complex ignition delay map can be convolved with the state history in other devices, like boosted SI



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

engines and particularly ACI engines to predict ignition characteristics and ultimately search for attractive configurations.

#### OVERALL IMPRESSIONS

- The MISR device for rapid throughput, lower cost blendstock analysis is intended to reduce the volume of material needed for analyses and increase throughput by orders of magnitude. If successful, this device will likely become a highly-desirable approach to analyzing small volumes of material for experimental testing and validation of modeling. It would be helpful to share a clear plan for making this device and/or testing capability available for the rest of the Co-Optima team.
- Once built, operated, and validated, MISR can provide a research tool to test labs on ignition properties of new bioblendstocks and components that is cost-effective and rapid.
- The premise of this work and the goals are exciting and lofty, but extremely important to revolutionizing the combustion characterization and flame diagnostics community, if successful. Here, a high-throughput screening (HTS) approach to running combustion experiments on the order  $10^3/day$  as compared to shock-tube data, which is of the lower order, is at stake. The issue then becomes data management and visualization to guide R&D and kinetic elucidation. If the parameters emerging from these experiments have a 1:1 design impact on MM, MCCI and kinetically control combustion modes, then this could be the path to accelerate the industry. The project has an enormous potential and promise. The project team has to do early benchmark and calibration work to show that this method can predict current and well known measurement methods for performance and prove that it is suitable for ACI. The team has a special expertise and unique hardware design for correlating with advanced engine evaluation rigs. This has long-term potential to enhance or even replace Cooperative Fuel Research (CFR) rigs which continues to be the dream for many stakeholders in the petroleum and automotive industry. The responsibility assignment matrix was clear in the project, and there has been good initial progress in building the operating regime maps. The team has been quite active in the literature, and there appears to be an automation opportunity to process the Livengood-Wu differentials into the activated ignition delay maps. The first step is to successfully build the MISR rig, and this will take time.
- The team is going to develop a new test rig for testing the ignition characteristics of Co-Optima fuels. The approach which is being adopted is new and will use a very small quantity of fuels to complete the testing. The number of tests done within a small duration of time would also increase. This project will indirectly aid in achieving BETO objectives and technology area goals.
- This project is a combined experimental and modeling effort with goals of (1) the development of a small-volume high-throughput ignition delay apparatus, (2) the use of that apparatus to measure characteristics of candidate fuels and blends in the Co-Optima program, and (3) the development of mechanistic-based modeling tools to describe and predict ignition characteristics, especially in ACI engines.
- Current methods for testing the ignition performance of fuel blends are slow, costly, and require large quantities of fuel. The goal of this project is to design, develop, and produce a high throughput ignition screening device capable of quickly assessing the properties of small quantities of fuels and blends.
- Barriers addressed: Co-Development of Fuels and Engines (ADO-E).

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The project is integrated with the fuel properties team and the kinetics small group. We intend to receive direction for various fuels and blends through this group. This structure has worked well for coordinating testing of fuels and blends in the past.

- We agree. MISR targets are at longer ignition delays under low-to-intermediate temperature conditions.
- We agree with all these points. We agree in particular that this will be one of the first truly large data apparatuses for kinetic studies and effort needs to be spent on data management. The team has already developed analysis approaches to interpret and correlate the acquired data with those from conventional large-size apparatus, as well as kinetic modeling methods to further demonstrate the data as useful and novel targets to compare and validate kinetics. With the large amount of ignition delay data, the team has demonstrated a general approach to qualitatively analyze the effect of operating condition and fuel property on auto-ignition in both SI knock and ACI conditions.

# **CO-OPTIMA OVERVIEW**

# **Co-Optimization of Fuels & Engines Consortium**

## **PROJECT DESCRIPTION**

The Co-Optima initiative is developing new highperformance fuels that can boost engine efficiency and cut emissions when combined with advanced combustion approaches. Internal combustion engines using liquid fuels will comprise a significant portion of the nation's vehicle fleet for the next several decades. Advanced combustion approaches have been identified that are capable of significantly improved efficiency and emissions, but new fuels are required to maximize benefits. There is an opportunity to exploit fuel properties and composition to enhance engine efficiency, particularly from biomassderived fuels that offer unique properties in addition to lower carbon-intensity.

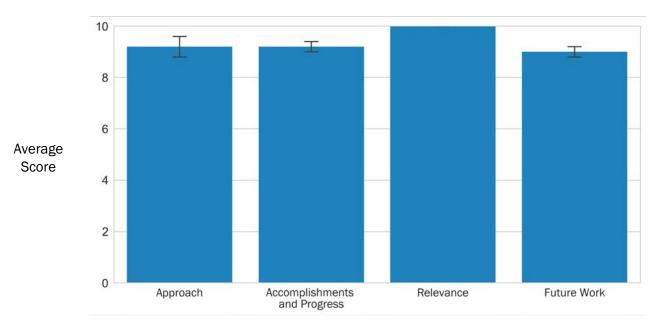
| WBS:                      | 3.5.1.4a            |
|---------------------------|---------------------|
| CID:                      | NL0029892a          |
| Principal Investigator:   | Dr. Daniel Gaspar   |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | N/A                 |
| DOE Funding FY16:         | N/A                 |
| DOE Funding FY17:         | N/A                 |
| DOE Funding FY18:         | N/A                 |
| DOE Funding FY19:         | N/A                 |
| Project Status:           | Ongoing             |
|                           |                     |

The Co-Optima team is composed of technical experts in analysis, biofuels, and engines from nine national laboratories and thirteen universities and funded by two DOE program offices. The team is supported by input and guidance from stakeholders and advisory boards.

Co-Optima is achieving its technical goals by (1) identifying fuel properties and engine operating parameters that enhance engine efficiency and reduce emissions for both light-duty and medium- and heavy-duty engines, (2) identifying high-performance blendstocks that are preferentially sourced from biomass, and (3) evaluating the potential economic and environmental impacts of the adoption of new engines and fuels.

# Weighted Project Score: 9.3

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $\square$  One standard deviation of reviewers' scores

Co-Optima is organized into technical teams possessing specific technical capabilities, with focused, integrated multi-team efforts centered on specific combustion approaches and enabling fuels for light-duty (BSI and multimode approaches combining compression ignition and SI) or medium- and heavy-duty (MCCI and kinetically controlled combustion) applications.

During the first three-year annual operating plan cycle, Co-Optima completed research on BSI fuel-engine technologies. Key outcomes include (1) quantification of fuel property impacts on efficiency, (2) identification of biomass-derived blendstocks imparting these fuel properties, and evaluation of impacts, including technoeconomic, life cycle, refinery integration and benefits analyses. Research octane number, octane sensitivity, and heat of vaporization were determined to be the most important properties for engine efficiency. A series of low molecular weight alcohols, iso-olefins, furans, and cyclopentanone were found to have the highest engineefficiency potential. An analysis of the benefits of adopting engines designed for fuels exhibiting these properties identified significant cost savings through higher efficiency and emissions reductions meeting or exceeding the advanced biofuel standard of 60%.

Co-Optima researchers will finish efforts in MCCI fuels and engines (diesel engines are the commercial example of this general class of engine) at the end of FY 2019. These MCCI efforts have identified key fuel properties including sooting tendency, cetane number, cold flow properties, and energy density. Research is ongoing to better understand how bioblendstock chemistry and properties can be leveraged for emissions reductions benefits in traditional and new MCCI approaches.

MM research builds upon the BSI approach and results and will conclude at the end of FY 2020. Several fuel properties, including octane sensitivity, flame speed, and phi sensitivity have been identified as important and blendstock measurements and evaluations are underway. Finally, nascent efforts in kinetically controlled combustion are underway to determine if reactivity control can be achieved by combining combustion approaches with bioblendstock fuel properties to meet operating and efficiency objectives.

Together, these efforts comprise the Co-Optima team's progress toward enhancing and understanding the value that can be provided by biomass-derived fuels.



Photo courtesy of Co-Optimization of Fuels & Engines Consortium

## OVERALL IMPRESSIONS

- The Co-Optima project uses an innovative approach to generating new opportunities for biofuel/engine advancement. The component elements are comprehensive and well-coordinated, and the tools and models being developed through the program will be valuable throughout the team but also for other researchers and stakeholders. The various tools and resources being developed are not assembled in one location as of yet. The review panel suggested that it would be valuable to create a Co-Optima landing page on the Bioenergy KDF website (http://www.bioenergykdf.net) that brings people to the Co-Optima website and also provides links to all the various tools, resources, and datasets that are being developed.
- Given the promising bioblendstocks identified thus far, it seems likely the team will meet the target of identifying three bioblendstocks that exhibit specific target fuel characteristics, but it may be more challenging to achieve cost parity and greenhouse gas emission (GHG) reduction targets. The team has indicated identification of fuels meeting all these criteria as a go-no-go milestone. However, a "no-go" result, in which the team is not able to identify three molecules that meet these targets, should not lead to abandonment of promising blendstocks or the program necessarily if the fuels provide most of the desired characteristics. The team should have a strategy in place to identify how those remaining characteristics could be met e.g., if only the GHG criterion is not met, how would the team go about identifying better pathways to reduce GHG emissions, or if cost were the remaining barrier, how could/would the team (or other teams in the BETO portfolio) refocus on cost drivers and reduction?
- The project does not want to be a future fuel recommendation tool, but rather a database for physical, chemical, and performance properties. This posture should continue allowing for objective research and analysis to occur while staying mindful/thoughtful of any negative implications on BETO milestones and targets. The program has a strong budget which shows a serious commitment from all funding sources. The portfolio manager on staff to deal with the Work Breakdown Structure (WBS) elements and act as a budgetary oversight along with structured weekly meetings is good. It seems like there is an opportunity in this program to take advantage of predictive software algorithms. Oak Ridge National Laboratory should have some insight on opportunities in this area. The program should continue to engage crossindustry organizations such as, CRC Industries, Southwest Research Institute, SAE International, any other engine OEMs, ASTM International, the U.S. Environmental Protection Agency, and additive companies that operate dedicated fleets. VTO may want to consider purchasing an inexpensive fleet of hybrid-electric vehicles for this work. A renewable lubricant product maybe from LanzaTech should be used in such a project with the same fleet. Multivariate modeling algorithms could take engine performance and correlate it back to molecular structure to design fuel-appropriate fuel molecules. Make sure to include baseline data showing what the merit function is for conventional fuels. Blending fuel properties are equally as important as pure component properties. Establishing a blending matrix visualization will be a good way to communicate the available blendstocks in future engine applications.
- The project provides an overall view of the Co-Optima initiative. The team is strong and has the right skills to deliver on the project. It is good to see that the team has selected 10 fuel blendstocks to proceed, which is an important step. Strong management structures are in place to make sure the project progresses well and delivers what it is intended to deliver. Technical progress to date has been provided with a clear future plan.
- This project is highly relevant and focuses on needed fuels (bio-based) to optimize advanced engines. As such, there are multidisciplinary efforts and resources required, which call for a great deal of management oversight.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We thank the reviewers for their insights and suggestions and are gratified that the reviewers found Co-Optima to be "fully aligned with BETO objectives and technology area goals," and have "outstanding technical accomplishments," with "a clear plan." The reviewers' assessment that Co-Optima has a strong team with the right skills and a sound management plan and structure, including our advisory boards, gives us confidence in the Co-Optima management approach.

• The reviewers' view that timelines are aggressive is consistent with our intent to provide foundational understanding that can lead to positive market and environmental impacts. Finally, we appreciate and will consider the suggestions to improve dissemination of results, models, and tools; evaluate more blendstocks composed of mixtures; consider biofuel/hybrid electric vehicle engines; and evaluate compatibility, toxicity, and environmental concerns sooner in our process.

# CO-OPTIMA BIOBLENDSTOCK STRUCTURE PROPERTY AND PREDICTIONS

# **Co-Optimization of Fuels & Engines Consortium**

# **PROJECT DESCRIPTION**

The structure-property relationship and property prediction work in the Co-Optima program determines which bioblendstocks will be evaluated by the broader Co-Optima effort. We do so by establishing principles that relate the chemical structure of bioblendstocks to the physical properties and combustion behavior most important in internal combustion engines. We create these structure-property relationships by: 1) evaluating chemical families and a range of structural variants using published data and available predictive tools and 2) determining the underlying relationships that confer certain properties to given structures.

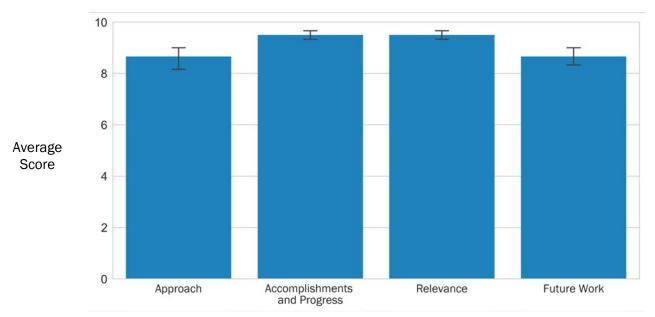
| WBS:                      | 3.5.1.4b            |
|---------------------------|---------------------|
| CID:                      | NL0029892b          |
| Principal Investigator:   | Dr. Anthe George    |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$16,473,000        |
| DOE Funding FY16:         | \$4,993,000         |
| DOE Funding FY17:         | \$4,290,000         |
| DOE Funding FY18:         | \$3,515,000         |
| DOE Funding FY19:         | \$3,675,000         |
| Project Status:           | Ongoing             |
|                           |                     |

We can thereby broadly evaluate if a chemical family is suitable or unsuitable for a given combustion mode. Specific structural variants within suitable chemical families are evaluated in greater detail for important physical properties, and combustion behavior such as research octane number, cetane number, and sooting propensity. This is done by developing and building predictive tools, and by using theoretical chemistry techniques, mathematical models, and machine learning.

Key outcomes have included:

# Weighted Project Score: 9.1

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 ${f I}$  One standard deviation of reviewers' scores

- Establishing important chemical families and identifying bioblendstocks for light-duty BSI and heavyduty MCCI engines
- Transferring data and information to the Co-Optima Bioblendstock Generation, Characterization, and Analysis efforts
- Using the scientific understanding around biofuel properties developed in this activity to inform stakeholders beyond Co-Optima, including other core BETO programs
- Developing tools, methodologies, and understanding of how structure affects properties that can be applied beyond biofuels, to wherever understanding of a compound's performance is required.

We will continue to expand our focus on multimode combustion approaches and kinetically-controlled combustion by applying the workflow developed. Key properties for these approaches are octane sensitivity, phi-sensitivity, and flame speed. More research is being conducted to identify additional key properties for these advanced combustion approaches. This work, conducted to establish structure-property relationships and predict properties of bioblendstocks, underpins fuel-candidate identification and evaluation in Co-Optima.

#### OVERALL IMPRESSIONS

- As a whole, the Co-Optima projects seem to be well thought out and planned. The outcome of their combined effort will provide the necessary analytical tools to policy developers as new biofuels are adopted in the liquid fuel sector and engine designers.
- This component of the Co-Optima project is crucial to the successful development of novel biofuel options in that it provides the predictive modeling and validation of blendstock characteristics, isolates the effects of specific functional groups on fuel properties, provides a method for high-throughput screening level analyses of blendstock candidates, and identifies unexpected structure-property relationships. The data and models from this project will be extremely useful within the Co-Optima team but also for industry and other researchers. The team could consider engagement at ASTM to enable use of these predictive models to facilitate new fuel qualification under the ASTM Committee D.02.
- This underlying premise for this project is notable. It enables both bio and petroleum refiners the opportunity to explore molecular management at a new level. A nuclear magnetic resonance approach to deal with complex mixtures in a high-throughput, small-volume environment was established. This work deals with correlating the properties with the engine performance at the first principles level using a variety of multivariate modeling and machine learning algorithms for HTS. The approach is quite sound and considers the critical parameters responsible for engine efficiency. It appears that there may be an opportunity to develop a compositional-based specification that provides a window of acceptable physical and performance characteristics. Significant progress was accomplished, and validation work should continue along with benchmarking against traditional hydrocarbons currently being used in the refinery to establish precision and accuracy metrics. The opportunity for fuel design also emerges when properties can be correlated down to the quantum descriptors for optimized molecular structures (i.e., MM2 force field). Stochastic approaches can be coupled with it to devise a distribution of molecules that provide aggregate values for the performance parameters of interest. Basically, the fuel is being "built from scratch." The project team has demonstrated the ability to predict synergistic non-linear behavior which is an extremely important capability. The team should continue to provide fundamental insights on such counter-intuitive fuel blending properties or behavior. Collaborations between the other projects that involve large databases is recommended as well (i.e., bio-information project, datahub project, RetSynth). AspenTech should be contacted to include the Statistically Associating Fluid Theory (SAFT) models after they are published highlighting the improvement in accuracy relative to classic activity coefficient theoretical approaches.

- Develop accurate chemical structure-fuel property relationships, and fuel property predictions from these, across a full set of chemical classes and structures. The structure-property relationship and property prediction work determines which bioblendstocks will be evaluated by the broader Co-Optima effort by establishing principles that relate the chemical structure of bioblendstocks to the physical properties and combustion behavior most important in internal combustion engines.
- Barriers addressed: Co-development of fuels & engines (ADO-E) and identifying new market opportunities for bioenergy and bioproduct (At-D).
- Property-structure relationships and selection of blends according to property required is an important approach of the whole Co-Optima initiative. Computational, experimental, chemical kinetics, and machine learning approaches are being used to deliver results. This would eventually help in speeding up the process of biofuels and engines for better efficiency. This is also assisting in taking steps forward for achieving BETO objectives and technology area goals.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

• The recipient chose not to respond to the reviewers' overall impressions of their project.

# CO-OPTIMA BIOBLENDSTOCK FUEL PROPERTY CHARACTERIZATION

# **Co-Optimization of Fuels & Engines Consortium**

## **PROJECT DESCRIPTION**

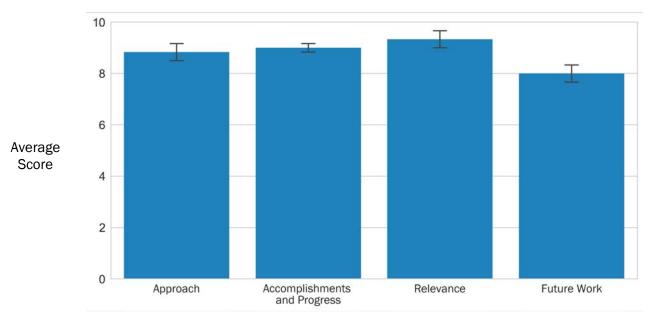
The Fuel Property Characterization (FPC) effort within the Co-Optima initiative focuses on the measurement of critical fuel properties. The goal of Co-Optima is to leverage unique fuel chemistries available from biomass to design more efficient engines, thereby reducing energy consumption and environmental impacts of transportation. FPC supports the on-going efforts of blendstock generation, structure-property relationships, and analysis, through multiple channels. FPC is responsible for the development, expansion, and, maintenance of the Fuel Properties Database (FPD), including acquisition of fuel property data. The FPD was heavily utilized during tieredscreening approaches to rapidly identify the most

| WBS:                      | 3.5.1.4c             |
|---------------------------|----------------------|
| CID:                      | NL0029892c           |
| Principal Investigator:   | Dr. Robert McCormick |
| Period of<br>Performance: | 10/1/2018-9/30/2021  |
| Total DOE Funding:        | \$8,952,000          |
| DOE Funding FY16:         | \$2,252,000          |
| DOE Funding FY17:         | \$1,935,000          |
| DOE Funding FY18:         | \$1,305,000          |
| DOE Funding FY19:         | \$3,460,000          |
| Project Status:           | Ongoing              |
|                           |                      |

promising blendstocks for BSI and MCCI combustion. A key outcome of this endeavor is that it directly led to the identification and more in-depth evaluation of ten of the most promising blendstocks for BSI as well as the initial selection of 12 MCCI candidates for further consideration. Future efforts will also rely on the FPD as a screening tool as additional combustion approaches are investigated. FPC supports analysis efforts through the performance of compatibility and toxicology assessment of promising candidates. Through fundamental experimental measurements in a flow reactor, FPC provides critical feedback to the mechanistic understanding of soot precursor formation and the validation of kinetic mechanisms. These experiments combined with quantum mechanical calculations showed mechanistically why different functional group location could lead

# Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



L One standard deviation of reviewers' scores

to widely varying soot production—even for very similar molecules such as positional isomers. Additionally, experiments are beginning to reveal the chemical basis for non-linear blending effects for octane number which will allow the design of molecules with desired blending octane behavior in future endeavors. The outcomes of these efforts will help ensure that the Co-Optima program can identify fuel-engine combinations which achieve Co-Optima's efficiency, environmental, and economic goals.

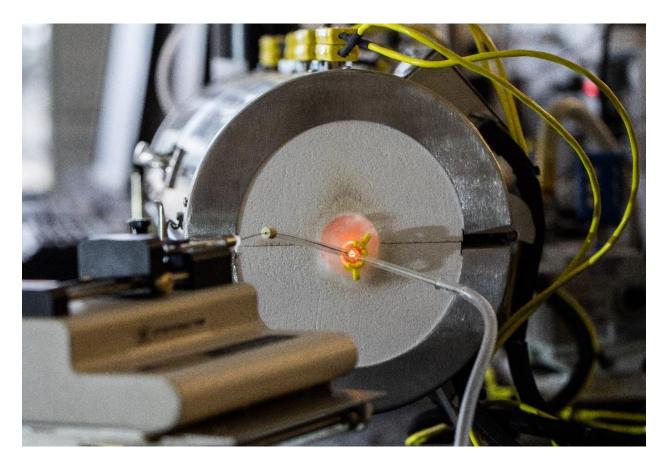


Photo courtesy of Co-Optimization of Fuels & Engines Consortium

#### **OVERALL IMPRESSIONS**

- This research will bring greater application of the existing and alternate biofuels that can be made and blended from the different fractions of biomass. This effort is greatly needed and can help inform the public, policy holders, governmental agencies, and departments as well as the auto and fuel industries.
- This project provides a tiered approach to the initial blendstock assessment, the results of which feed into most if not all of the other Co-Optima projects. The team has successfully narrowed a large field of candidates to a key set of highly likely candidates, incorporating not only chemical characteristics but also certain environmental performance criteria. Given the importance of biodegradability and low toxicity for these blendstocks, for which sustainability and improved environmental performance will be critical, it makes sense to evaluate these elements of the blendstocks as an early screening i.e., these should be part of the Tier 1 screening rather than waiting until Tier 3.
- The FPD has made really important progress. It includes over 800 compounds and mixtures. The team is working with next-level detection methods like vacuum ultraviolet spectroscopy. The concept of the

FPD will be essential for the success of Co-Optima and ChemCatBio. The project team should continue to coordinate efforts with the Bio-Information and Data Hub projects to leverage capabilities. Great progress has been made so far on publishing this database. There was a significant work effort here making blends and testing them. The team should continue to characterize real blends that include ethanol which is the foundational biofuel blendstock. The team should be applauded for looking at the toxicology and health, safety, and environment impacts early, as well as, fluoroelastomer responses. This is good progress. The ASTM outcome with D8076 is a very significant deliverable establishing the original working group and completing the statistics. The project team should make comments on future OEM partnerships and interactions as well as SAE collaboration with groups working on boosted direct injection spark ignition. The analytical scientific progress was evident with results from the flow reactor kinetic modeling showing the soot formation mechanisms in collaboration with the Consortium for Computational Chemistry and Physics team. The project team should consider both thermal oxidative and storage stability characterization opportunities.

- The FPC effort within the Co-Optima initiative focuses on the measurement of critical fuel properties. The goal of Co-Optima is to leverage unique fuel chemistries available from biomass to design more efficient engines, thereby reducing energy consumption and environmental impacts of transportation.
- The approach of providing one online location solution for all fuel properties is good. Interaction of different linear and non-linear properties while mixing is very important and has been covered. The database has been made easily accessible and easy to search. Providing fuel properties in an easy and accessible way is an important part of the Co-Optima initiative, as this helps in quick downselection of the final biofuels to be used. This would eventually help in speeding up the process of biofuels and engines for better efficiency.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their insights, recommendations, and strong endorsement of our project approach that "is clearly defined" and "is crucial for team collaboration and future modeling." We are grateful that the reviewers felt that "this work supports BETO's mission to provide a fuel/engine pair," and that "the relevance to the Co-Optima project is clearly defined."
- Additionally, we appreciate and will consider the reviewers' thoughtful suggestions for improvements to the project which include: potential upgrades to the flow reactor system to function under elevated pressures that are more relevant to real engine operating conditions, a more in-depth assessment of blendstock biodegradability and toxicology earlier in the evaluation process, and improvement of the distribution of information by a centralization of resources.

# CO-OPTIMA BIOBLENDSTOCK GENERATION

# **Co-Optimization of Fuels & Engines Consortium**

# **PROJECT DESCRIPTION**

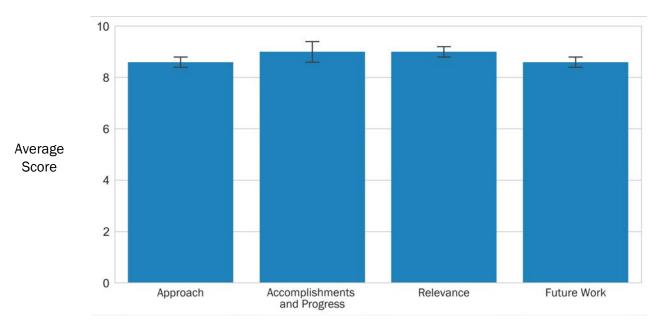
This project is part of the Co-Optima initiative that is working to identify blendstocks derived from biomass that can provide critical fuel properties and assess their benefits and barriers to adoption. The project provides a key function within Co-Optima by addressing gaps in fuel property and conversion knowledge for promising noncommercial bioblendstocks. This is done by (1) generating bioblendstock samples for fuel property characterization and (2) supplying preliminary conversion data for feasibility analysis. Project team members work with input provided by other Co-Optima researchers to determine which chemical families and molecular structures to target for advantaged fuel properties. We utilize in-house

| WBS:                      | 3.5.1.4d            |
|---------------------------|---------------------|
| CID:                      | NL0029892d          |
| Principal Investigator:   | Dr. Derek Vardon    |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$16,473,000        |
| DOE Funding FY16:         | \$4,993,000         |
| DOE Funding FY17:         | \$4,290,000         |
| DOE Funding FY18:         | \$3,515,000         |
| DOE Funding FY19:         | \$3,675,000         |
| Project Status:           | Ongoing             |
|                           |                     |

retrosynthetic analysis tools to help evaluate possible conversion pathways to investigate, and we produce bioblendstocks samples at increasing scales using a tiered approach that is informed by results from fuel property testing and pathway viability analysis. Efforts are coordinated with the BETO Conversion R&D program to ensure a focus on novel production pathways using the latest conversion tools and knowledge base. In concert with other Co-Optima teams, this project addresses the need to (1) provide a framework to derisk and evaluate novel bioblendstocks, (2) develop conversion pathway assessment tools, and (3) inform future conversion targets for the BETO core program. To date, this multi-year effort has generated novel and promising bioblendstocks that address both light-duty and heavy-duty vehicle applications. Key outcomes

# Weighted Project Score: 8.8

Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $\square$  One standard deviation of reviewers' scores

include the (1) development of a scalable algorithm for the retrosynthetic analysis of potential conversion pathways, (2) evaluation of under-explored bioblendstocks with scaled production to validate their advantaged fuel properties, and (3) the development of new bioblendstock production routes for single and mixed compounds that can be tailored based on desirable fuel properties. Moving forward, our approach will be applied to emerging light-duty and heavy-duty combustion strategies that include multimode and kinetically controlled modes of combustion, respectively. Collectively, this project will help ensure the success of Co-Optima's mission for enhancing and understanding the value of blendstocks that can be obtained from biomass.



Photo courtesy of Co-Optimization of Fuels & Engines Consortium

# OVERALL IMPRESSIONS

- This project is innovative and offers a unique opportunity to identify and generate novel bio-based blendstocks that meet chemical, economic, and sustainability criteria. There would also be value in executing predictive modeling on blendstock components from fuel producers who want to get them analyzed and perhaps ASTM qualified. I'm very glad to see that the data and retrosynthetic analysis (RSA) tool have been made publicly available on GitHub. It would be great to incorporate life cycle emissions, sustainability considerations, and economics into the selection process to prioritize the retrosynthetic pathways.
- Overall, the project is very comprehensive with a lot of moving activities, results, and deliverables which at a glance can appear disjointed. However, the mission to tie pathway discovery to advance engine fuel discovery under the same project is not an easy task, and team should be applauded for the breadth of space being pursued in this work. The project team has already shown proof that they can connect feedstock, process, and engine with physical samples. Now, additional resources and project organization efforts should be bolstered to balance out the discovery work with the process design engineering considerations. Significant progress has been accomplished in this project thus far and the amount of hard work given to this point is evident. This is a very large program especially when one has to generate their own blendstocks to study and send to collaborators.

- This research addresses gaps in fuel property and conversion knowledge for promising non-commercial bioblendstocks by (1) generating bioblendstock samples for fuel property characterization, and (2) supplying preliminary conversion data for feasibility analysis.
- The team has done good work towards bio blendstock generation. It is good to see that the team has done a detailed risk analysis of potential options. The team gets information on which bioblendstock is most desirable and can develop the method of producing it. This project directly aligns with BETO objectives and technology area goals.

# RECIPIENT RESPONSE TO REVIEWER COMMENTS

• We appreciate that the reviewers found value in our approach to produce and evaluate novel bioblendstocks. Per the reviewers' suggestions, the project team will continue to assess novel bioblendstock candidates via retrosynthetic analysis and provide samples for fuel property testing and conversion data for production viability. In addition, future efforts will ensure the retrosynthetic analysis tools are publicly available and integrate sustainability and economic considerations. By working closely with the other Co-Optima teams, this effort will help address initial process design engineering considerations for promising bioblendstocks that are identified through the tiered screening process. The team thanks the reviewers for their support of this effort and constructive feedback for project next steps.

# INTEGRATED ANALYSIS OF EFFICIENCY-ENHANCING BIOBLENDSTOCKS

# **Co-Optimization of Fuels & Engines Consortium**

# **PROJECT DESCRIPTION**

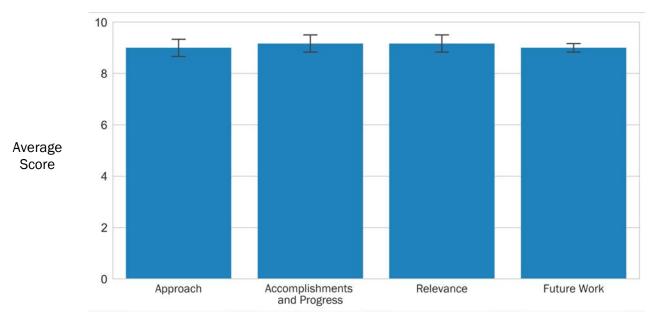
The Co-Optima ASSERT team carries out integrated analysis of efficiency-enhancing bioblendstocks that also reduce emissions. ASSERT supports Co-Optima by evaluating environmental and economic drivers and the scalability potential of perspective bioblendstocks, sharing these key outputs with the teams and stakeholders, and guiding Co-Optima's R&D. ASSERT leverages expertise at the national laboratories in TEA, LCA, refinery modeling, job creation modeling, and modeling of the biofuel industry. The team interacts extensively with other Co-Optima teams to gather data for use in analysis, to receive feedback on analysis parameters, scenarios, and assumptions, and to disseminate analysis results that inform research and development direction.

| WBS:                      | 3.5.1.4e            |
|---------------------------|---------------------|
| CID:                      | NL0029892e          |
| Principal Investigator:   | Dr. Jennifer Dunn   |
| Period of<br>Performance: | 10/1/2018-9/30/2021 |
| Total DOE Funding:        | \$13,270,000        |
| DOE Funding FY16:         | \$3,631,000         |
| DOE Funding FY17:         | \$3,120,000         |
| DOE Funding FY18:         | \$3,394,000         |
| DOE Funding FY19:         | \$3,125,000         |
| Project Status:           | Ongoing             |
|                           |                     |

Initially, ASSERT's focus was on analysis of bioblendstocks co-optimized with BSI engines. ASSERT screened 24 BSI bioblendstock candidates with desirable fuel properties, diverse functional groups, and diversity in production method. Each bioblendstock was categorized as exhibiting favorable, neutral, or unfavorable performance against 17 total technology readiness, economic viability, and environmental sustainability metrics. Isobutanol and aromatic rich hydrocarbons, based on significant technology readiness



Weighting for Ongoing Projects: Approach-25%; Accomplishments and Progress-25%; Relevance-25%; Future Work-25%



 $oldsymbol{I}$  One standard deviation of reviewers' scores

and economic and environmental feasibility, were the subject of detailed TEA and LCA. Furthermore, with a modeling suite customized for Co-Optima that estimates how the vehicle fleet and fuel consumption will evolve with the availability of co-optimized fuels and engines, the team estimated that as an upper bound, considering isopropanol as a bioblendstock at 30 vol%, 12% annual GHG emissions could be achieved in 2050 from the light-duty fleet.

Additional analyses characterized the potential economic value of bio-based blendstocks with favorable fuel properties for BSI engines to refiners. When octane was the only property considered, less bioblendstock than traditional high-octane fossil reformate was needed to boost fuel octane from the standard 88 RON to 95 RON. Furthermore, using actual product compositions from 15 different petroleum refineries in the United States, the analysis showed Co-Optima bioblendstocks would increase the refiners' profitability for every refinery studied.

ASSERT began to evaluate the potential value in pursuing bioblendstocks for the MCCI combustion approach that would limit engine-out emissions of oxides of nitrogen (NOx) and particulate matter (PM). We explored the range in potential aftertreatment device capital and operating cost savings through co-optimization of MCCI engines and fuels with a new modeling tool. We concluded that a smaller diesel oxidation catalyst, a diesel particulate filter, and selective catalytic reduction devices can reduce capital costs and lowering selective catalytic reduction urea use cuts operating costs. In an optimistic scenario, costs per mile for a heavy-duty truck could be reduced by over \$0.50.

Going forward, ASSERT will continue to develop analyses for the MCCI combustion approach as well as for multimode (MM) and kinetically-controlled combustion approaches. This fiscal year, we will screen between eight and 12 bioblendstocks for MCCI or MM combustion approaches and explore the role of co-optimized engines and fuels in vehicles with hybridized power trains. Furthermore, the refinery analysis will expand to include bioblendstocks for MCCI and MM combustion approaches and integrate sustainability considerations.

Overall, ASSERT's research aims to enhance the bioenergy value proposition by identifying scalable, economically viable bioblendstocks that maximize engine performance and energy efficiency and minimize environmental impacts.

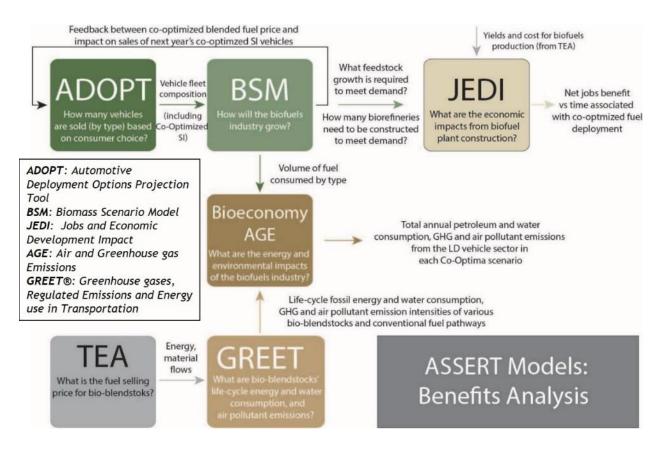


Photo courtesy of Co-Optimization of Fuels & Engines Consortium

# OVERALL IMPRESSIONS

- The Co-Optima approach to bio-blends is relatively new but is necessary in light of the range of potential products that can be derived from biomass carbohydrate and lignin fraction. Looking at ways to develop a tool that integrates LCA and TEA makes a lot of sense as so far these two seem to be treated separately. I applaud the team of collaborators in working together in this effort. Looking at 8–12 potential bioblendstocks also is the right approach to develop sound research on properties and feasibility of these different feedstocks as biofuels. Process inputs can be optimized as more information and research is done and results are made available. The ASSERT approach is comprehensive and BETO should continue to develop such models that can be used to assess the wide range of impacts of increased uses of biofuels and other uses for biomass feedstocks and products derived from biomass.
- This project executes a critical aspect of the highly valued Co-Optima project, which is the screening of potential blendstocks to assess economic and sustainability implications. I strongly agree with the idea raised during the review of using both economic and environmental considerations into the retrosynthetic analysis tool in order to generate the most environmentally-sound production pathway for targeted blendstocks.
- Most existing advanced biofuel processes generate multiple products that are often directed to different markets. There may be value in assessing coproducts as part of this analysis.
- Given the potential to adapt/tweak some of the non-favored blendstocks that the Co-Optima team have identified if they offer other benefits (e.g., improved sustainability, etc.), it would be helpful to know if

there is a strong GHG LCA or other sustainability reason to focus on the slightly lower priority blendstocks.

- This is one of the most powerful projects in the Co-Optima portfolio. The use of Aspen PIMS<sup>™</sup> along with ASSERT (TEA, GREET<sup>®</sup>, JEDI, ADOPT, BSM, BA) provides a realistic scenario on the possible outcomes and benefits to the nation when advanced engines are mapped strategically to high-performing biofuel candidates. This is an extremely comprehensive modeling approach. The team should continue their sound approach of engaging stakeholders. Pipeliners should come to the table (e.g., the Association of Oil Pipe Lines) in conjunction with the U.S. Department of Energy, American Petroleum Institute (API), SAE International, American Chemistry Council (ACC), and ASTM. This will be the "stakeholder village" necessary to increase the accuracy of the modeling scenarios. The project team is already highly collaborative and takes informs from across BETO and VTO.
- The team evaluates the blendstock and vehicle technologies under consideration within the Co-Optima program from environmental and economic perspectives while conducting R&D-guiding analyses.
- Barriers Addressed: Co-Development of Fuels and Engines (ADO-E) and Analysis to inform strategic direction (At-A).
- The team is helping the Co-Optima team complete TEA and LCA. The strategies and methodologies taken by the team to evaluate TEA and LCA are strong. The work of crosscutting teams is good. Their response to last year's reviewer views is good. There is a clear plan of future analysis. Screening of different bioblendstock candidates has been planned, in addition to co-deployment of co-optimized and hybridized vehicles.

#### RECIPIENT RESPONSE TO REVIEWER COMMENTS

Reviewers of the ASSERT team of the Co-Optima initiative found value in the TEA and LCA of bioblendstocks under consideration within the program. Furthermore, the reviewers found the overall ASSERT analysis suite that includes the Biomass Scenario Model, the Automotive Deployment Options Projection Tool, the Jobs and Economic Development Impact model, the Greenhouse gases, Regulated Emissions, and Energy use in Transportation model, the Bioeconomy Air and Greenhouse gas Emissions model, and Aspen PIMS<sup>™</sup> to be powerful and of value to BETO overall. The ASSERT team thanks the reviewers for the affirmation of the importance of the team's work. Per the reviewers' suggestions, ASSERT will continue to evaluate co-product influence on economics and sustainability of bioblendstocks, consider the interplay between biorefineries and petroleum refineries, and engage with additional stakeholders around the quantification of infrastructure costs and evaluation of bioblendstock viability based on infrastructure considerations.

# PROGRAMMATIC EVALUATION AND RESPONSE

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# **BIOENERGY TECHNOLOGIES OFFICE PROGRAMMATIC EVALUATION**

Prepared by the Bioenergy Technologies Office 2019 Peer Review Steering Committee

The Steering Committee was tasked with observing the technology peer review process performed by the technical review panels and with reviewing the Bioenergy Technologies Office (BETO) project portfolio for relevance in developing transformative and revolutionary bioenergy technologies to enable sustainable, domestically produced biofuels, bioproducts, and biopower.

The Steering Committee based its review of the BETO project portfolio on information collected from several resources: plenary presentations that provided the overall context and goals for the portfolio technology areas; direct observations of the different technology area reviews; a closed-door session involving the lead reviewers and discussions between the Steering Committee and BETO management; a review of the BETO *Strategic Plan for a Thriving And Sustainable Bioeconomy* and the draft *Multi-Year Plan* (MYP) for 2019; and supplemental information detailing the breakdown of the types of projects in the portfolio, who is performing the work, and barriers being addressed. We attempted to keep our evaluation focused on issues pertaining to the portfolio and not duplicate comments from the individual technology reviewers detailed elsewhere in this report.

The members of the Steering Committee thank BETO for the opportunity to review the progress and direction of the program portfolio. We are unanimous in our appreciation of the depth of thought and expertise shown by the BETO staff in the program management and incorporation of independent advisor feedback, including the 2017 Steering Committee, and in the development of the multiyear and strategic plans.

The Steering Committee members express their condolences to the family of Don Stevens. Stevens was a member of the 2019 Steering Committee, and he was profoundly impactful during his short time with us. Stevens and his insights will be missed in the bio-industry community.

#### PEER REVIEW OBSERVATIONS

Based on our observations during the Project Peer Review, the project technology review sessions were performed reasonably similarly and fairly across the portfolio and allowed enough time for questions from the review panel; however, minimal time was allowed for audience questions. We noted that the quick pace of the review process did not allow enough time for all reviewers to record their evaluations and suggestions in the review tool. We recommend that BETO allow additional time between individual project reviews for the audience to ask questions and provide time for the reviewers to complete their entries. Also, guidance on slide limits should be given to principal investigator presenters to help ensure that presentations fit into allocated time slots and allow enough time for questions. Reviewers voiced their appreciation for receiving project presentations ahead of time so that they could be better prepared for the review. Reviewers also favored slide content that focused more on the technical approach, data, lessons learned, and results instead of aspects of project management. The preference toward more results-oriented information could be a result of BETO's direction toward more projects with lower technical readiness levels (TRLs) that are focused on research. As discussed in the following sections, however, we believe that the project management information should be enhanced, particularly regarding progress and relevance.

Some review panels had trouble distinguishing between similar projects. It would be helpful to reviewers for similar projects within a technology area to be grouped together and for any complementary relationship or key differences between them to be explained by the BETO lead technology manager. Generally, the panel reviewers were excellent, very knowledgeable, and offered many thoughtful questions. Recognizing that many of the reviewers are taking time away from other commitments, we recommend that BETO consider reducing the significant demand on the reviewers that occurs when preparing for the peer review, during the week of the review, and when preparing feedback after the review by enlisting additional reviewers or downselecting which projects are fully reviewed.

The closed-door program review session was a very useful and informative open exchange between the BETO team and the Steering Committee. It provided a critical forum for frank discussion and nuanced discussion that would not otherwise be possible during the peer review or in conjunction with another public meeting or conference. It worked well as a stand-alone meeting. BETO technology managers comprehensively and satisfactorily addressed the recommendations made in the review panel summary reports and encouraged the Steering Committee to provide feedback in an open and nonprescriptive way.

## LEVERAGING KNOWLEDGE AND COLLABORATION

Based on the amount of work being managed and the expertise and commitment of the BETO staff we observed, it is clear to us that BETO has an exceptional group of people who have a tremendous amount of knowledge and dedication toward advancing the bioeconomy. To supplement the BETO expertise, BETO has been implementing consortia comprising industry advisory boards (IABs) and national laboratories that are dedicated to specific technology areas. The consortia comprise experts who can meet several times per year to discuss progress on projects.

BETO is active in understanding domestic and international markets and drivers for bio-based commodities, in promoting collaborative efforts to harmonize domestic and international codes and standards and regulations for alternative fuels, and in fostering responsible sustainability practices and metrics. On a project level, we identified several individual projects that brought in international resources to help with specific technical issues. We believe it is appropriate that the individual projects identify and collaborate with international experts and for BETO's international role to be focused on understanding markets and regulations to aid in directing U.S. bio-industry efforts. On a domestic level, it was clear that BETO works closely with other relevant agencies, such as the U.S. Department of Agriculture, National Science Foundation, and the U.S. Environmental Protection Agency (EPA). An example of this is the initiative taken by BETO, with EPA, to develop and approve an analytical pathway to cellulosic ethanol renewable identification numbers for starch ethanol plant residuals. BETO has a strong history of developing standardized methods that have been widely accepted. BETO has shown to be a leader for federal interagency collaboration and coordination on bioenergy and bioproducts research. BETO played a strong role in the development of the Biomass Research and Development (BR&D) Board's Bioeconomy Initiative: Implementation Framework, which is now guiding and coordinating research at BETO and among numerous other key federal agencies and offices. BETO has also demonstrated strong collaboration with other U.S. Department of Energy (DOE) offices within the Office of Energy Efficiency and Renewable Energy (EERE), Office of Fossil Energy, and Office of Science. The Steering Committee recommends that BETO continue to communicate and showcase its intra- and interagency work at future peer reviews.

#### COMMERCIAL RELEVANCE AND MARKET TRENDS

In 2018 and early 2019, several firsts occurred, and some bold announcements were made. Expanded and distributed electricity generation and vehicle electrification are some of the energy transitions anticipated in the coming decades, and they demonstrate a growing movement away from coal- and petroleum-based liquid fuels, whether or not the specific commitments are fully realized. Such trends are likely to impact the BETO portfolio, but other end-use areas, such as air and marine transportation, might require different approaches to reduce their carbon footprint, including bioenergy. A few of the milestones and trends we noted include:

- BETO supported a major milestone in sustainable jet fuel for commercial aviation: the first commercial flight (a Virgin Airlines Boeing 747 from Orlando, Florida, to London, England) using fuel from recycled waste carbon.
- Increasing numbers of U.S. states have pledged to become carbon neutral or carbon free and are codifying a commitment to renewable energy sources. Action at the state level to remove greenhouse gas emissions from the electric grid is becoming increasingly common.

- Such policies have the potential to reshape local/state energy sectors with wind and solar but also technologies employing carbon capture and reuse, sequestration, or storage.
- Major automakers—such as the Volkswagen Group, Toyota, Nissan, and Honda—have committed to achieving 90%–100% carbon neutrality by 2050, in large part by producing only battery electric and/or fuel cell electric vehicles (EVs). Volvo announced that every vehicle produced from 2019 and beyond will involve some level of electrification, and the company has set a goal for 50% of sales volume to be fully electric vehicles by 2025. Some countries—such as India, France, the United Kingdom, and Norway—are making bold statements about transitioning from internal combustion to fully EVs. BETO's programmatic expansion to include more diverse biomass sources, bioenergy alternatives, and diverse end-use markets is consistent with current trends, including increased electrification of the light-duty vehicle fleet. It will be important that energy generation and energy storage from clean and renewable sources matches increased demand.
- New applications of algae and lignin are exciting and have the long-term potential to increase the profitability and sustainability of technologies formerly focused only on bioenergy generation. Although new markets and products take time to establish, these are technology areas where BETO has taken a lead in recent years. In the lignin area, a diverse group of projects is addressing the use of lignin in composite form and as isolated components.

Recycling and reuse of plastics continues to have popular support, and both local and national governments are introducing policy initiatives, such as various restrictions on single-use plastics. New solutions are needed, and the background technology that BETO brings is well positioned to contribute to this difficult problem.

BETO has an important role in translating renewable energy technologies in relation to incumbent technologies for policymakers and the public. The transformative work being funded by BETO should be championed in the public forum. BETO has the "basic data" and expertise to infuse the advanced fuel conversation with fact-based comparisons of life cycle assessments, economics, job creation, and sustainability as an economic opportunity for rural America to participate in generating domestic energy security. BETO-supported technologies and approaches can generate income for farmers, provide an outlet for forest residues (fire-prone states are ramping up their forest management practices), and diversify municipal waste disposal options.

# **DIVERSE PORTFOLIO**

As part of the review process, the Steering Committee was asked to review the mix of projects in the BETO portfolio. During the 2013, 2015, and 2017 peer reviews, the number of projects reviewed was between 190 and 277, representing total DOE investments of between \$400 million and \$1.6 billion, depending on the review cycle. The 2019 Project Peer Review included 447 projects across five technology areas, representing a combined DOE investment of nearly \$860 million. This is an extraordinary number of projects, and the increase in 2019 was a result of the inclusion of projects not previously reviewed or presented in poster sessions, including related projects that are not managed by BETO, as well as the recent emphasis of BETO to focus on smaller research-and-development (R&D) projects instead of larger demonstration or pioneer projects.

The 2019 project breakdown by participant included:

- 13 projects conducted by research institutions (representing 3% of the portfolio)
- 58 by academic institutions (representing 13% of the portfolio)
- 84 by industrial companies (representing 19% of the portfolio)
- 292 by national laboratories (representing 65% of the portfolio).

Additionally, there were 333 annual operating plan (AOP) projects led by the national laboratories and managed by BETO. The AOP projects addressed 55 of BETO's 59 identified barriers. The four barriers not addressed were (1) investigation into the productivity and robustness of energy crops, (2) characterization of energy crop production, (3) development of selective harvesting machines, and (4) development of algal harvesting technologies. In addition, the AOP projects addressed 25 of the 33 BETO milestones listed in the draft 2019 MYP. There are another 55 projects not directly related to any single milestone but are considered to be enabling, analysis, or emerging technology projects. It was apparent to us, however, that at least some technical barriers not being addressed by the AOPs are addressed through BETO's Fiscal Year 2019 funding opportunity announcement (FOA) process, but the full analysis of the most recent FOA projects was not yet available at the time of our review. In addition to the projects presented, we reviewed the draft 2019 MYP and found it to be an excellent resource to aid in understanding the focus of BETO, development of the technical pathways, and programmatic milestones.

We reviewed the number of projects and planned spending for the identified technical barriers. In general, we believe the research supports the key areas in a biomass-to-bioenergy supply chain. Barriers with the least number of projects and planned spending are appropriately on the low end of priorities. Additionally, the two technical barriers with the most projects (82 total) are appropriately focused on increasing the product and coproduct yields from biological and catalytic processes. These two technical barrier descriptions are broad and contain many different topic areas. We believe that the large focus on these areas is appropriate; however, we found that our brief exposure, the number of projects, and the variety of technologies employed made it difficult to grasp the full scope of BETO's portfolio and to offer a further opinion on BETO's priorities in overcoming technical barriers.

We recognized a consistent theme from the preceding and current peer review panels inquiring into how BETO measures progress and how is it reported; how projects are chosen to be funded; which issues justify parallel efforts; where efforts are being unnecessarily duplicated; how work is being leveraged among participants; and whether the assumptions across the different projects are consistent in reporting costs, product values, risks, market sizes, environmental benefits, and progress. Past and present panels have recommended that BETO incorporate standard measurement and reporting tools for all portfolio projects, such as the use of Work Breakdown Structures (WBS), techno-economic analysis (TEA) models, and Gantt charts. It is clear to us that BETO incorporates a WBS for its projects and for the technical barriers that are being addressed. BETO has required the projects to incorporate TEA, as noted in the 2013 review process and earlier. The 2015 review process noted that major improvements had been made in the rigor and depth of the TEA since 2013 and were increasingly integrated into the decision-making process. The 2017 review process did not raise a concern; however, some 2019 review panels noted that the use of TEA models by individual projects were inconsistent or missing, leading to potentially erroneous conclusions regarding potential commercial applicability. We believe that during the 2019 review process a significant factor toward the inconsistent or misuse of the TEA model could be attributed to the recent BETO emphases on projects with lower technology risk, where comprehensive economic models are less applicable.

We appreciate the past panels recommending the use of very useful tools, such as TEA models; however, given the diversity of projects located in a variety of environments, such as universities and national laboratories, it is not unexpected that the rigor and assumptions used in the models continue to be inconsistent. In addition, it is not obvious to us that TEA or Gantt charts should be used equally among all projects in the portfolio. Instead, we recommend that BETO focus on the panel questions we mentioned—such as how progress is measured, the criteria for making choices, and consistency in assumptions (to name a few)—and that the BETO project managers and researchers in individual technology areas should determine the best way to communicate to stakeholders and technical reviewers.

Given the vast complexity of the BETO portfolio, we would like BETO to consider what they want the program and peer review process to accomplish. It appears to us that the current methodology of reviewing the portfolio every 2 years, using temporary panel members, is not optimally effective in evaluating the technical

aspects, relevance, or progress of the projects currently in the portfolio or understanding the historical effort BETO has accomplished. We suggest that BETO consider using the IABs (which can meet several times per year, if appropriate) to evaluate the program and project objectives and that BETO might want to use the biannual peer review process for communication purposes and to review a smaller and more focused set of barriers.

#### CLOSING OUT OLD AND NEW ISSUES

In the latter part of the last century, private and public researchers performed transformative research into addressing some important bio-industry technical challenges. Because of changing world events and changing of emphasis on both private and public efforts in the U.S. bioenergy realm, some past subject matter experts are no longer available or are not being used as a resource. Consequently, we have seen some repeating of past work by both the private and public communities and a reidentification of previously identified technical barriers.

BETO and the bioenergy industry are at a unique point in history that is experiencing renewed interest and investment in renewable energy, fuels, and products. This investment has resulted in developing a new generation of subject matter experts in renewable fuels and chemicals that are proficient in developing new technologies, assessing risk, and performing project management, and the experts have accumulated a working knowledge of lessons learned and deficiencies in the technologies and equipment that must be overcome.

We recognize that one of BETO's primary focuses has been to identify and mitigate technical barriers that have been identified through the multitude of projects BETO has participated in developing. We also recognize that BETO, through coordination with some national laboratories, has been active in publishing commercially relevant results. It also appears to us, however, that some technical barriers and potential solutions identified around equipment choice and how the equipment choice affects a facility's technical and financial performance might not be well communicated to the industry at large in all cases. It is our experience that we continue to see private industries encounter equipment issues (notably around solids handling in the areas of bale deconstruction and solids cleaning, transporting, and feeding) that were identified decades ago and were not fully addressed at that time, in addition to new issues BETO has identified. We understand that in some cases BETO might be hindered from publishing private industry results because of concerns about intellectual property protection; however, we recommend that BETO make a concentrated effort to find commercially applicable solutions for these lingering issues that have hindered the industry while we have the subject matter experts, vendors, and companies with the knowledge to solve these issues and not need to rediscover and readdress them again in the future.

#### BETO GOALS AND COMMERCIAL SUCCESS

BETO has long recognized the benefits of producing valuable coproducts to improve the economic viability of a biorefinery and to provide an incentive for private industry to develop these projects. We appreciate that BETO's stated strategic goal in the draft 2019 MYP "is to enable use of America's abundant biomass and waste resources for advanced biofuels, bioproducts, and biopower. …" We believe that to achieve this strategic goal, a bioeconomy must exist that creates an environment that motivates investment in the industry. We recommend that BETO broaden its focus to include higher value products—not only as byproducts but as primary products. The production of higher value bioproducts reduces the economic investment risk and provides funding for solving technical risks (availability, scale-up, yields, and reduction in operation-and-maintenance [O&M] costs), which can be applied to the fuel production pathway when economics dictate. This approach can be seen in the oil refinery and chemical business.

During the project reviews, we noted two items which we believe BETO could apply from the oil refinery business. The first item is the value and focus on products. We appreciate DOE's mandate and focus on fuel production and the strides BETO has made in promoting coproduct production. However, as demonstrated in the oil refining business, a biorefinery with the ability to divert, or further convert, the reactants in the

feedstock from fuel to valuable products can be a key element in its economic viability. We believe the current limitation set on BETO to focus on fuels and only make byproducts with the more difficult to convert elements of the feedstock unnecessarily hinders the potential commercial success of these efforts.

The second item we believe BETO could apply from the oil refinery business revolves around the quality of feedstock the biorefineries should be willing to take. We noted that there was discussion from some project presenters and peer reviewers regarding the need to require (in particular, from farmers delivering stover) a certain feedstock quality to make processing the stover easier for the biorefinery. For example, the presence of rocks and grit is hard on the front-end stover deconstruction equipment and fouls facility equipment. The oil refining business faced a similar issue and determined that low-price feedstock is key. Such low-price feedstock might have a low degree of American Petroleum Institute gravity or be high in sulfur. Feedstock costs comprise a significant portion of the product selling price. Refiners made the necessary improvements to the refineries to accept and process heavy and contaminated feedstocks. The biorefinery should ultimately be designed to do the same and take and use low-priced feedstocks. For example, these feedstocks could be distressed fats or recycled oils and greases (which are currently used in some biorefineries), second-pass field residues, or overwintered material. We believe that efforts to avoid cheaper, dirty feedstock is a shortcut to solving equipment processing issues that will be reflected in the future economic viability of the facility.

The draft 2019 MYP also describes BETO's performance goals to verify models showing the production of hydrocarbon biofuels that achieve a mature modeled minimum fuel selling price (MFSP) of \$3/gallons gasoline equivalent (GGE) with a minimum 60% reduction in emissions relative to petroleum-derived fuels by the year 2022 and \$2.5/GGE with a minimum 60% reduction in emissions relative to petroleum-derived fuels by the year 2030. Based on our suggestion that BETO place increased emphasis on the production of more valuable coproducts, the target price for fuels becomes less important to the development of a viable bio-industry. We suggest that BETO consider that a more appropriate goal would be verifying models showing an economically viable commercial bio-facility that produces biofuels and bioproducts.

#### SUMMARY

The members of the Steering Committee thank BETO for the opportunity to review the progress and direction of the program portfolio. We recognize that BETO comprises an exceptional group of subject matter experts, visionaries, and leaders who are executing an extraordinary program. We appreciate BETO's use of consortia comprising IABs and national laboratories that are dedicated to specific technology areas. We believe BETO has an important role in translating renewable energy technologies in relation to incumbent technologies for policymakers and the public.

In our role as the Steering Committee, we reviewed the number of projects and planned spending for the identified technical barriers. In general, we believe that the barriers with the lowest number of projects and planned spending are appropriately on the low end of priorities. Additionally, the two technical barriers with the most projects are appropriately focused on increasing the product and coproduct yields from the biological and catalytic processes. These two technical barrier descriptions are large and contain many different topic areas; however, given the number of projects and the variety of technologies employed, we found it difficult to grasp the full scope of BETO's portfolio to develop a detailed opinion on BETO's priorities in overcoming technical barriers beyond the cursory findings of the technical review panels. Given the complexity of the BETO portfolio, we would like BETO to consider what is it they want the program and peer review process to accomplish. It appears to us that the current methodology of reviewing the entire portfolio every 2 years using temporary panel members is not effective in evaluating the technical aspects, relevance, or progress of the projects currently in the portfolio or understanding the historical effort BETO has accomplished. We suggest that BETO consider using the IABs to evaluate the program and project objectives and to develop criteria for communicating the measurement means, status of progress, and decision-making.

We recommend that BETO make a concentrated effort to find commercially applicable solutions for the known lingering issues that have commercially hindered the industry while we have access to the subject

matter experts, vendors, and companies with the knowledge to solve these issues and not need to rediscover and readdress them in the future.

We recommend that BETO broaden its focus to include higher value products—not only as byproducts but as primary products—to reduce the economic investment risk and provide funding for solving technical risks that can be applied to the fuel production pathway when economics dictate.

Sincerely,

The 2019 Steering Committee

# **BETO PROGRAMMATIC RESPONSE**

Prepared by BETO Leadership

#### **INTRODUCTION**

BETO leadership would thanks the Steering Committee for its work, technical support, and critical insights throughout the implementation of the 2019 Project Peer Review and Program Management Review. BETO appreciates all the feedback provided and is encouraged by the Steering Committee's support for many of BETO's current research activities and plans for future directions as well as the Steering Committee's appreciation for the strength and dedication of the BETO staff.

This section represents BETO's response to the Steering Committee's final report. In the coming years, BETO will work with the program and technology managers to implement several of the recommendations and address many of the Steering Committee's concerns. BETO will consider these in managing its portfolio based on systematically prioritizing R&D in technology opportunities across a range of emerging scientific breakthroughs and TRLs.

#### **Steering Committee Recommendations Overview**

The Steering Committee provided several recommendations covering a broad spectrum of areas, from portfolio scope and focus to the peer review process and implementation. BETO appreciates the Steering Committee's acknowledgement of BETO's international and federal intra and interagency engagement and plans to apply the Steering Committee's recommendation that BETO showcase this work in the future. Further, BETO appreciates the Steering Committee's robust support of BETO's new R&D directions exploring plastics and recycling improvements.

#### **Peer Review Recommendations**

The Steering Committee made several recommendations toward improving the peer review experience and process. BETO thanks the Steering Committee and agrees that the review panels were knowledgeable and thoughtful in their recommendations. BETO appreciates that the peer review takes a significant time commitment for both the Steering Committee and technical reviewers and will consider ways to alleviate this burden in planning future reviews. BETO will also consider how best to balance this against the recommendation that additional time be allotted for audience questions, additional explanation of technology portfolios, and administration.

BETO is glad that the Steering Committee found the revised program review format productive and will note this when planning future program reviews.

#### Leveraging Knowledge and Collaboration

"The Steering Committee recommends that BETO continue to communicate and showcase its intra- and interagency work at future peer reviews."

BETO thanks the Steering Committee for their positive acknowledgement of staff dedication, knowledge, and commitment. We agree that our consortia enhance our knowledge and provide valuable input to our various technology areas.

We are glad that the Steering Committee approves of BETO's current levels of international, intra-, and interagency engagement. BETO will implement the Steering Committee's recommendation to continue to highlight intra- and interagency work. With work in support of the goals laid out in the *Bioeconomy Initiative: Implementation Framework* now underway, BETO and the other offices and agencies of BR&D are actively seeking opportunities to discuss and amplify the initiative, its accomplishments, and its activities.

#### **Commercial Relevance and Market Trends**

"Recycling and reuse of plastics continues to have popular support. ... New solutions are needed, and the background technology that BETO brings is well positioned to contribute to this difficult problem. BETO has an important role in translating renewable energy technologies in relation to incumbent technologies for policymakers and the public. The transformative work being funded by BETO should be championed in the public forum."

BETO agrees that new solutions are needed for recycling and plastics and appreciates the Steering Committee's support of this effort. BETO plans to expand its support of this area into Fiscal Year 2020 and beyond.

#### **Diverse Portfolio**

BETO presented a total of 447 projects (an investment of more of than \$700 million) at the 2019 Project Peer Review and acknowledges that the breadth and diversity of this portfolio is vast. We are glad that the Steering Committee feels that the portfolio is appropriately focused.

"Past and present panels have recommended that BETO incorporate standard measurement and reporting tools for all portfolio projects, such as the use of Work Breakdown Structures (WBS), techno-economic analysis (TEA) models, and Gantt charts. ... Instead, we recommend that BETO focus on the panel questions we mentioned—such as how progress is measured, the criteria for making choices, and consistency in assumptions (to name a few)—and that BETO project managers and researchers in individual technology areas should determine the best way to communicate to stakeholders and technical reviewers."

Increased use of TEA to evaluate project feasibility and progress has been heavily encouraged by steering committees and peer review panels during the past decade. The Steering Committee noted that as BETO moves toward lower TRL projects, the use of TEA to guide project management is not as advisable. BETO appreciates this sentiment and is currently having—and will continue to have—internal discussions about revising our strategy for monitoring progress. The Steering Committee suggested that BETO work to standardize assumptions across the different projects, including "reporting costs, product values, risks, market sizes, and environmental benefits." BETO implemented a consortium approach to many of its research areas that allows for standardization of assumptions among project performers. BETO will continue to work on

standardizing assumptions among projects in the portfolio. Further, BETO will investigate how to best communicate how progress is measured, the criteria for making choices, and underlying assumptions for our technical audience.

"We would like BETO to consider what is it they want the program and peer review process to accomplish. It appears to us that the current methodology of reviewing the portfolio every 2 years, using temporary panel members, is not optimally effective in evaluating the technical aspects, relevance, or progress of the projects currently in the portfolio or understanding the historical effort BETO has accomplished. We suggest BETO consider using the IABs ... to evaluate the program and project objectives and ... the biannual peer review process for communication purposes and to review a smaller and more focused set of barriers."

BETO appreciates the Steering Committee's thoughtful consideration of review standards and practices and welcomes suggestions for improving the process for reviewers, performers, Steering Committee, and BETO staff. DOE EERE guidance requires that BETO review at least 80%–90% of its portfolio via a rigorous, formal, and documented evaluation process using qualified and independent reviewers not less than every other year. Outputs of the peer review should inform BETO planning and must be considered when determining whether projects should continue, continue with adjustments, or no longer be funded. BETO could investigate the feasibility of narrowing the focus of the peer review while continuing to comply with EERE guidelines.

Although BETO project performers use IABs within their projects, BETO employs only one external advisory board: the BR&D Federal Advisory Committee Act. Because of federal statute, BETO cannot be advised (and hence our projects cannot be reviewed) by an unapproved advisory committee. Further, assembling a review team consisting only of individuals who work with BETO on an ongoing basis could compromise or appear to compromise the objective/external nature of the peer review process.

BETO agrees with the Steering Committee that the peer review process is suboptimal, and we will continue to explore strategies to streamline, shorten, and enhance the process.

#### **Closing Out Old and New Issues**

The deep understanding of both science and the bioenergy industry are among the reasons that BETO selected this Steering Committee; the insight into both the current and past industry is highly valuable.

"We recommend that BETO make a concentrated effort to find commercially applicable solutions for the known lingering issues [regarding equipment choice and how the equipment choice affects a facility's technical and financial performance] that have commercially hindered the industry while we have access to the subject matter experts, vendors, and companies with the knowledge to solve these issues and not need to rediscover and readdress them again in the future." Areas of note include: "solids handling in the areas of bale deconstruction and solids cleaning, transporting, and feeding."

BETO recently launched the Feedstock-Conversion Interface Consortium (FCIC) to address some of these issues. The Advanced Development and Optimization portfolio is also addressing this issue. As the Steering Committee mentioned, it is sometimes difficult for BETO to share proprietary successes and failures of BETO projects. BETO will continue to investigate methods to bring together project performers with subject matter experts, vendors, and companies to help solve these problems.

#### **BETO Goals and Commercial Success**

BETO recognizes and agrees with the Steering Committee's assessment that high-value bioproducts are critical to growing the bioeconomy, and BETO appreciates the Steering Committee's strong support of this research direction.

"We recommend that BETO broaden its focus to include higher value products—not only as byproducts but as primary products. The production of higher value bioproducts reduces the economic investment risk and provides funding for solving technical risks (availability, scale-up, yields, and reduction in operation-and-maintenance [O&M] costs), which can be applied to the fuel production pathway when economics dictate. ... We believe the current limitation set on BETO to focus on fuels and only make byproducts with the more difficult to convert elements of the feedstock unnecessarily hinders the potential commercial success of these efforts."

BETO recognizes the importance of R&D to support the bioeconomy as part of a strategy to develop pricecompetitive biofuels. As the Steering Committee notes, the BETO program resides at DOE, and thus our mission must focus on addressing energy challenges. BETO understands the role that producing high-value coproducts can play in improving the commercial viability of a biorefinery and will seek to appropriately balance and communicate this in support of our current goals of energy storage, reliability, and affordability.

The second item we believe BETO could apply from the oil refinery business revolves around the quality of feedstock the biorefineries should be willing to take. ... The oil refining business ... determined that low-price feedstock is key. ... The biorefinery should ultimately be designed to do the same and take and use low-priced feedstocks.

BETO appreciates this recommendation. BETO conversion projects are aimed at converting a variety of types and qualities of feedstocks, and these efforts can be expanded. The FCIC is also evaluating strategies for using lower priced feedstocks that meet necessary conversion specifications.

#### Conclusion

BETO reiterates its thanks of the Steering Committee for their time and recommendations. BETO appreciates that the Steering Committee took the time to not only consider BETO's original questions and guidelines but went above and beyond the call of duty. The Steering Committee continually considered ways to add value to not only the 2019 Project Peer Review but also BETO peer reviews for years to come. The 2019 Steering Committee has been highly engaged, collaborative, and thoughtful throughout the planning process, and it was a pleasure to execute the peer review with them.

Though a challenging, full, and fast-paced week, the BETO peer review is invaluable to the success and future of BETO. We thank the Steering Committee, reviewers, BETO staff, and attendees for their interest in and commitment to BETO's mission of advancing applied research and experimental development to reduce the price of producing of biofuels, biopower, and bioproducts and grow the bioeconomy.



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