BETO 2021 Peer Review:

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

Josh Schaidle, NREL

CO_2 Utilization

March 11th, 2021

Project Overview

Goal: ***Guide existing and future R&D*** efforts by defining key technical challenges, risks, cost/carbon intensity drivers, and future technical targets for utilizing renewable electricity and CO_2 to improve biorefinery economics and carbon utilization

Outcomes: (1) FY20 – Develop a ***roadmap of strategic R&D needs to accelerate CO_2 utilization*** and (2) FY23 – Develop and publish a ***comprehensive design report*** for the integration of CO_2 utilization into two existing conceptual biorefinery designs

- Critical literature review and subject matter expert interviews
- Collaboration with experimental projects
- High-level comparative and detailed techno-economic analysis coupled with biorefinery integration
- Carbon intensity assessment through partnership with ANL (GREET)
- Risk identification and evaluation

Impact: ***Foundational analysis to guide decarbonization*** of fuels and chemical production

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

Quad Chart Overview: 2.1.0.304

Timeline
- Prior AOP Cycle: Oct. 1, 2018 – Sept. 30, 2020
- Current AOP Cycle: Oct. 1, 2020 – Sept. 30, 2023

	FY20	Active Project
DOE Funding	$400,000	$1,200,000

Project Collaborators
- Electrocatalytic CO_2 Utilization (2.3.1.316)
- ANL Life-Cycle Analysis (4.1.1.10)

Barriers addressed
Emerging BETO Direction: Develop strategies for adding value to waste gases
- Ot-B: Cost of Production
- At-E: Quantification of Economic, Environmental, and Other Benefits and Costs

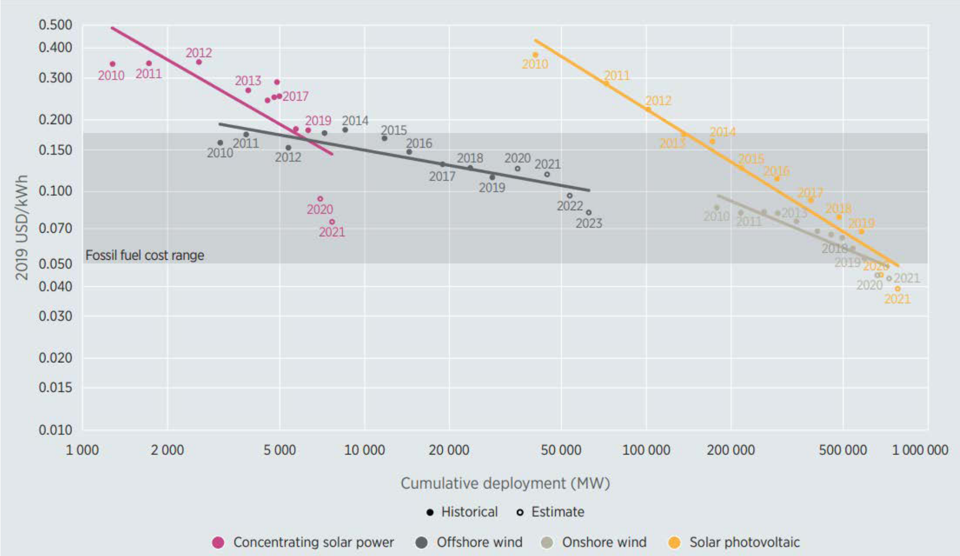
Project Goal
Guide existing and future research and development efforts by defining key technical challenges, risks, cost/carbon intensity drivers, and future technical targets for utilizing renewable electricity and CO_2 to improve biorefinery economics and carbon utilization

End of Project Milestone
Develop and publish a comprehensive design report for the integration of CO_2 utilization into two existing conceptual biorefinery designs, which will include conceptual process models, pioneer and n^{th} plant economics, identification and quantification of technological risks, and projections for future cost reductions

Funding Mechanism
Annual Operating Plan

Project Overview: Convergence of Trends

Increasing Deployment and Decreasing Costs of Renewable Electricity



IRENA, Renewable Power Generation Costs in 2019

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

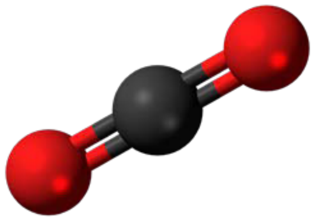
$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$$

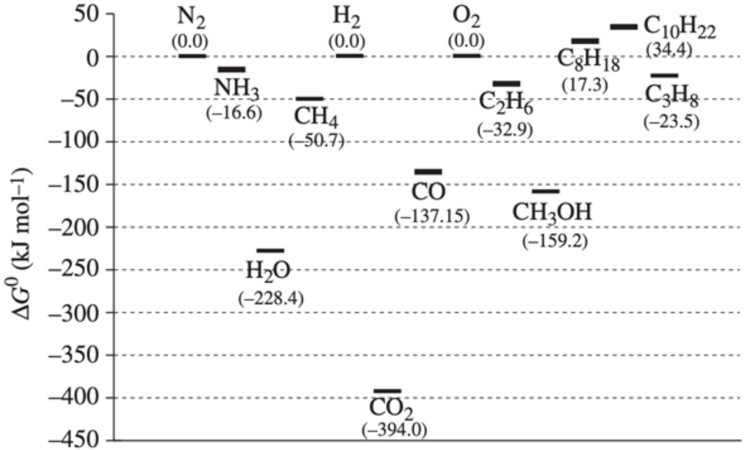
216 US Biorefineries Emit 45Mt CO_2/year*

***Opportunity:** Decarbonization of fuels and chemicals production*

Project Overview: Brutal Reality of CO_2 Reduction

- CO_2 is 73wt% O and is neither free nor pure
- CO_2 is abundant, but has no heating value
  - Energy demand for converting CO_2 to ethylene is ca. 7 – 20 kWh/kg[#]
  - Ammonia synthesis: ca. 8 kWh/kg*
  - Converting 45Mt/y of CO_2 from ethanol fermentation to hydrocarbon fuels requires ca. 35 – 50 GW of power
- Pipeline availability is limited
- CO_2 as feedstock ≠ lower carbon intensity than the incumbent





Z. Jiang, et al., *Phil. Trans. R. Soc. A,* 2010, **368**, 3343-3364.

[#]Depends upon energy efficiency of specific process

*K. Kermeli, Energy Efficiency and Cost Saving Opportunities for Ammonia and Nitrogeneous Fertilizer Production, 2017.

Market Trends

Product	Anticipated decrease in gasoline/ethanol demand; diesel demand steady
	Increasing demand for aviation and marine fuel
	Demand for higher-performance products
	Increasing demand for renewable/recyclable materials
Feedstock	Sustained low oil prices
	Decreasing cost of renewable electricity
	Sustainable waste management
	Expanding availability of green H_2
	Closing the carbon cycle
Capital	Risk of greenfield investments
	Challenges and costs of biorefinery start-up
	Availability of depreciated and underutilized capital equipment
Social Responsibility	Carbon intensity reduction
	Access to clean air and water
	Environmental equity

NREL's Bioenergy Program Is Enabling a Sustainable Energy Future by Responding to Key Market Needs

Value Proposition

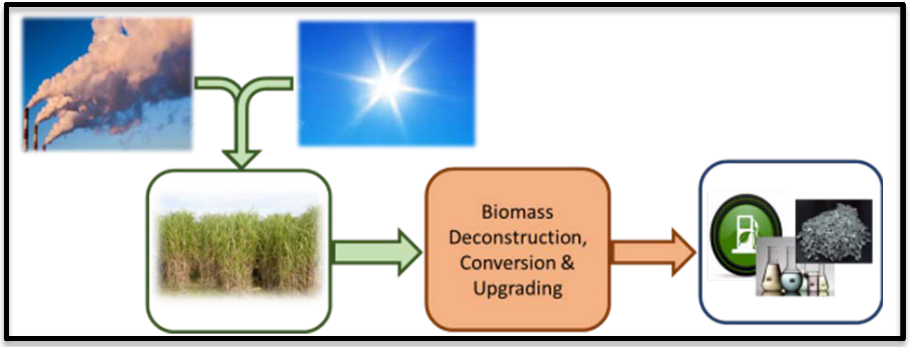
Guide future R&D by defining the key technical challenges, risks, and cost/carbon intensity drivers for utilizing electricity and CO_2 to improve biorefinery carbon utilization

Key Differentiators

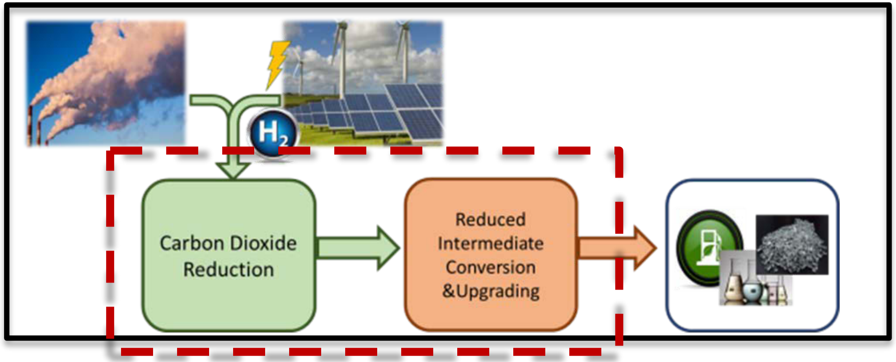
- Focus on the intersection of electricity and biorefinery streams (CO_2)
- Cross-cutting analysis, followed by technology-specific deep dives
- World-class analysis team with deep expertise in modeling emerging technologies with complex chemistry
- In-house chemical and biological conversion experts

1. Management: Key Challenge

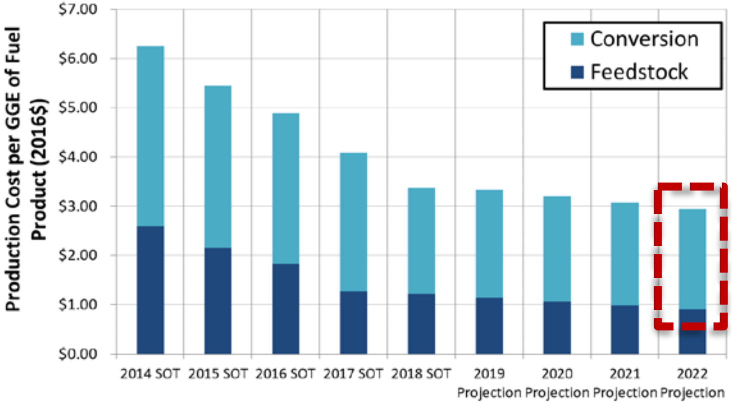
Traditional Biomass System Carbon Flow



Future Vision of Carbon Flow



Biofuel Production Cost (MFSP)



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

1. Management: Project Structure

Focused on linking technical challenges and risks with impacts on cost and carbon intensity

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
- Identify and evaluate ***technological risks*** by developing a risk register, quantifying probability and impact, and developing mitigation strategies with experimental teams

Task 2: Economic Feasibility

Task Lead: Ling Tao

- Develop conceptual process designs and perform TEA
- Integrate CO_2 upgrading strategies with existing biorefinery designs to evaluate impact on MFSP and carbon utilization
- Perform sensitivity/uncertainty analyses based on identified technological risks
- Provide life-cycle inventory data to ANL for ***carbon intensity assessment***

Communication: Weekly/biweekly team meetings and monthly meetings with experimental teams and grid integration analysts

1. Management: Collaboration and Community Engagement

Broad community engagement addresses key risk of siloed analysis

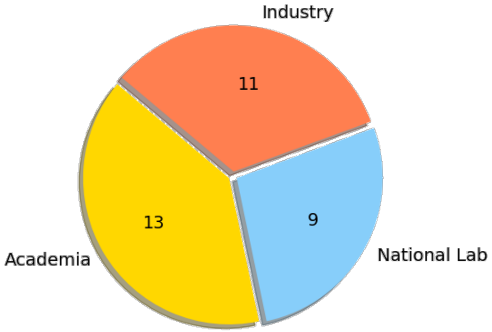
- Life-cycle analysis in partnership with ANL (WBS: 4.1.1.10)
  - Provide life-cycle inventory data to ANL based on process designs
- Global CO_2 Initiative (GCI)
  - Includes members from across North America and Europe
  - Josh Schaidle serves on the GCI advisory board
  - Co-organize annual workshop on harmonizing TEA/LCA for CO_2 utilization
  - Contribute to task teams on TEA/LCA integration, defining comparison cases/scenarios, and assessment of emerging technologies
- USDRIVE Tech Team on Net-Zero Carbon Fuels
  - Ling Tao provides process design and analysis support

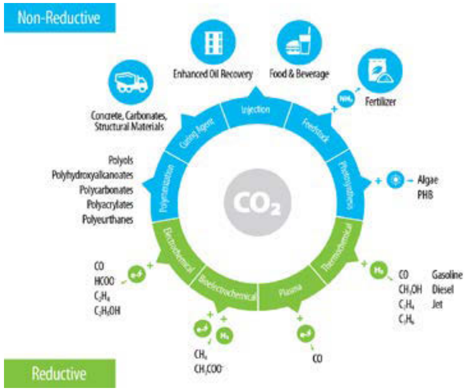
2. Approach: Overarching Strategy

Cross-cutting evaluation of emerging and existing CO_2 reduction technologies followed by deep dives into specific pathways

Assessed technical feasibility of 5 CO_2 reduction technologies

- Interviewed over 30 subject matter experts
- Direct and indirect technologies across electrochemical, biological, and thermochemical approaches
- Identified key technical challenges and accessible products





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Assessed technical feasibility of 5 CO_2 reduction technologies

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- Direct and indirect technologies across electrochemical, biological, and thermochemical approaches
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Assessed economic feasibility of generating 11 products from 5 CO_2 reduction technologies

- Identified products based on technical feasibility study
- Developed Aspen Plus process designs (nth plant)
- Calculated minimum product selling price (MSP) using discounted cash flow analysis (consistent BETO assumptions)
- Performed sensitivity analysis to identify key cost drivers

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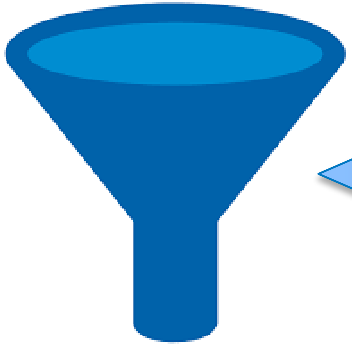
Generated a roadmap report identifying strategic R&D needs to accelerate CO_2 utilization

2. Approach: Overarching Strategy

Cross-cutting evaluation of emerging and existing CO_2 reduction technologies followed by deep dives into specific pathways

1st AOP Cycle

- FY18
- FY19
- FY20



Utilized 3-year AOP merit review cycle in 2020 to respond to 2019 Peer Review feedback

- Encouraged to "narrow the scope of our study"
- "Net carbon balance (intensity) should be analyzed"
- "Quantitative metrics are desired and uncertainty analysis will be helpful when making assumptions"

2nd AOP Cycle

- FY21
- FY22
- FY23

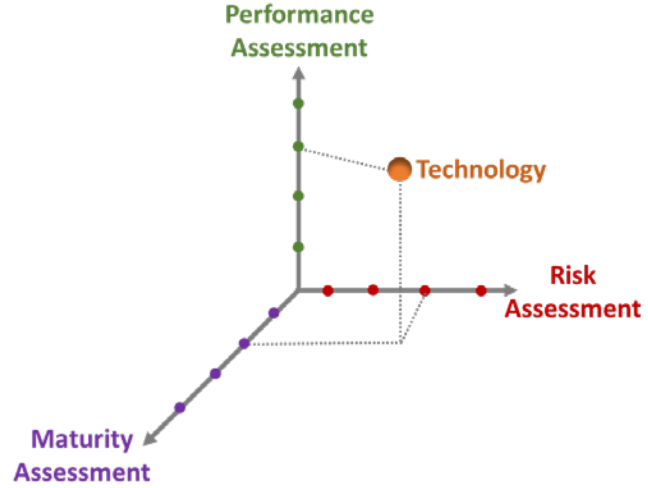
2. Approach: Overarching Strategy

Cross-cutting evaluation of emerging and existing CO_2 reduction technologies followed by deep dives into specific pathways

Establish state-of-technology (SOT) for 2 pathways to end products (FY21, FY22), culminating in a comprehensive design report with biorefinery integration in FY23

- Pathways selected based on technology maturity, prior technical and economic feasibility assessment, R&D opportunity, and relevance to BETO mission
- Establish SOT in close collaboration with experimentalists, industry, and subject matter experts:
    - *Performance:* Cost, carbon intensity (ANL), technical metrics
    - *Maturity:* TRL (unit op and systems level)
    - *Risks:* Technical risk register with mitigation strategies
- Quantify impact of risks through uncertainty and sensitivity analysis

Technology = f (performance, maturity, risks)



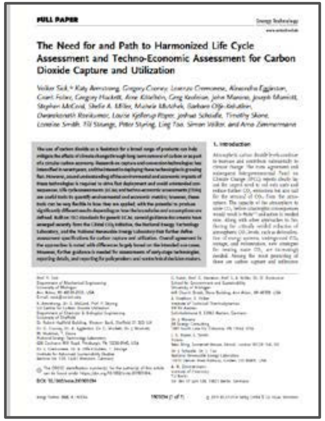
3. **Impact:** Bioenergy and CO_2 Utilization Communities

Providing foundational analysis to guide decarbonization of fuels and chemical production

Identifying and disseminating key technical challenges for CO_2 reduction

R. Grim, et al., *Energy Environ. Sci.* 13 (2020) 472.
[Selected by editors as a 2020 HOT Article]

Partnering with other analysts around the globe to harmonize TEA/LCA for CO_2 utilization


FULL PAPER

The Need for and Path to Harmonized Life Cycle Assessment and Techno-Economic Assessment for Carbon Dioxide Capture and Utilization

GLOBAL CO_2 INITIATIVE
UNIVERSITY OF MICHIGAN

V. Sick, et al., *Energy Technol.* 8 (2020) 1901034.
[Top Downloaded Paper in *Energy Technology*]

3. Impact: Establishing State-of-Technology and Future Targets

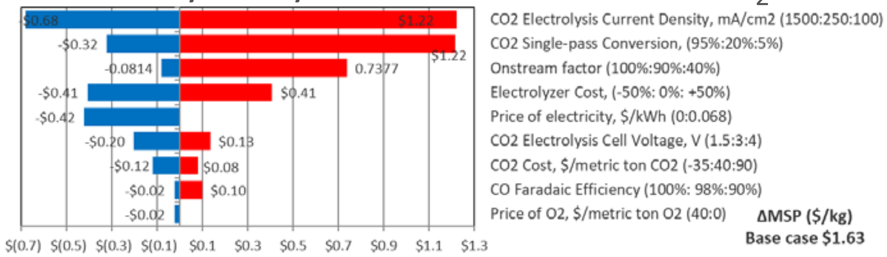
Supporting BETO's pursuit of converting gaseous waste streams into revenue-generating streams

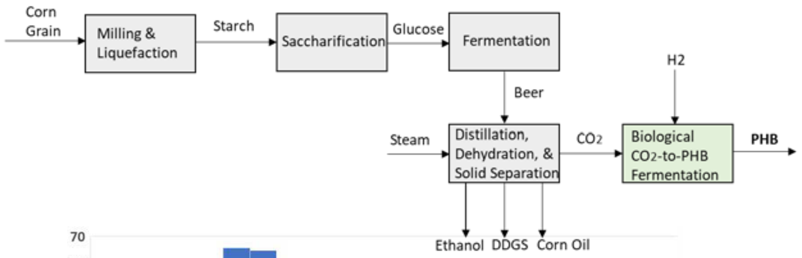
Guiding R&D through identification of key cost and carbon intensity drivers

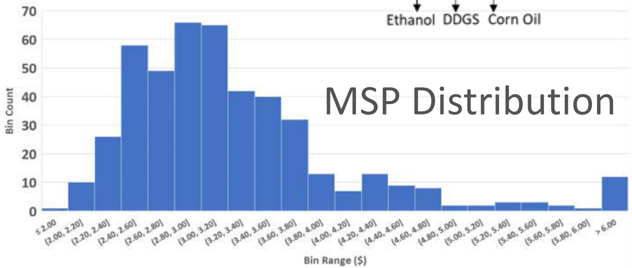
Integrating CO_2 utilization with biorefinery models to assess impact on MFSP and carbon intensity

Incorporating risk evaluation and uncertainty analysis into state-of-technology assessments

Sensitivity Analysis for Electrochemical CO_2-to-CO







4. Progress: Cross-Cutting Technical Feasibility

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
Major Technical Challenges	• Scale up reactor / supporting systems • Increase long-term system stability	• Improve energy efficiency; reduce cell overpotential • Increase selectivity to individual C_{2+} products • Increase single-pass CO_2 conversion	• Develop fundamental understanding of electron transfer mechanism(s) • Raise CO_2 reduction rates • Increase product titers and cell toxicity limits • Increase CO_2 solubility / current density	• Decouple energy efficiency / conversion correlation • Raise yield to C_{2+} products • Develop commercially viable reactor design	• Increase solubility of gaseous reactants • Reduce separation costs • Increase product titers and cell toxicity limits	• Process intensification and scale-down • Develop multi-functional water and CO_2 tolerant catalysts • Improve product selectivity
Research Needs	• Transition to gas-phase, membrane electrode assemblies • Standardize testing protocols • Develop accelerated degradation testing methods • Test possible anodic chemistries to replace OER • Optimize reaction conditions (electrolyte, pH, mass transport) • Develop of new catalytic materials and membranes		• Expanded testing of mixed and pure cultures • Develop bio-compatible gas diffusion electrodes • Genetic engineering	• Develop specialized packed-bed catalysts for plasma conditions • Electronics development • Scalable reactor design	• Raise product titers • Improve reactant delivery / mixing • Develop low-cost *in-situ* separations	• Rapid screening of active materials • Improve catalyst performance through promoter additives • Intelligent systems integration and reactor design
Advantages	• Commercially deployed for C_1 species • Tunable distribution of over 20+ products • 100% theoretical conversion of CO_2 • High theoretical energy conversion efficiency • Access to high-value, high-volume intermediates & products		• Can form C-C bonds at ~100% selectivity • Specialized chemistry accessible through genetic modifications • ~98.6 % theoretical conversion of CO_2 • High theoretical energy conversion efficiency	• Adaptable to transient usage; quick to reach steady-state • Feedstock flexible • 100% theoretical conversion of CO_2	• Can form C-C bonds at ~100% selectivity • High TRL, deployed commercially • ~98.6 % theoretical conversion of CO_2	• Direct access to high volume fuels and chemicals markets • Highest TRL; deployed commercially at large-scale • Long history of R&D investments; existing infrastructure
Limitations	• Low selectivity to C_{2+} products • Reported products limited in carbon number ≤ 4 • Low TRL to C_{2+} products • Rapid deactivation and limited testing on long-term stability		• Low productivity • Limited number of direct C_1-C_3 products • Poorly understood reaction mechanisms	• Low TRL • High power demand • Low selectivity to C_{2+} products	• Poor mass transfer • Limited number of direct C_1-C_3 products • Large system footprint • Lower theoretical energy conversion efficiency	• Challenged economics at small-scale • Limitations in CO_2 equilibrium conversion • Lower theoretical energy conversion efficiency

R. Grim, et al., *Energy Environ. Sci.*, 2020, **13**, 472-494.

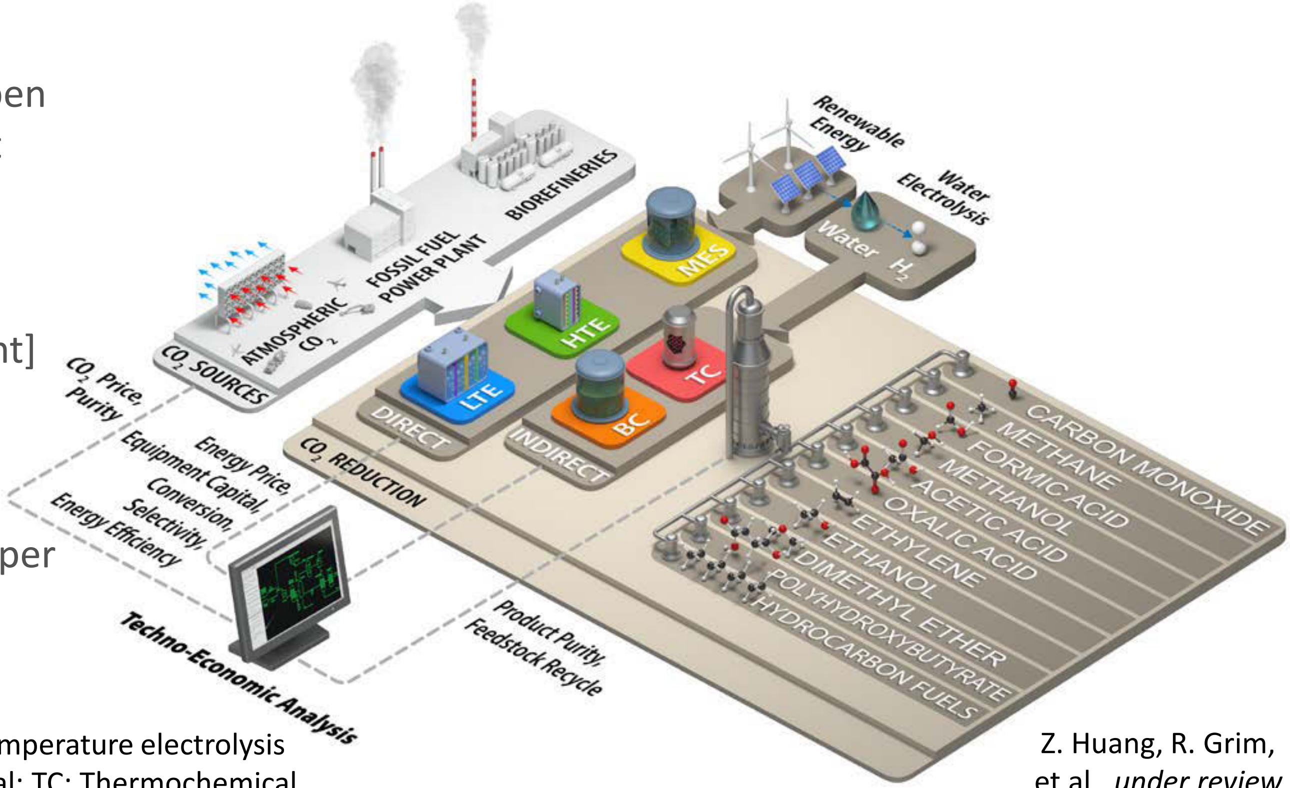
4. Progress: Cross-Cutting Economic Feasibility

Calculated MSP values for products across 5 different (direct and indirect) CO_2 reduction technologies

Three scenarios:

- *Current:* Results published in open literature [$0.068/kWh; $40/mt CO_2]
- *Future:* Attainable process improvements or engineering judgements [$0.03/kWh; $20/mt]
- *Theoretical:* Thermodynamic limitations [$0.02/kWh; $0/mt]

Scale Basis: CO_2 from 200M gallon per year ethanol biorefinery

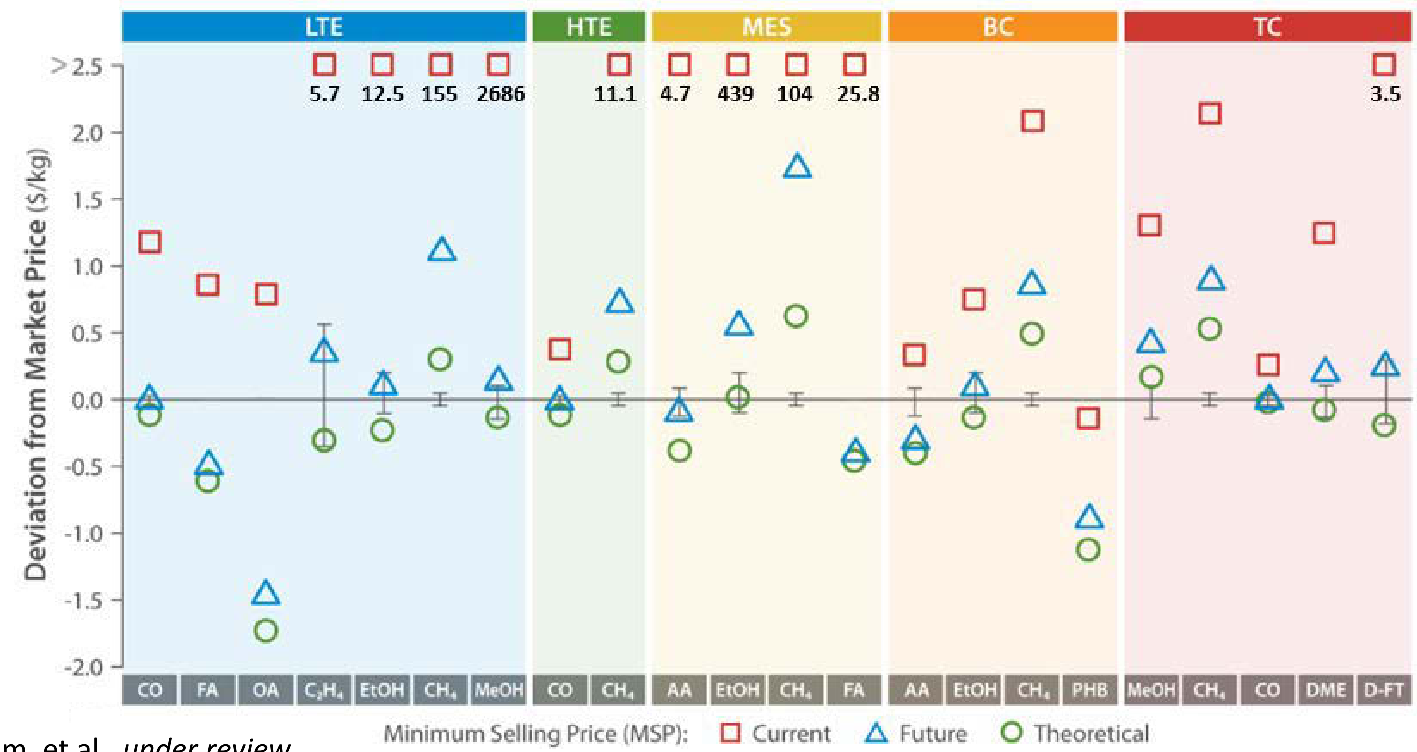


LTE: Low-temperature electrolysis; HTE: High-temperature electrolysis
MES: Microbial Electrosynthesis; BC: Biochemical; TC: Thermochemical

Z. Huang, R. Grim, et al., *under review*

4. Progress: Cross-Cutting Economic Feasibility

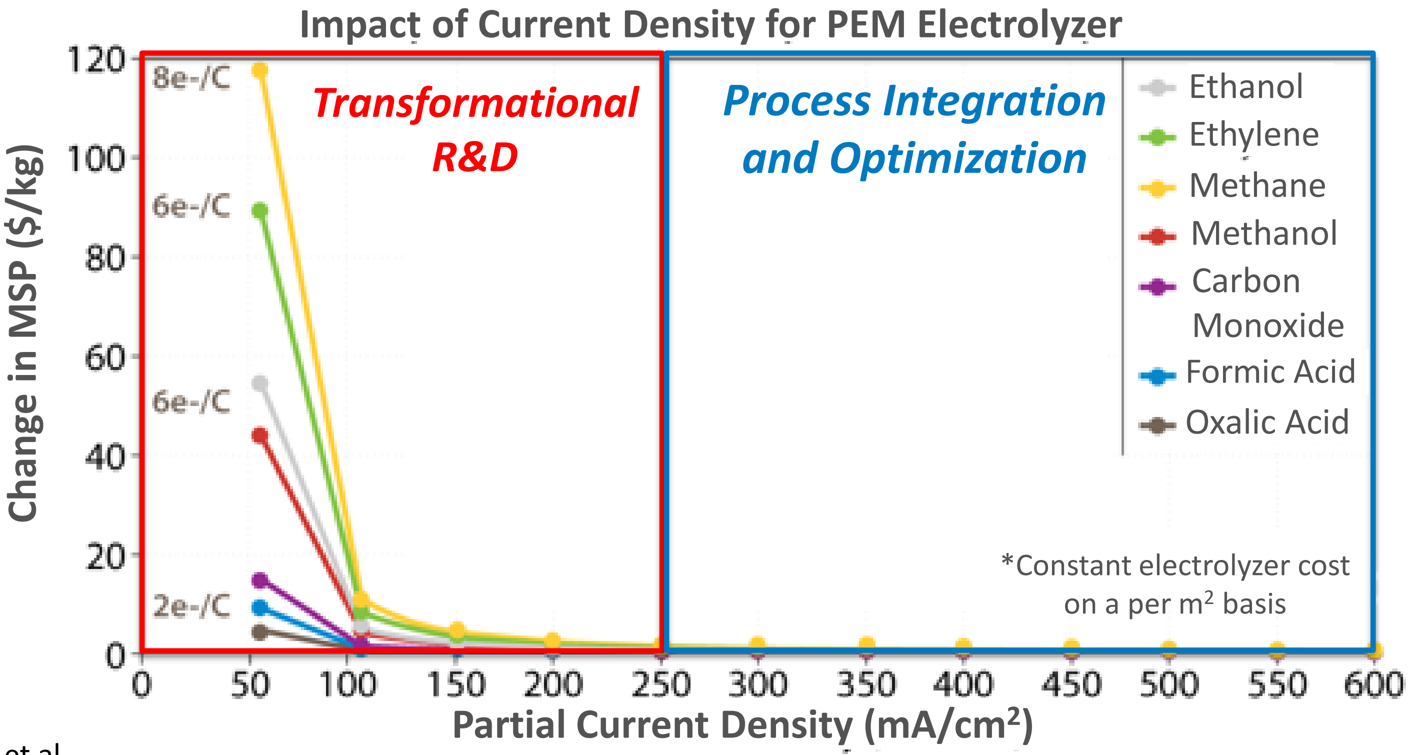
Assessed near-term product viability by comparing MSP of 11 products from 5 technologies to market price under Current, Future, and Theoretical scenarios



Z. Huang, R. Grim, et al., *under review*

4. Progress: Cross-Cutting Economic Feasibility

Identified key cost drivers and quantified opportunities for transformational R&D through sensitivity analysis



Z. Huang, R. Grim, et al., *under review*

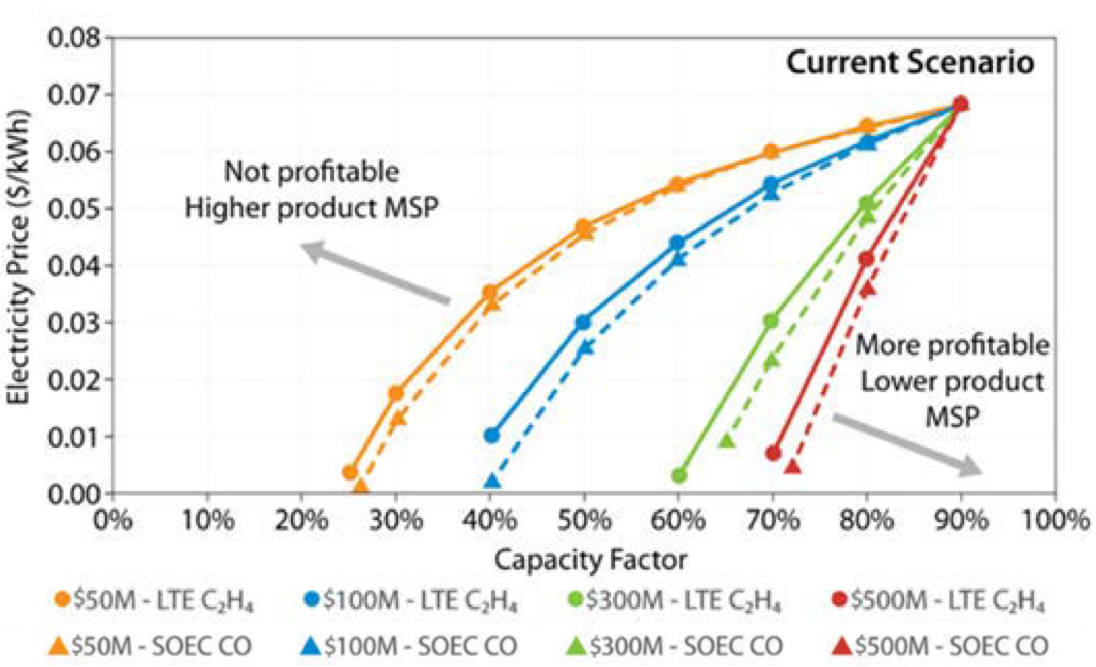
Level-off point dependent upon number of electrons transferred

4. Progress: Impact of Intermittency and Onstream Factor

Assessed impact of intermittency on MSP as a function of capital costs and electricity price

Approach:

- Two Cases:
  - LTE C_2H_4 – 6e$^-$/C
  - HTE CO – 2e$^-$/C
- Defined a range of values for fixed capital (\$50M - \$500M)
- Same models and assumptions as shown earlier for current scenario
- Plotted lines of constant MSP as a function of capacity factor and electricity price



Z. Huang, R. Grim, et al., *under review*

4. Progress: Roadmap of Strategic R&D Needs

Identified strategic R&D needs to accelerate CO_2 utilization by distilling findings across subject matter expert interviews, technical feasibility assessment, and economic feasibility assessment

Identified Strategic R&D Needs

- Assess renewable energy demand and feedstock supply chain for CO_2 reduction at scale
- Continue to advance sustainable hydrogen production
  - Key cost driver for indirect routes
- Raise single-pass CO_2 conversion (avoid CO_2 loss) through improved electrolyzer designs
  - Including electrolytes, electrocatalysts, and membranes
- Pursue opportunities for transformational R&D
- Integrate TEA/LCA to evaluate tradeoffs between cost and carbon intensity
- Accelerate the development of CO_2 electrolyzers
  - Durability testing of industrially-relevant cell architectures
- Establish standardized metrics and performance guidelines
- Assess technical, economic, and carbon intensity risks and uncertainties

Report submitted to BETO in FY20 Q4

Summary

Goal: ***Guide existing and future R&D*** efforts by defining key technical challenges, risks, cost/carbon intensity drivers, and future technical targets for utilizing renewable electricity and CO_2 to improve biorefinery economics and carbon utilization

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

Outcomes: (1) FY20 – Develop a ***roadmap of strategic R&D needs to accelerate*** CO_2 ***utilization*** and (2) FY23 – Develop and publish a ***comprehensive design report*** for the integration of CO_2 utilization into two existing conceptual biorefinery designs, with inclusion of outyear targets

Impact: ***Foundational analysis to guide decarbonization*** of fuels and chemical production

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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Transforming ENERGY

Acronyms

- AA – Acetic Acid
- ANL – Argonne National Laboratory
- AOP – Annual Operating Plan
- BC – Biochemical
- CD – Current density
- DDGS – Distiller's dried grains with solubles
- D-FT – Direct Fischer-Tropsch Hydrocarbons
- DME – Dimethyl Ether
- EtOH - Ethanol
- FA – Formic Acid
- FE – Faradaic Efficiency
- FY – Fiscal Year
- GCI – Global CO_2 Initiative
- HTE – High-temperature electrolysis
- LCA – Life-cycle assessment
- LTE – Low-temperature electrolysis
- MeOH - Methanol
- MES – Microbial electrosynthesis
- MESP – Minimum Ethanol Selling Price
- MFSP – Minimum Fuel Selling Price
- MGY – Million gallons per year
- MSP – Minimum Product Selling Price
- mt – Metric ton
- Mt – million tons
- OA – Oxalic Acid
- PHB - Polyhydroxybutyrate
- SOT – State of Technology
- TEA – Technoeconomic Analysis
- TC - Thermochemical
- TRL – Technology Readiness Level

Additional Slides

Responses to Previous Reviewers' Comments

Our Overarching response to 2019 Peer Review:

"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 initial study is fairly broad (spanning across five different direct and indirect CO_2 reduction technologies), we believe that the cross-cutting nature of this analysis is critical to its value creation for the research community. Moving forward, we plan to dive deeper into specific technologies, especially in regards to integration of these technologies with existing biorefinery designs."

Please also see slide 13.

Publications, Patents, Presentations, Awards, and Commercialization

- Publications:
  - G. Grim, Z. Huang, M. Guarnieri, J. Ferrell, L. Tao, J. Schaidle, "Transforming the Carbon Economy: Challenges and Opportunities in the Convergence of Low-Cost Electricity and CO_2 Utilization", *Energy & Environmental Science*, 13 (2020) 472-494.
  - V. Sick, K. Armstrong, G. Cooney, L. Cremonese, A. Eggleston, G. Faber, G. Hackett, A. Katelhon, G. Keoleian, J. Marano, J. Marriott, S. McCord, S. Miller, M. Mutchek, B. Olfe-Krautlein, D. Ravikumar, L. Roper, J. Schaidle, T. Skone, L. Smith, T. Strunge, P. Styring, L. Tao, S. Volker, A. Zimmerman, "The Need for and Path to Harmonized Life Cycle Assessment and Techno-economic Assessment for Carbon Dioxide Capture and Utilization", 8 (2020) 1901034.
  - Z. Huang, G. Grim, J. Schaidle, L. Tao, "Using Waste CO_2 to Increase Ethanol Production from Corn Ethanol Biorefineries: Techno-Economic Analysis", *Applied Energy* 280 (2020) 115964.
  - F. Lucas, G. Grim, S. Tacey, C. Downes, J. Hasse, A. Roman, C. Farberow, J. Schaidle, A. Holewinski, "Electrochemical Routes for the Valorization of Biomass-Derived Feedstocks: From Chemistry to Application", *ACS Energy Letters*, in press.
  - Z. Huang, G. Grim, J. Schaidle, Ling Tao, "The Economic Outlook for Converting CO_2 and Electrons to Molecules", under review.
- Selected Presentations:
  - Z. Huang, G. Grim, J. Ferrell, M. Guarnieri, L. Tao, J. Schaidle, "Assessing the Technical and Economic Feasibility of Electron-Driven CO_2 Reduction", Closing the Carbon Cycle Webinar Series, Idaho National Lab, December 11th, 2020.
  - Z. Huang, G. Grim, J. Ferrell, M. Guarnieri, L. Tao, J. Schaidle, "What is the Technical and Economic Feasibility of Utilizing Electricity-Driven CO_2 Reduction to Transform our Carbon Economy?", European Biomass Conference and Exhibition, July 8th, 2020.
  - Z. Huang, G. Grim, J. Ferrell, M. Guarnieri, L. Tao, J. Schaidle, "Technical and Economic Feasibility of Electron-Driven CO_2 Reduction", AICHE Annual Meeting, Orlando FL, November 19th, 2019.
- Other Relevant Activities:
  - Organizer for a workshop titled "Reactive CO_2 Capture: Process Integration for the New Carbon Economy", February 17th-19th, 2020 – attended by over 100 subject matter experts across industry, academia, and national labs
  - Co-Chair of "CO_2 Upgrading: Reduction and Hydrogenation" session at AICHE Annual Meeting in Fall 2020