NREL
Transforming ENERGY

DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

Feasibility Study of Utilizing Electricity to Produce Intermediates from CO_2 and Biomass

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March 2019
CO_2 Utilization

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Goal Statement

Goal: Assess the ***technical and economic feasibility*** of utilizing electricity for (1) the reduction of CO_2 to C_1-C_3 intermediates and (2) the generation and upgrading of biomass-derived intermediates

Outcome: Develop a ***roadmap for the effective utilization of electricity within existing and emerging biorefinery designs*** that can guide ongoing research and development activities towards cost reductions and carbon/energy efficiency improvements

- Critical literature review
- Subject matter expert interviews
- Collaboration with experimental projects
- High-level comparative and detailed techno-economic analysis coupled with biorefinery integration

Relevance to Bioenergy Industry: Identify risks and opportunities for leveraging low-cost electricity to improve biorefinery carbon utilization

Quad Chart Overview

Timeline

- Project start date: October 1st, 2017
- Project end date: September 30th, 2020
- Percent complete: 47%

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	N/A	N/A	$400k	$800k
Project Cost Share	N/A			

Related Projects: 2.3.2.106 CO_2 Valorization via Rewiring Metabolic Network; 2.3.1.316 CO_2 Utilization: Thermo- and Electro-catalytic Routes to Fuels and Chemicals; 2.2.3.500 Electrocatalytic Oxidation of Lignin Oligomers

Barriers addressed

Emerging BETO Direction: Develop strategies for adding value to waste gases → Conversion of CO_2 into intermediates for subsequent upgrading to fuels/bioproducts

Objective

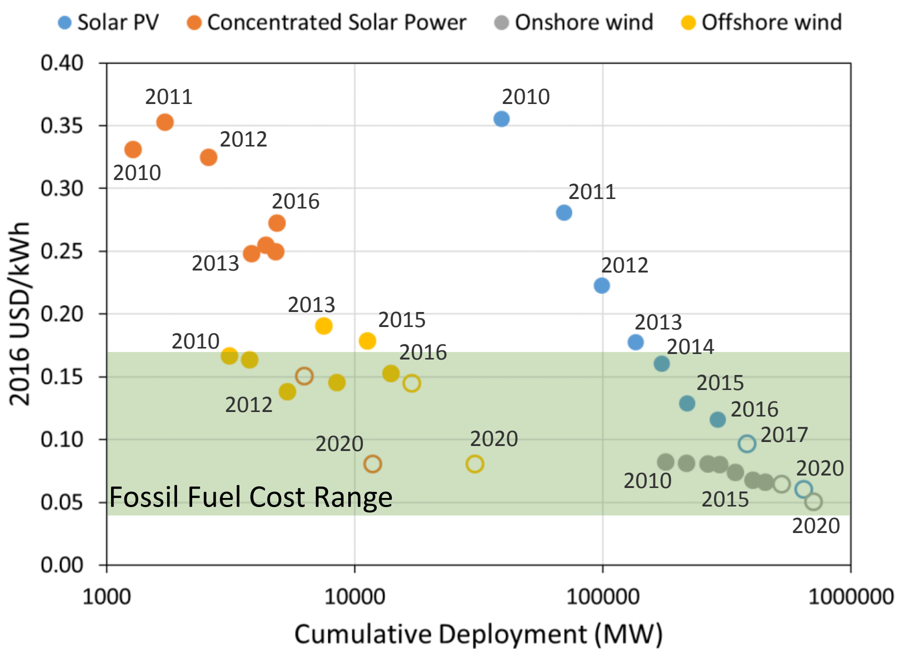
Assess the technical and economic feasibility of utilizing electricity for (1) the reduction of CO_2 to C_1-C_3 intermediates and (2) the generation and upgrading of biomass-derived intermediates

End of Project Goal

By September 2020, through critical literature review, subject matter expert interviews, collaboration with experimental projects, and both high-level comparative and detailed techno-economic analysis 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 research and development activities towards cost reductions and carbon/energy efficiency improvements

Project Overview: Convergence of Trends

Increasing Deployment and Decreasing Costs of Renewable Electricity



IRENA, Renewable Power Generation Costs in 2017

Future Levelized Costs:
\$0.02 - \$0.07/kWh

Growing Need and Opportunity for Utilizing Gaseous Carbon Waste Streams

Government, NGO, Industry, Academia, NAS

Ethanol Fermentation

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + \mathbf{2CO_2}$$

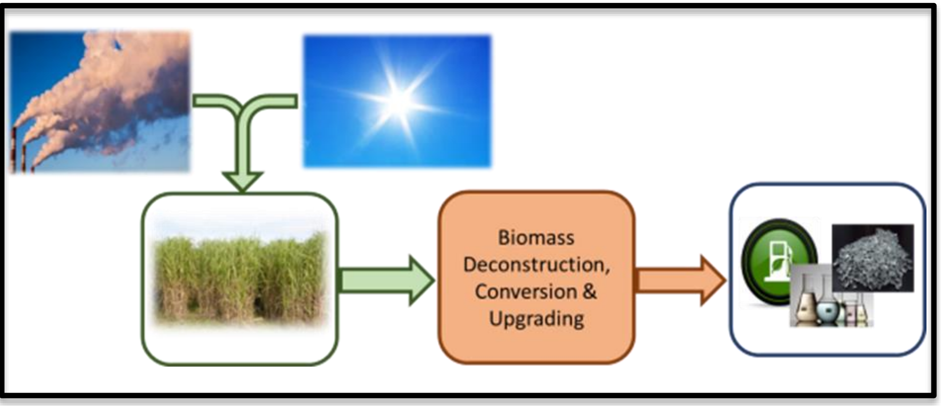
216 Existing US Biorefineries
Emit 45Mt CO_2/year*

Opportunity: *Improve Biorefinery Carbon Utilization*

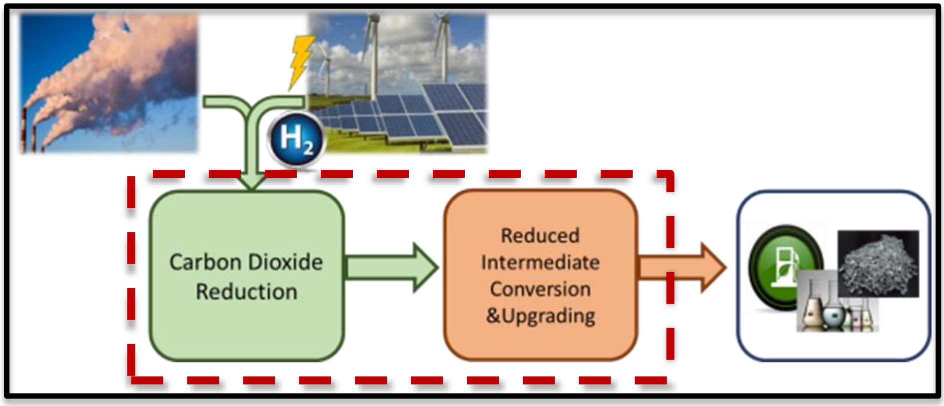
*D. Sanchez, et al., *PNAS* 115 (2018) 4875.

Project Overview: Same Story, Different Starting Point

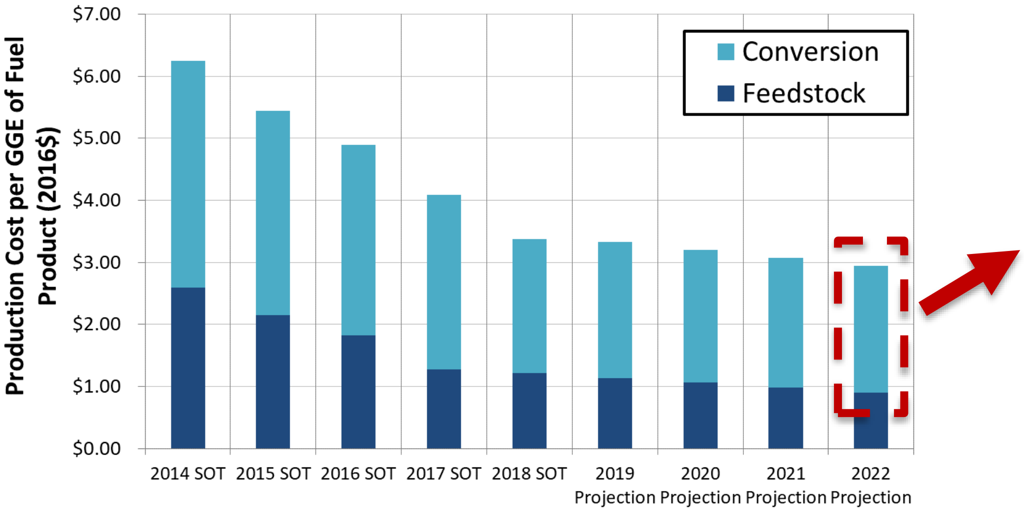
Traditional Biomass System Carbon Flow



Future Vision of Carbon Flow



Biofuel Production Cost (MFSP)



***Challenge:** Significant uncertainty exists around cost and technical challenges associated with electron-driven CO_2 reduction*

Project Overview: Value Proposition

***Value Proposition:** Guide future R&D by defining the key technical challenges and cost drivers for electron-driven CO_2 reduction*

Objectives:

- Assess and characterize technical barriers for electron-driven CO_2 reduction, identify accessible C_1-C_3 intermediates (oxygenates and hydrocarbons), and rank these intermediates based on ease of production
- Perform high-level comparative economic analysis across existing electron-driven CO_2 reduction technologies
- Perform rigorous TEA of selected CO_2 reduction technologies integrated with existing biorefinery designs to evaluate impact on MFSP

Differentiators:

- Strict focus on the intersection of electricity and biorefinery streams (CO_2)
- World-class analysis team with deep expertise in modeling emerging technologies (low TRL) with complex chemistry
- In-house chemical and biological conversion experts

Management Approach

Focused on linking technical challenges with major cost drivers

Task 1: Technical Feasibility
Task Lead: Josh Schaidle

- Perform critical literature review and subject matter expert interviews
- Characterize major technical challenges and highlight critical R&D needs
- Compare existing and emerging technologies based on cross-cutting metrics and TRL

Task 2: Economic Feasibility
Task Lead: Ling Tao

- Develop process designs for all technology pathways and products
- Perform comparative economic analyses for the integration of CO_2 upgrading strategies with existing biorefinery designs
- Evaluate key process parameters with clear cost implications through sensitivity analyses

Literature review

Subject Matter Experts

Experimentalists

Identify and Evaluate Technical Barriers

Prepare and Refine Technical Feasibility Report

External and BETO Review (Go/No-Go)

Establish SOT and Prepare Process Designs

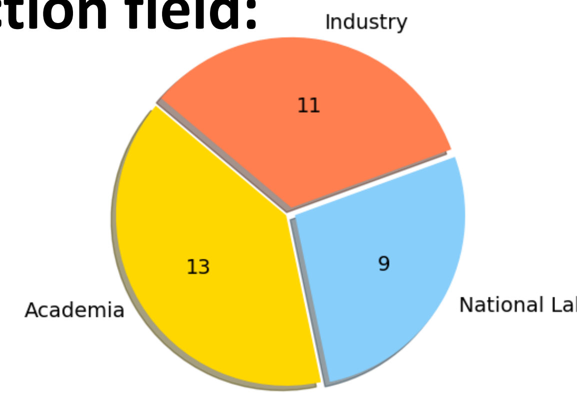
Comparative Economic Analysis

Integration with Biorefinery

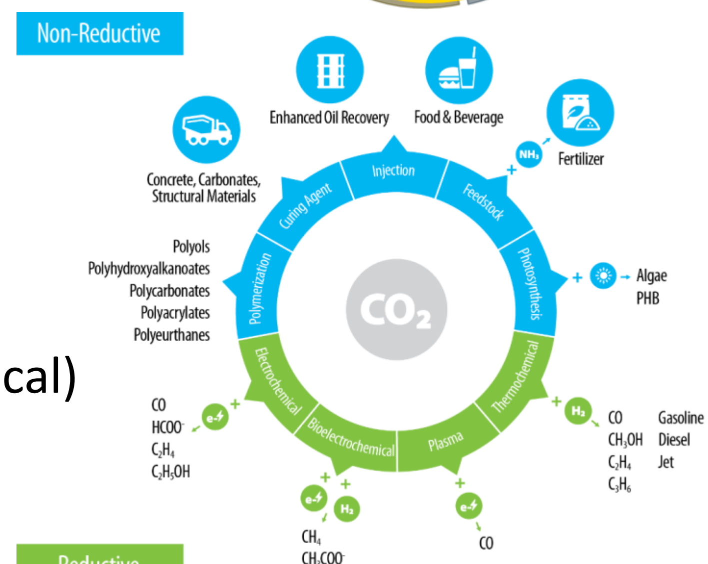
Identification of Major Cost Drivers

Technical Approach: Technical Feasibility

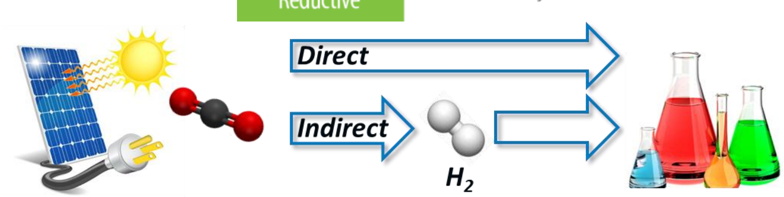
Driven by 2 core components to address the major challenge of capturing the breadth and depth of CO_2 reduction field:



- *Energy I-Corps Philosophy of "Getting out of the Lab"*
  - Interviewed over 30 subject matter experts
  - These experts covered all technologies and spanned from academia to industry



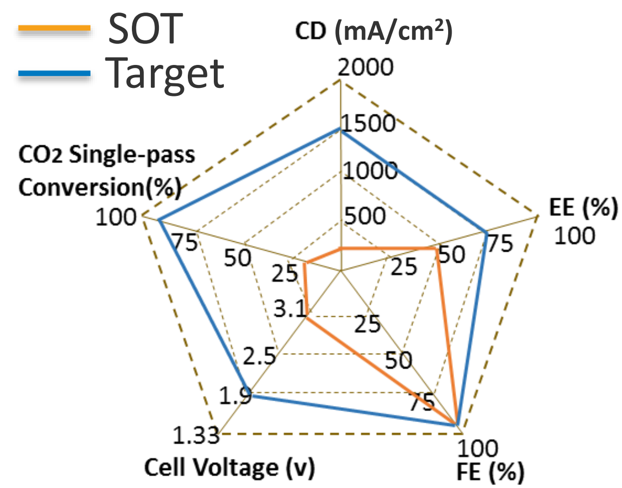
- *Cross-cutting Evaluation of Emerging and Existing CO_2 Reduction Technologies*
  - Spanned technological approaches (electrochemical, biological, thermochemical)
  - Included both direct and indirect (i.e., H_2) electron utilization
  - Excluded multi-step processing, focused on intermediates
  - Ranked accessibility of products



Technical Approach: Economic Feasibility

Addressing uncertainty by leveraging world-class analysis team, technical feasibility assessment, and existing industry-vetted models

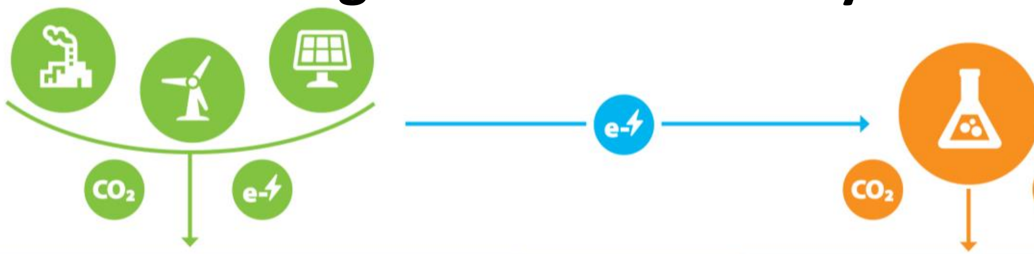
- Build upon prior CO_2-to-chemicals survey work at NREL in FY16
- Identify targeted products for technologies
  - Guided by technical feasibility report
- Establish cases:
  - SOT: Published in open literature
  - Target: Attainable process improvements
  - Theoretical: Thermodynamic limitations
- Develop Aspen-based process designs
  - Basis: CO_2 generated from 200MM gallon/y ethanol biorefinery
- Calculate Minimum Product Selling Price (MSP)
  - Consistent BETO economic assumptions
- Perform sensitivity analysis to identify key cost drivers



Success Factor: *Accurately identify process parameters with greatest impact on cost and connect to technical barriers, then disseminate*

Progress: Technical Feasibility
Final Report

Successfully captured technical challenges, research needs, and TRL of 5 CO_2 reduction technologies in an externally-reviewed report



	DIRECT			FLEXIBLE	INDIRECT	
	Electrochemical		Bioelectrochemical (MES)	Plasma	Bioelectrochemical (Fermentation)	Thermochemical
	C_1 (TRL: 4–6)	C_{2+} (TRL: 1–3)	TRL: 1–3	(TRL: 1-3)	TRL: 4-7	TRL: 5-8
Technical Challenges (Timeline)	• Reactor design and scale-up (Near) • Improved system stability (Intermediate)	• High overpotential, low energy efficiency (Long) • Poor selectivity to individual C_{2+} products (Intermediate) • Ion transport / pH gradient (Intermediate) • Low single-pass CO_2 conversion (Intermediate)	• Poor fundamental understanding of electron transfer (Long) • Slow CO_2 reduction rates (Long) • Product separation and toxicity (Near) • Low CO_2 solubility / GDE compatibility (Intermediate)	• Poor efficiency / low conversion (Long) • Low yield to C_{2+} products (Long) • Process scale-up (Intermediate) • High power demands at scale (Long)	• Poor solubility of reactants (Intermediate) • Product separation and toxicity (Near)	• Process intensification and scale-down (Intermediate) • Developing multi-functional water and CO_2 tolerant catalysts (Intermediate) • Improving product selectivity (Near)
Critical Research Needs	• Transition to gas phase, membrane electrode assemblies • Standardized testing protocols	• Increasing stability of known catalysts • Optimizing reaction conditions (electrolyte, pH, mass transport) • Developing new catalytic materials and membranes	• Expanded testing of mixed and pure cultures • Biocompatible gas diffusion electrodes • Genetic engineering of microorganisms	• Development of specialized packed-bed plasma catalysts • Electronics development • Scaling reactor design	• Genetic engineering of microorganisms • Systems engineering for improved mixing • In-situ separations development	• Rapid screening of active materials • Promoter additives to improve catalyst performance • Systems integration and reactor design for efficient process scale-down
Advantages	• Commercially deployed • Easily combined with downstream upgrading	• Tunable distribution of over 18+ products • Can have high productivities	• Capable of forming C-C bonds at ~100% selectivity • Specialized chemistry accessible through genetic modifications	• Adaptable to transient usage; quick to reach steady state • Feedstock flexible	• Capable of forming C-C bonds at ~100% selectivity • High TRL, deployed commercially	• Direct access to high volume fuels and chemicals markets • High TRL, deployed commercially at large-scale • Long history of R&D investments
Limitations	• Limited viable products • Suboptimal system durability	• Wide product range can lead to challenging product separation	• Low productivity • Limited number of direct products • Complicated, poorly understood	• Low TRL • High power requirements • Selectivity challenges	• Poor mass transfer • Limited number of direct products • Large system footprint	• Challenged economics at small-scale • Competition from non-renewable routes

Progress: Technical Feasibility
Direct Electrochemical (EC) Reduction Example

Identified top technical challenges for direct EC CO_2 reduction:

- Reducing overpotential to limit energy loss
- Forming C-C bonds with high faradaic efficiency
- Reaching commercially-viable durability in industrially-relevant reactors
- Maintaining stable ion concentration (pH) at the interface when operating at commercially-relevant current density

SOT Process Parameters

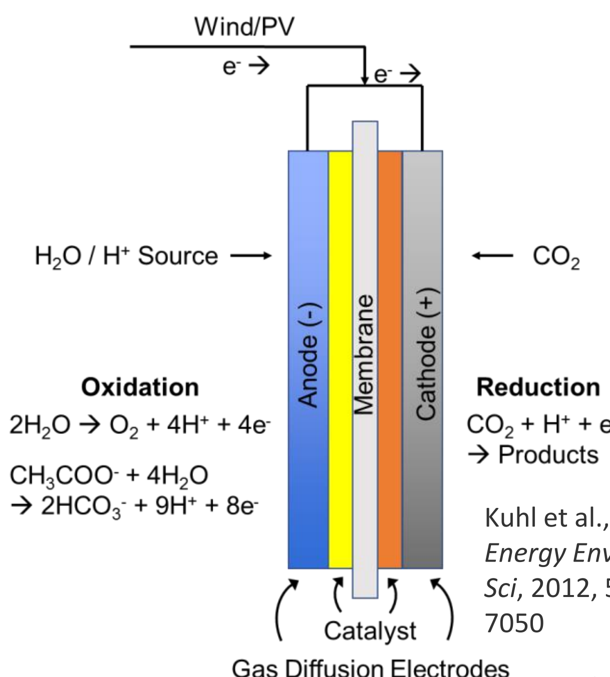
<u>C_1 Products:</u>
Overpotential: 150-1670 mV
Current Density: 0.2 – 870 mA/cm^2
FE: 76 to 99.9%
TRL: 4 – 6

<u>C_{2+} Products:</u>
Overpotential: 830 – 1520 mV
Current Density: 0.2 – 170 mA/cm^2
FE: 0.1 – 55%
TRL: 1 - 3

Over 16+ Unique Products

Product	# e⁻	E	Product	# e⁻	E
Formate	2	−0.02	Acetaldehyde	10	0.05
Carbon monoxide	2	−0.10	Ethanol	12	0.09
Methanol CH_3OH	6	0.03	Ethylene	12	0.08
Glyoxal	6	−0.16	Hydroxyacetone	14	0.46
Methane CH_4	8	0.17	Acetone	16	−0.14
Acetate	8	−0.26	Allyl alcohol	16	0.11
Glycolaldehyde	8	−0.03	Propionaldehyde	16	0.14
Ethylene glycol	10	0.20	1-Propanol	18	0.21

Conversion System



Kuhl et al., *Energy Environ. Sci*, 2012, 5, 7050

Progress: Technical Feasibility
Evaluating Accessible Products and Ease of Formation

Evaluated 23 products across 5 CO_2 reduction technologies to assess ease of formation:

- Metrics: Formation rate, selectivity, energy efficiency and TRL
- Identified six products with the highest near-term viability

Qualitative Evaluation of Product Ease of Formation

Species	Rate of Formation[a]	Selectivity[b]	Energy Efficiency[c]	Current Commercial Level[d]
CO	High	High	High	High
Ethylene	High	Intermediate	Low	Low
Formate	Intermediate	High	Intermediate	Low
Methane	High	High	Intermediate	High
Acetate	Low	High	Intermediate	Low
Methanol	High	High	High	High

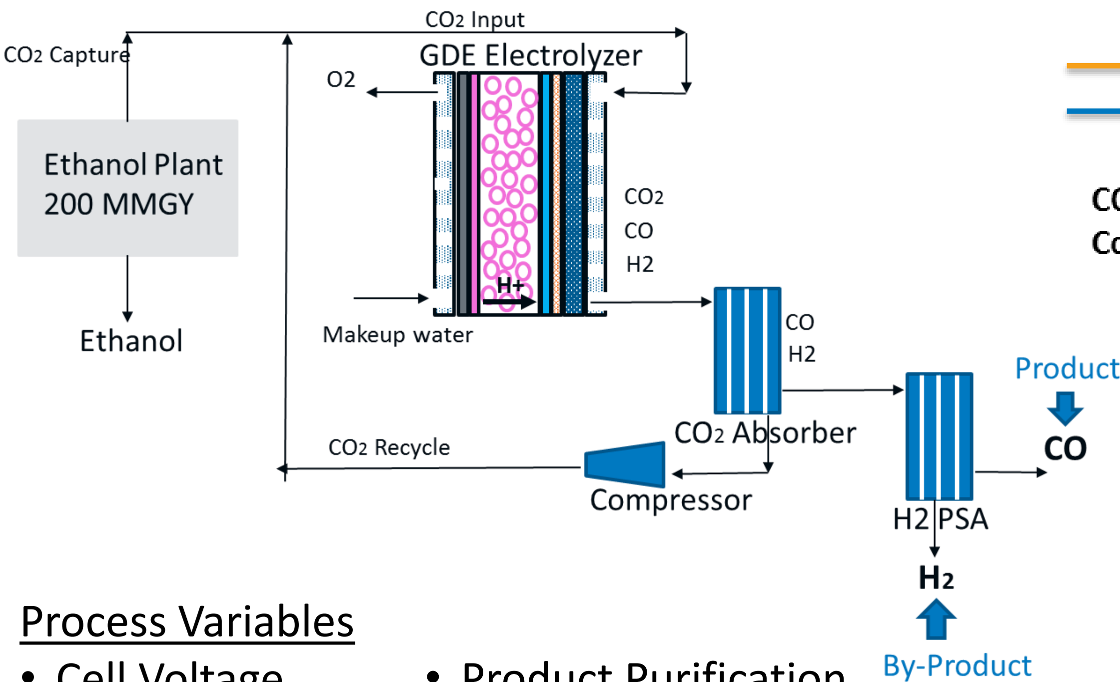
a: High: >200 mA/cm^2 (or commercial TC), Intermediate: 200 > j > 100 mA/cm^2, Low: < 100 mA/m^2
b: High: >80%, Intermediate 80% > FE > 60%, Low: < 60%
c: High: >60%, Intermediate: 60%> EE >40%, Low: <40%
d: High: Operated at TRL > 6, Intermediate: Operated TRL 4-6, Low: Operated TRL 1-3

Species	#e-	Pathway
CO	2	EC, TC, P
CO(syngas)	2	EC, TC, P
Formic Acid	2	EC, TC
Carbon Nanotubes	4	EC
Methanol	6	EC, TC
Methane	8	EC, TC, BC
Acetic Acid	8	EC, BC
Ethylene Glycol	10	EC
Acetaldehyde	10	EC
Dimethyl Ether	12	TC
Ethanol	12	EC, TC, BC
Ethylene	12	EC, TC, BC
Acetone	16	EC
Propionaldehyde	16	EC
Propylene	18	TC
1-Propanol	18	EC
Isopropanol	18	BC
Oxalate	2	EC
Glyoxal	6	EC
Glycolaldehyde	8	EC
Hydroxyacetone	14	EC
Propionate	14	BC
Allyl Alcohol	16	EC

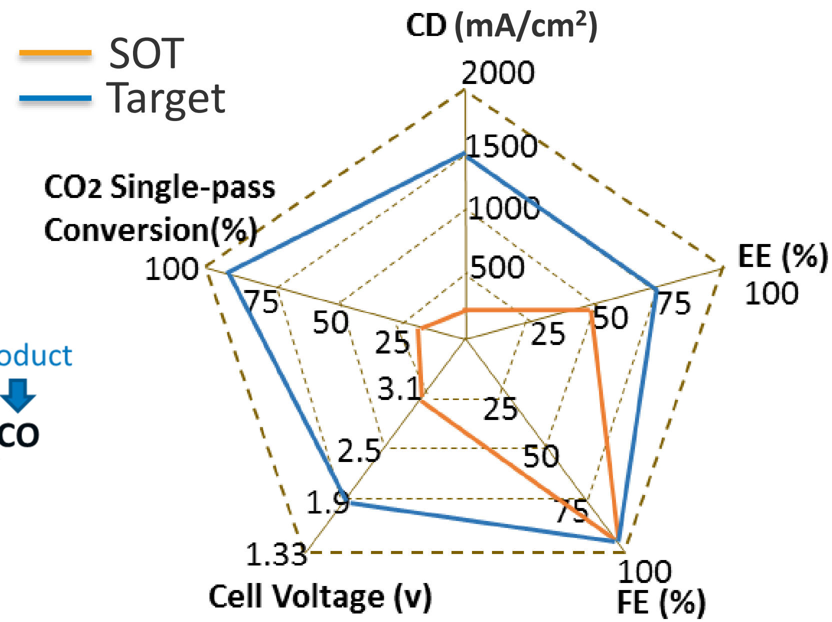
Progress: Economic Feasibility
Direct EC CO_2-to-CO Example

Developed process design and established SOT, Target, and Theoretical Cases

Process Flow Diagram



Key Process and Technology Metrics



Process Variables

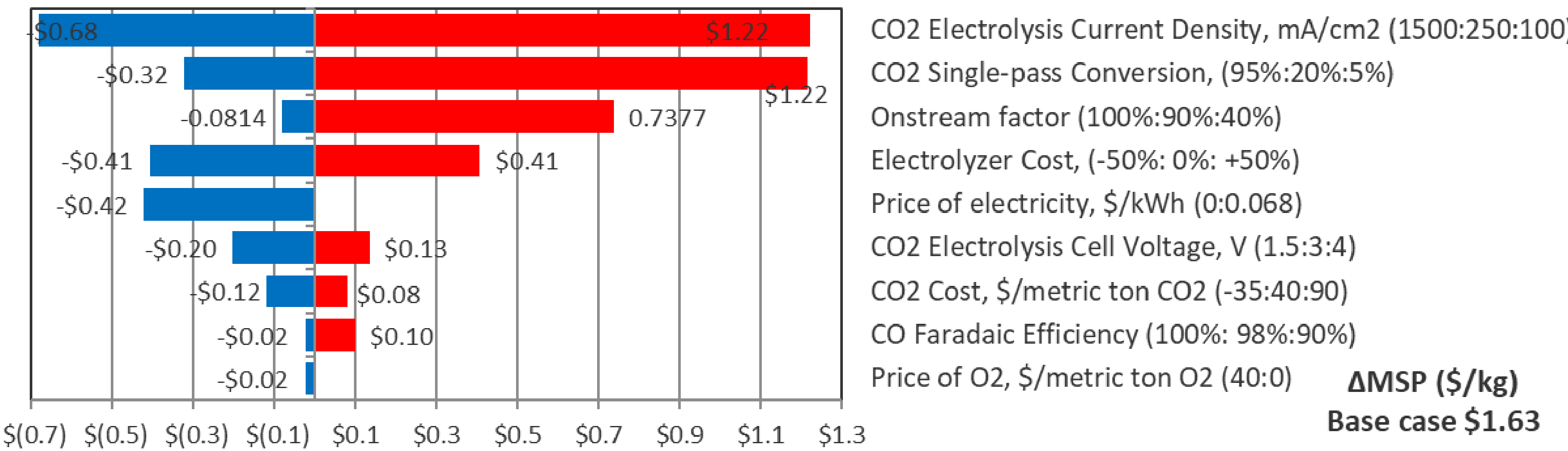
- Cell Voltage
- Current Density
- Faradaic Efficiency
- CO_2 Conversion
- Electrolyzer Cost
- Electricity Price
- Product Purification
- Compression
- CO_2 Capture Cost
- Catalyst Lifetime
- By-product Credits

*FE=Faradaic Efficiency
*EE=Energy Efficiency
*CD=Current Density
Theoretical values on the edge

Progress: Economic Feasibility
Direct EC CO_2-to-CO Example

Calculated MSP for CO and identified major cost drivers

Minimum Selling Price	SOT	Target	Theoretical	Market
$/MMBtu	169.68	21.86	7.29	
$/Kg	1.63	0.21	0.07	$0.23



- Key cost drivers are current density, single-pass CO_2 conversion, onstream factor, electrolyzer cost, and electricity cost
- Potential to be cost-competitive with CO market price

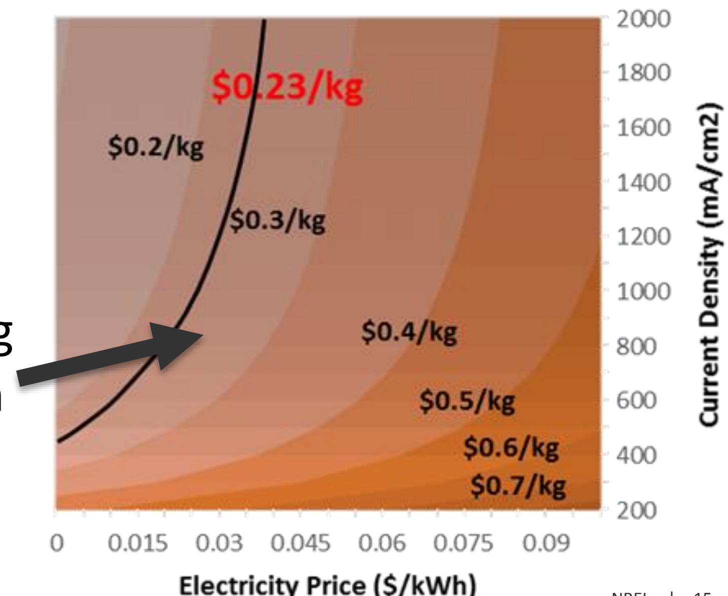
Relevance: Expanding BETO Feedstock Slate

Guiding future R&D by defining the key technical challenges and cost drivers for electron-driven CO_2 reduction

- BETO is pursuing strategies for converting gaseous waste streams into revenue-generating streams:

  2018 MYP: "BETO is investigating strategies for adding value to waste gases such as biologically derived CO_2. BETO is exploring catalytic, electrocatalytic, and biological conversion routes to reduce these species into intermediates that can be subsequently converted to fuels and bioproducts."

- *This feasibility project supports and advances this effort by:*
  - Defining critical technology- and product-specific technical challenges and research needs for electron-driven CO_2 reduction
  - Identifying major cost drivers and mapping process parameter space that will result in cost reduction, ***guiding R&D targets***
  - Integrating with biorefinery models to ***assess impact on MFSP***



Relevance: Bioenergy Industry

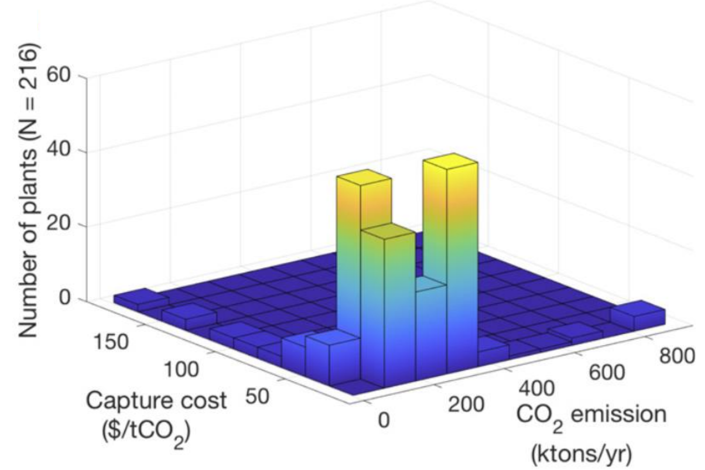
Improving commercial viability by identifying risks and opportunities for leveraging low-cost electricity to improve biorefinery carbon utilization

Ethanol Fermentation

$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$

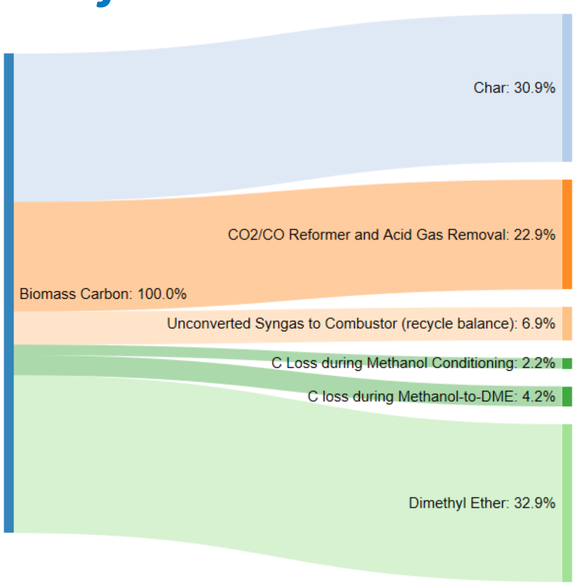
~33% of carbon lost to CO_2 [45Mt/y in US]

60% available for pipeline transport at <$25/tonne (nearly free if utilized on-site)



*D. Sanchez, et al., *PNAS* 115 (2018) 4875.

Gasification Carbon Flow



Greater than one-third of biomass carbon emitted as CO_2

***C utilization is typically most impactful process parameter on overall economics** – this project identifies and evaluates routes to improve C efficiency by leveraging low-cost electricity*

Future Work: Technical Feasibility

Assess the technical feasibility of utilizing electricity to drive the generation and upgrading of biomass-derived intermediates

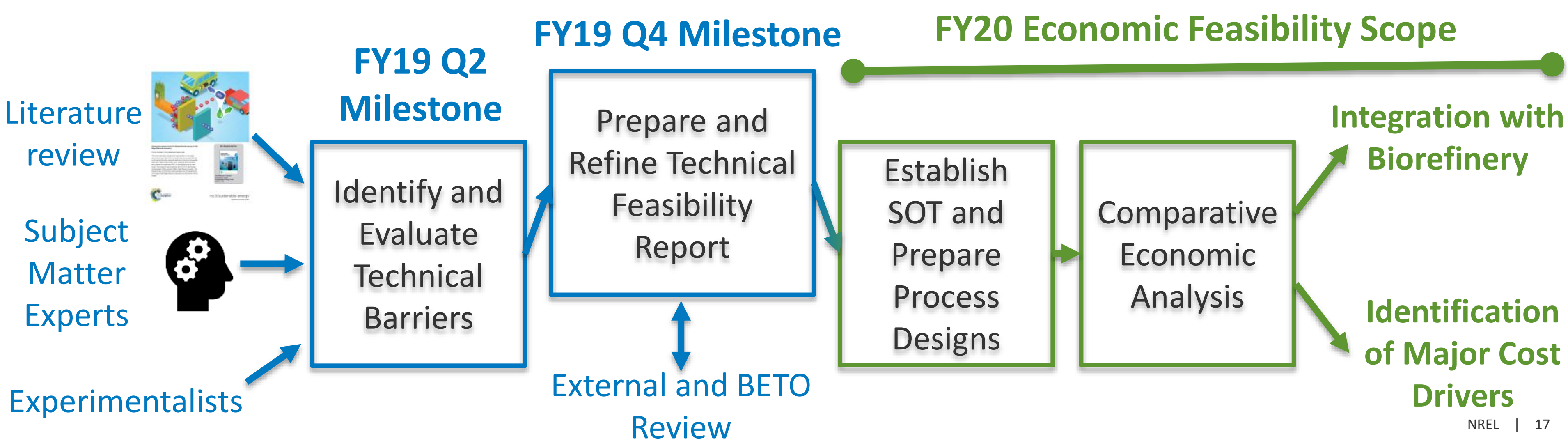
Scope:

- Identify and characterize technologies
- Focus on processes relevant to existing BETO biomass conversion pathways
- Describe top technical barriers, R&D needs, and TRL

Direct EC examples:

- Coupled upgrading of CO_2 and ethanol
- Reductive catalytic fractionation of biomass
- Lignin depolymerization and oxidation

Electron-Driven Biomass Conversion



Future Work: Economic Feasibility

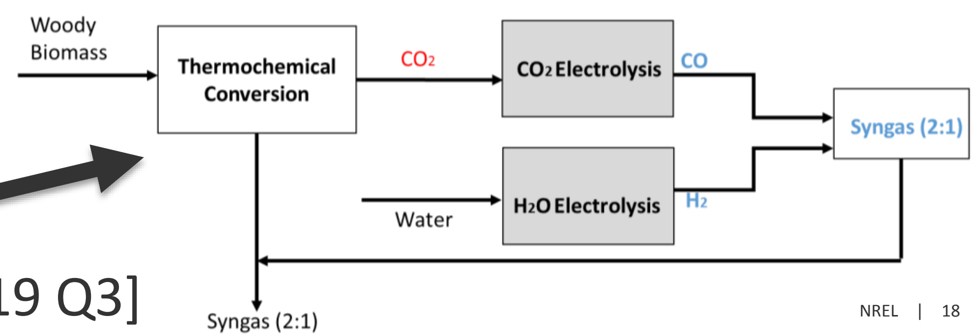
Finalize comparative economic analyses for electron-driven CO_2 reduction technologies and products

FY19 Scope:

	Selected Products												
	CO	CH_4	Formic Acid	MeOH	Acetic Acid	C_2H_4	Ethanol	DME	Isopropanol	Butanol	PHB	HC	CNT
Electrochemical (EC)	v	v	v	v		v	v						
Biological (BC)		v			v		v		v		v		
Thermochemical (TC)	v	v		v				v				v	
MES (BC+EC)		v	v		v		v			v			
SOEC (TC+EC)	v	v											v

- Disseminate key findings on cost drivers and attainable future targets by ***publishing results in peer-reviewed journal articles*** and developing a ***public-website with powerful visualizations of cost distributions***
- Select specific CO_2 utilization cases and perform rigorous TEA with biorefinery integration to ***evaluate impact on MFSP***

[FY19 Q3]



Future Work: Integrated Roadmap

Integrate results across technical and economic assessments to form a R&D roadmap for biorefinery electricity utilization

Task 1: Technical Feasibility

Described major technical challenges, critical R&D needs, and TRLs for electron-driven CO_2 reduction and biomass conversion/upgrading

Task 2: Economic Feasibility

Developed process designs, calculated MSPs, identified major cost drivers, and assessed impact on MFSP for electron-driven CO_2 reduction and biomass conversion/upgrading

FY20 Outcome: *Develop a roadmap for the effective utilization of electricity within existing and emerging biorefinery designs that can guide ongoing research and development activities towards cost reductions and carbon/energy efficiency improvements*

Summary

Goal: Assess the ***technical and economic feasibility*** of utilizing electricity for (1) the reduction of CO_2 to C_1-C_3 intermediates and (2) the generation and upgrading of biomass-derived intermediates

Approach and Progress: Connecting key technical challenges with major cost drivers as a means to ***provide actionable information*** to R&D teams within BETO and the broader scientific community

Outcome: Develop a ***roadmap for the effective utilization of electricity within existing and emerging biorefinery designs*** that can guide ongoing research and development activities towards cost reductions and carbon/energy efficiency improvements

Relevance to Bioenergy Industry: Identify risks and opportunities for leveraging low-cost electricity to improve biorefinery carbon utilization

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Thank You

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Acronyms

- BC – Biochemical
- CD – Current Density
- EC – Electrochemical
- EE – Electrical Efficiency
- FE – Faradaic Efficiency
- FY – Fiscal Year
- GDE – Gas Diffusion Electrode
- GGE – Gasoline Gallon Equivalent
- MES – Microbial Electrosynthesis
- MFSP – Minimum Fuel Selling Price
- MSP – Minimum Product Selling Price
- P – Plasma
- SOEC – Solid Oxide Electrochemical Cell
- SOT – State of Technology
- TC – Thermochemical
- TRL – Technology Readiness Level

Go/No-Go Highlights (June 2018)

In FY18 Q3, we subjected our technical feasibility report to a thorough and critical review by 18 external subject matter experts ranging from industry, national labs, and academia. We asked the reviewers to directly edit and comment on the report and also provided them with a questionnaire that solicited targeted feedback on areas including the strengths and weaknesses of the report, report scope, identification of any data gaps, and to what degree the report would be of value to the CO_2 community. Based on their feedback, we made significant updates to the report and identified components that needed to be further developed over the next few quarters. These components fell into three main categories: (1) additional techno-economic analysis, (2) incorporation of additional pathways, and (3) knowledge dissemination. To-date, we have now performed an economic feasibility assessment, incorporated additional pathways (i.e., plasma), and are preparing two manuscripts for publication (as well as developing a companion website for easy visualization of the economic results).

Publications, Patents, Presentations, Awards, and Commercialization

Publications:

- Two manuscripts are in preparation that will present our results of the technical and economic feasibility assessments; these manuscripts are targeted for submission to peer-reviewed journals in FY19

Collaborations:

- We are working with the Global CO_2 Initiative to host a workshop in 2019 to help harmonize technoeconomic analyses and life-cycle assessments in the field of CO_2 utilization