DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

Feasibility Study of Utilizing Electricity to Produce Intermediates from CO$_2$ and Biomass

Josh Schaidle, NREL
March 11$^{th}$, 2021
CO$_2$ Utilization
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 CO₂ to improve biorefinery economics and carbon utilization

Outcomes: (1) FY20 – Develop a **roadmap of strategic R&D needs to accelerate CO₂ utilization** and (2) FY23 – Develop and publish a **comprehensive design report** for the integration of CO₂ 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**

<table>
<thead>
<tr>
<th>FY20</th>
<th>Active Project</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Funding</td>
<td>$400,000</td>
</tr>
<tr>
<td></td>
<td>$1,200,000</td>
</tr>
</tbody>
</table>

**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 CO₂ to improve biorefinery economics and carbon utilization.

**End of Project Milestone**
Develop and publish a comprehensive design report for the integration of CO₂ utilization into two existing conceptual biorefinery designs, which will include conceptual process models, pioneer and nth plant economics, identification and quantification of technological risks, and projections for future cost reductions.

**Project Collaborators**
- Electrocatalytic CO₂ 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

**Funding Mechanism**
Annual Operating Plan
Project Overview: Convergence of Trends

Increasing Deployment and Decreasing Costs of Renewable Electricity

- Cumulative deployment (MW)
- Historical, Estimate
- Concentrating solar power, Offshore wind, Onshore wind, Solar photovoltaic

Growing Need and Opportunity for Utilizing Gaseous Carbon Waste Streams

Government, NGO, Industry, Academia, NAS

Ethanol Fermentation

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

IRENA, Renewable Power Generation Costs in 2019

Future Levelized Costs: $0.02 - $0.07/kWh

216 US Biorefineries Emit 45Mt CO₂/year*

Opportunity: Decarbonization of fuels and chemicals production
Project Overview: Brutal Reality of CO₂ Reduction

- CO₂ is 73wt% O and is neither free nor pure
- CO₂ is abundant, but has no heating value
  - Energy demand for converting CO₂ to ethylene is ca. 7 – 20 kWh/kg#
  - Ammonia synthesis: ca. 8 kWh/kg*
  - Converting 45Mt/y of CO₂ from ethanol fermentation to hydrocarbon fuels requires ca. 35 – 50 GW of power
- Pipeline availability is limited
- CO₂ as feedstock ≠ lower carbon intensity than the incumbent

#Depends upon energy efficiency of specific process

### Market Trends

<table>
<thead>
<tr>
<th>Product</th>
<th>Feedstock</th>
<th>Capital</th>
<th>Social Responsibility</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anticipated decrease in gasoline/ethanol demand; diesel demand steady</td>
<td>Decreasing cost of renewable electricity</td>
<td>Risk of greenfield investments</td>
<td>Carbon intensity reduction</td>
</tr>
<tr>
<td>Increasing demand for aviation and marine fuel</td>
<td>Sustainable waste management</td>
<td>Challenges and costs of biorefinery start-up</td>
<td>Access to clean air and water</td>
</tr>
<tr>
<td>Demand for higher-performance products</td>
<td>Expanding availability of green H₂</td>
<td>Availability of depreciated and underutilized capital equipment</td>
<td>Environmental equity</td>
</tr>
<tr>
<td>Increasing demand for renewable/recyclable materials</td>
<td>Closing the carbon cycle</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Sustained low oil prices**

**Value Proposition**

Guide future R&D by defining the key technical challenges, risks, and cost/carbon intensity drivers for utilizing electricity and CO₂ to improve biorefinery carbon utilization.

**Key Differentiators**

- Focus on the intersection of electricity and biorefinery streams (CO₂)
- 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 CO₂ 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 CO₂ 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 CO₂ 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
Assessed technical feasibility of 5 CO₂ 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
2. Approach: Overarching Strategy

Cross-cutting evaluation of emerging and existing CO₂ reduction technologies followed by deep dives into specific pathways

- 1st AOP Cycle
  - FY18
  - FY19
  - FY20

- 2nd AOP Cycle
  - FY21
  - FY22
  - FY23

Assessed technical feasibility of 5 CO₂ 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

Assessed economic feasibility of generating 11 products from 5 CO₂ 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
2. Approach: Overarching Strategy

Cross-cutting evaluation of emerging and existing CO\textsubscript{2} reduction technologies followed by deep dives into specific pathways

1st AOP Cycle

FY18
FY19
FY20

Assessed technical feasibility of 5 CO\textsubscript{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

Assessed economic feasibility of generating 11 products from 5 CO\textsubscript{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

2nd AOP Cycle

FY21
FY22
FY23

Generated a roadmap report identifying strategic R&D needs to accelerate CO\textsubscript{2} utilization
2. Approach: Overarching Strategy

Cross-cutting evaluation of emerging and existing CO\textsubscript{2} reduction technologies followed by deep dives into specific pathways

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”
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 CO₂ Utilization Communities

Providing foundational analysis to guide decarbonization of fuels and chemical production

Identifying and disseminating key technical challenges for CO₂ reduction

Partnering with other analysts around the globe to harmonize TEA/LCA for CO₂ utilization


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 CO₂ utilization with biorefinery models to assess impact on MFSP and carbon intensity

Incorporating risk evaluation and uncertainty analysis into state-of-technology assessments
## 4. Progress: Cross-Cutting Technical Feasibility

Captured technical challenges, research needs, and TRL of 5 CO₂ reduction technologies in an externally-reviewed report.

### Major Technical Challenges

<table>
<thead>
<tr>
<th>DIRECT</th>
<th>FLEXIBLE</th>
<th>INDIRECT</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Electrochemical</em></td>
<td><em>Bioelectrochemical (MES)</em></td>
<td><em>Plasma</em></td>
</tr>
<tr>
<td><em>Bioelectrochemical (Fermentation)</em></td>
<td><em>Thermochemical</em></td>
<td></td>
</tr>
<tr>
<td>C₂ (TRL: 1–3)</td>
<td>C₂ (TRL: 1–3)</td>
<td>(TRL: 1–3)</td>
</tr>
<tr>
<td>(TRL: 1–3)</td>
<td>(TRL: 1–3)</td>
<td>(TRL: 1–3)</td>
</tr>
</tbody>
</table>

- **Scale up reactor / supporting systems**
- **Increase long-term system stability**
- **Improve energy efficiency; reduce cell overpotential**
- **Increase selectivity to individual C₂ products**
- **Increase single-pass C₂ conversion**
- **Develop fundamental understanding of electron transfer mechanism(s)**
- **Raise CO₂ reduction rates**
- **Increase product titers and cell toxicity limits**
- **Increase C₂ solubility / current density**
- **Decouple energy efficiency / conversion correlation**
- **Raise yield to C₂ products**
- **Develop commercially viable reactor design**
- **Increase selectivity of gases / reactants**
- **Reduce separation costs**
- **Increase product titers and cell toxicity limits**
- **Process intensification and scale-down**
- **Develop multi-functional water and CO₂ 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 chemicals to replace OER
- Optimize reaction conditions (electrolyte, pH, mass transport)
- Develop 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
- Electronic development
- Scalable reactor design
- Raise product titers
- Improve reactant delivery / mixing
- Develop low-cost on-site separations
- Rapid screening of active materials
- Improve catalyst performance through promoter additives
- Intelligent systems integration and reactor design

### Advantages

- Commercially deployed for C₂ species
- Tunable distribution of over 20+ products
- 100% theoretical conversion of CO₂
- High theoretical energy conversion efficiency
- Access to high-value, high-volume intermediates & products
- Can form C₂ bonds at ~100% selectivity
- Specialized chemistry accessible through genetic modifications
- ~98.6 % theoretical conversion of CO₂
- High theoretical energy conversion efficiency
- Adaptable to transient usage; quick to reach steady-state
- Feedstock flexible
- 100% theoretical conversion of CO₂
- Can form C₂ bonds at ~100% selectivity
- High TRL deployed commercially
- ~98.6 % theoretical conversion of CO₂
- 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 C₂ products
- Reported products limited in carbon number ≤ 4
- Low TRL to C₂ products
- Rapid deactivation and limited testing on long-term stability
- Low productivity
- Limited number of direct C₂ products
- Poorly understood reaction mechanisms
- Low TRL
- High power demand
- Low selectivity to C₂ products
- Poor mass transfer
- Limited number of direct C₂ products
- Large system footprint
- Lower theoretical energy conversion efficiency
- Challenged economics at small-scale
- Limitations in CO₂ equilibrium conversion
- Lower theoretical energy conversion efficiency
4. Progress: Cross-Cutting Economic Feasibility

Calculated MSP values for products across 5 different (direct and indirect) CO₂ reduction technologies

Three scenarios:
- **Current**: Results published in open literature [$0.068/kWh; $40/mt CO₂]
- **Future**: Attainable process improvements or engineering judgements [$0.03/kWh; $20/mt]
- **Theoretical**: Thermodynamic limitations [$0.02/kWh; $0/mt]

Scale Basis: CO₂ 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.
Identified key cost drivers and quantified opportunities for transformational R&D through sensitivity analysis

**Impact of Current Density for PEM Electrolyzer**

- **Transformational R&D**
- **Process Integration and Optimization**

*Constant electrolyzer cost on a per m² basis*

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\textsubscript{2}H\textsubscript{4} – 6e\textsuperscript{-}/C
  - HTE CO – 2e\textsuperscript{-}/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 CO₂ 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 CO₂ utilization* and (2) FY23 – Develop and publish a *comprehensive design report* for the integration of CO₂ 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.
Acknowledgements

Team members and contributors:

Ling Tao       Mike Guarnieri
Zhe Huang      Jack Ferrell
Gary Grim      Randy Cortright
Abhijit Dutta  Dwarak Ravikumar

Special thanks to 35+ reviewers and subject matter experts!
Thank You

www.nrel.gov
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 CO₂ 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
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 CO₂ 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:

• Selected Presentations:

• Other Relevant Activities:
  – Organizer for a workshop titled “Reactive CO₂ 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 “CO₂ Upgrading: Reduction and Hydrogenation” session at AICHE Annual Meeting in Fall 2020