CO_2 Reduction and Upgrading for e-Fuels Consortium

U.S. DEPARTMENT OF ENERGY

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

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

4/7/2023

Carbon Dioxide Utilization

Gary Grim

National Renewable Energy Laboratory

Project Overview

Goal: ***Guide ongoing and future R&D*** in CO_2 reductive utilization by defining:

- Technical Challenges
- Opportunities
- Cost Drivers
- Carbon Intensity Drivers
- Future Technical Targets
- Scaling Risks

Outcomes: (1) FY21 – Analyzed ***promising bolt-on compatible CO_2 reduction pathways*** to fuels or products from standalone biorefineries and (2) FY22 –Published a ***comprehensive strategic plan*** for achieving industrial decarbonization goals via CO_2 conversion, with inclusion of outyear technical, cost, and carbon intensity targets (3) FY23 – Performing integrated TEA/LCA Analysis of CO_2 conversion

Relevance to BETO/Bioenergy Industry: Identify risks and opportunities for leveraging low-cost renewable electricity to improve biorefinery carbon utilization. Directly in support of BETO-EERE goals of (1) industrial decarbonization and (2) low-carbon strategic fuels (e.g., sustainable aviation fuel)

Quad Chart – Project Details and Financials

Timeline

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

	FY22 Costed	Total Award
DOE Funding	$400,000	$1,200,000

Project Partners

- *CO_2RUe Project:* Thermo- and Electro-catalytic routes to fuels and chemicals (WBS: 2.3.1.316)
- *CO_2RUe Project:* Economics and Sustainability of CO_2 Utilization Technologies with TEA and LCA (WBS: 2.1.0.506 / 2.1.0.507)

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

Integrate TEA/LCA models and determine key trade-offs for the CO_2 reduction field spanning different technological approaches. This will help identify and understand key decision points based on TEA and LCA implications.

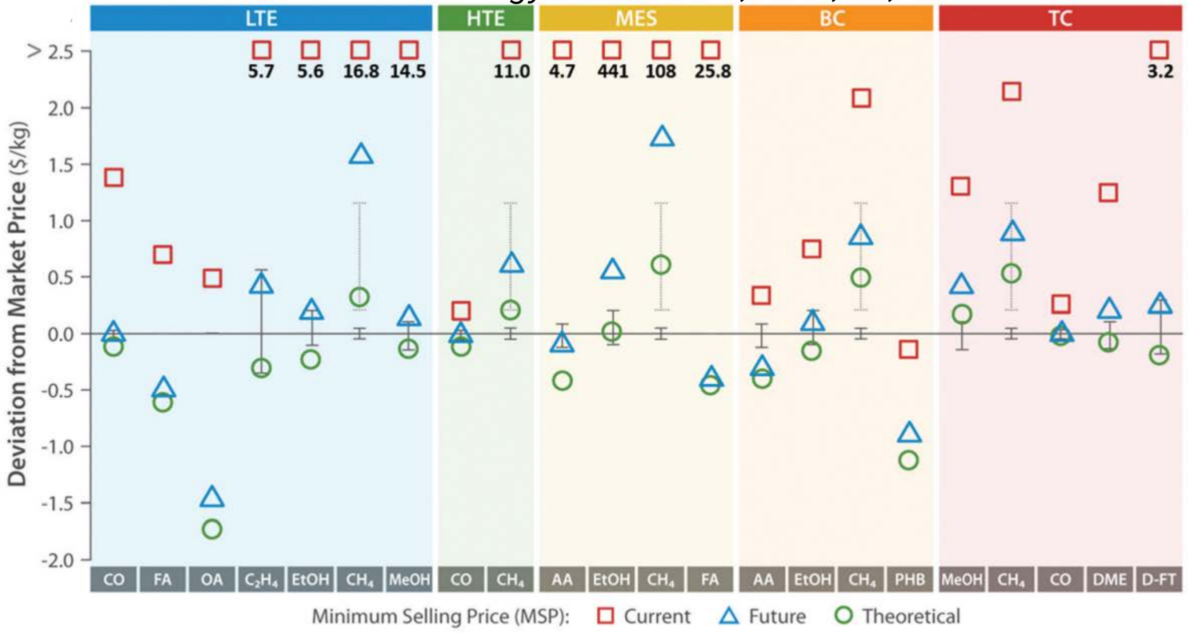
Funding Mechanism

Annual Operating Plan (AOP)

Project Overview: *Realities and Barriers of CO_2 Conversion*

- 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 (50% EE) is ca. >90 kWh/kg*
  - *Ammonia synthesis: ca. 8 kWh/kg*
- Transportation infrastructure is limited
- <u>CO_2 as feedstock does not guarantee a lower carbon intensity than the incumbent</u>

FY 21 Publication: *Energy Environ. Sci.*, 2021, **14**, 3664-3678



CO_2 products are expensive relative to the market

Challenge: *Overcome thermodynamic barriers to reach cost-competitive and environmentally-friendly fuels and chemicals for hard to abate sectors*

Project Overview: *Many Questions on CO_2 Conversion Feasibility*

Technical Feasibility

1. *Relative TRL of conversion technologies?*
2. *What kinds of products accessible?*
3. *Unique advantages & disadvantages?*

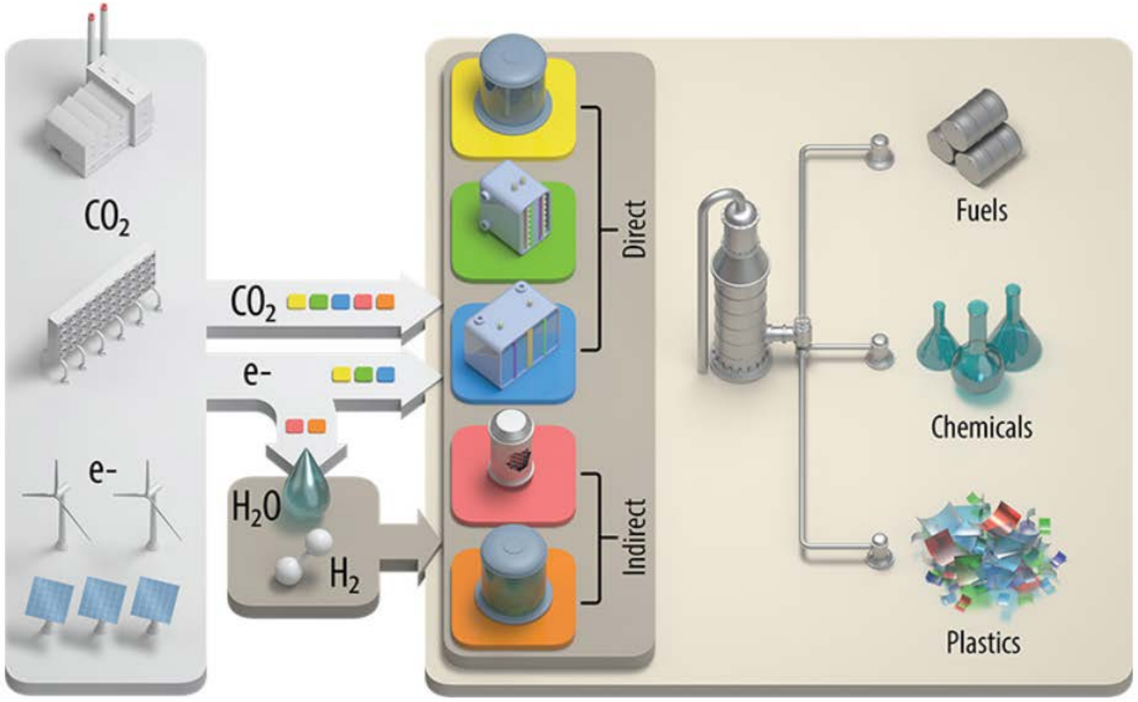
Economic Feasibility

1. *What are current and future cost estimates?*
2. *Greatest R&D needs? Cost drivers?*

Environmental Considerations

1. *Carbon and energy intensity*
2. *Sources and footprint of energy*

FY 21 Milestone: *Interactive Website Launched*



Opportunity: *Use analysis to baseline technologies, products, and identify best practices to accelerate CO_2 utilization deployment*

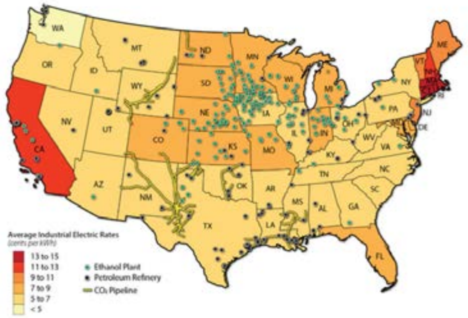
1. Approach

Collaboration & Info. Gathering

- Critical literature review and subject matter expert interviews
- Collaboration with CO_2RUe consortium members and projects

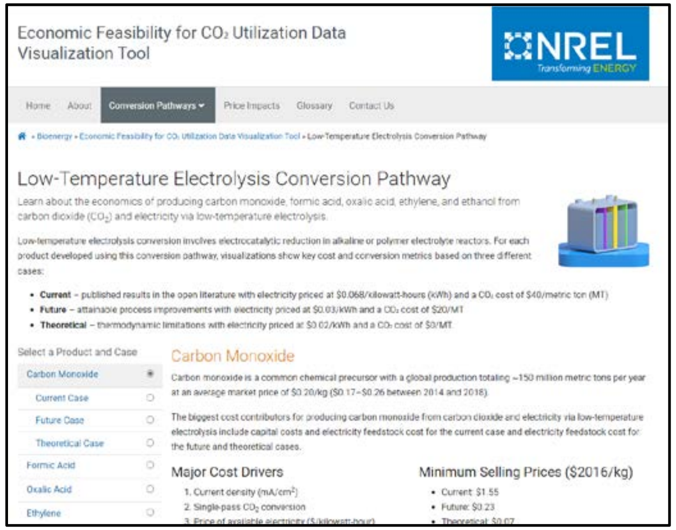
Analysis

CO₂ Source



- Comparative and detailed techno-economic/life-cycle analysis coupled with point-source integration
- Risk identification and uncertainty analysis

Public Outreach



- Peer-reviewed publications
- Online interactive toolkit
- Strategic roadmaps
- International consortia representation

Energy Environ. Sci., 2021, **14**, 3664-3678

1. Approach: FY22-FY23 Milestones

FY22 Milestones

Milestone Name/Description	Criteria	End Date
Manuscript Outline Development	Prepare outlines for manuscripts on (1) a generalized approach to integrating TEA, LCA, and uncertainty analysis and (2) a case study evaluating CO_2-to-ethylene technologies using integrated TEA/LCA.	12/30/2021
Establish CO_2-to-SAF Process Alternatives	Establish technological alternatives to our existing SOT CO_2-to-SAF pathway (CO_2 electrolysis → gas fermentation to ethanol → catalytic conversion of ethanol to SAF) and quantify reductions in cost and carbon intensity of these alternatives. This milestone is in response to risks identified in FY21 Q3 from subject matter expert interviews regarding the complexity of the existing SOT process and the commercial status of specific steps of the process (i.e., gas fermentation to ethanol).	3/31/2022
Interview Subject Matter Experts and Draft CO_2 to Fuels Strategic Plan	Using both past and new analysis combined with subject matter expert feedback, draft document summarizing opportunity space for delivering low-carbon fuels and products by 2050.	6/30/2022
Finalize Internal Draft of CO2 to Fuels Strategic Plan	Building on efforts in Q3, finalize and submit draft of CO_2-to-fuels strategic plan to internal and external advisory board members for feedback.	9/30/2022

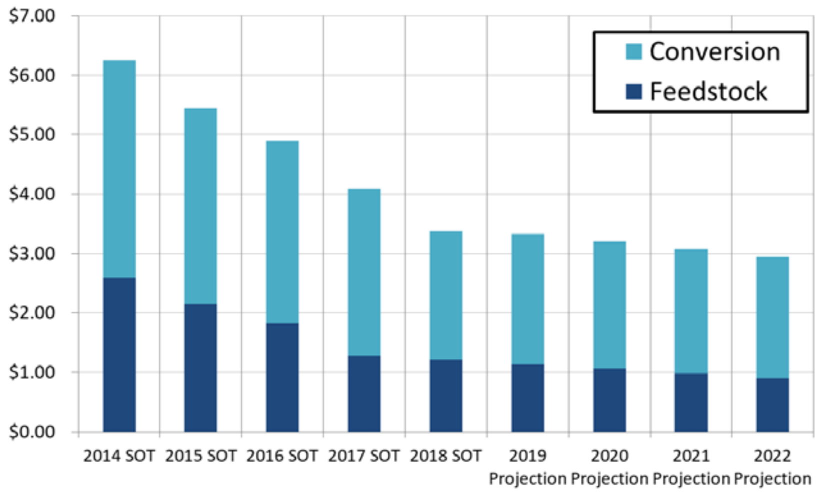
FY23 Milestones

Milestone Name/Description	Criteria	End Date
Publish Strategic Plan on CO_2 to Fuels	Incorporate internal and external advisory board feedback and BETO guidance in CO_2 to fuels strategic plan. Prepare separate manuscript for peer review journal publication capturing high-level perspectives.	12/30/2022
Update Existing TEA Models with current SOT data	Review and update existing CO_2-to-X process models (electrochemical, thermochemical, and biological) from our prior economic feasibility manuscript (Energy Environ. Sci., 2021, 14, 3664-3678) based on latest state of technology data.	3/31/2023
Assessment of Carbon Intensity and Life-Cycle Impacts Across CO_2 Reduction Technologies	Assess the carbon intensity and life-cycle impacts for the diverse CO_2 reduction technologies established in Q2. This work will leverage spreadsheet-based models developed in prior years to compare carbon intensity across technological approaches.	6/30/2023
Determination of TEA/LCA Trade-offs for the Field of CO_2 Reduction	Integrate TEA/LCA models and determine key trade-offs for the field of electron-driven CO_2 reduction spanning different technological approaches. This work will leverage our TEA and LCA from Q2 and Q3, respectively, and heuristics mined from the literature. This milestone will help the CO_2 reduction field identify and understand key decision points based on TEA and LCA implications	9/30/2023

1. Approach: Analysis Methodology

Approach:

- Design conceptual process including all major steps; build model in Aspen PLUS/Excel
- ***Scale basis:*** CO_2 stream generated from a 90M gallon per year ethanol biorefinery
- Calculate ***minimum selling price (MSP)*** using discounted cash-flow analysis
- Evaluate 3 scenarios with major assumptions and technical metrics based on:
  - ***SOT***: Results published in the open literature [$0.068/kWh; $40/mt CO_2 cost]
  - ***Future***: Attainable process improvements or engineering judgements [$0.03/kWh; $20/mt CO_2 cost]
  - ***Theoretical***: Thermodynamic limitations [$0.02/kWh; $0/mt CO_2 cost]
- Calculate ***carbon intensity (CI)*** from vetted references and databases
  - GREET
  - SimaPRO EcoInvent

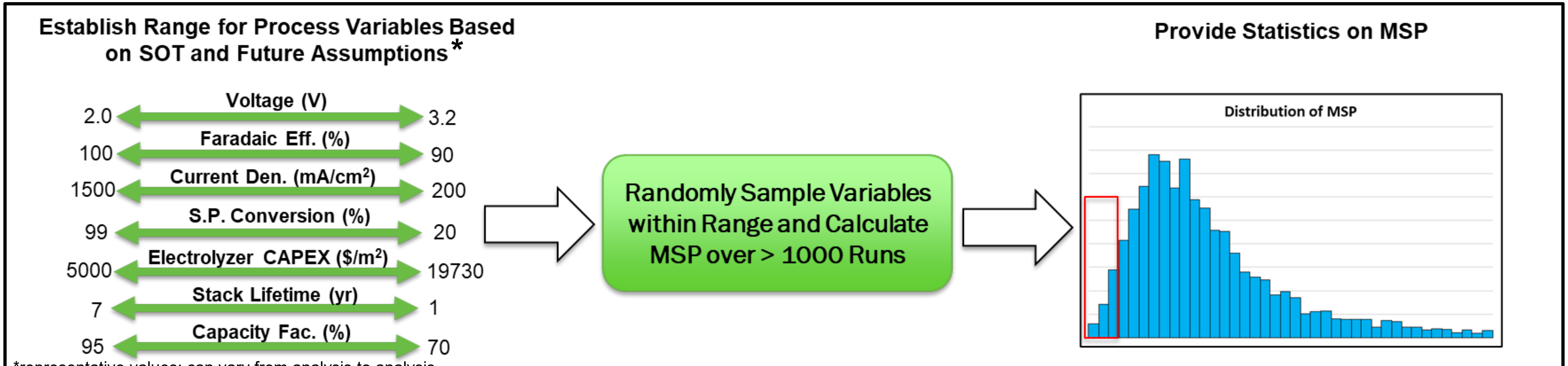


1. Approach: Analysis Methodology

Incorporating Uncertainty:

- Production cost and carbon intensity estimates often reported as “point values”
- Significant uncertainty in input values and future assumptions often present

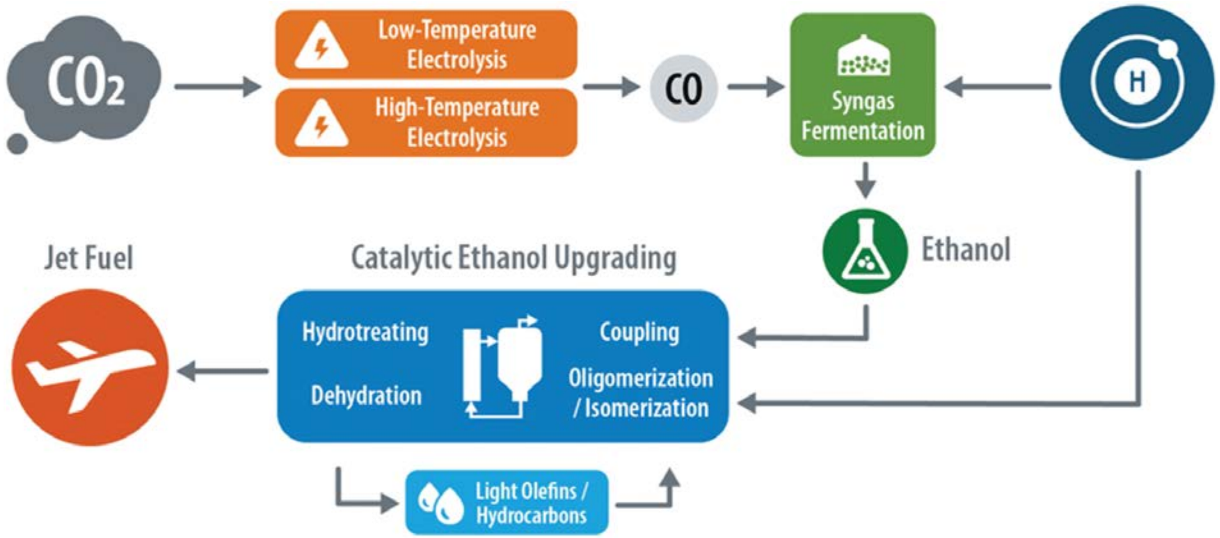
○ ***Monte Carlo Analysis*** offers a pathway towards minimally-biased analysis results

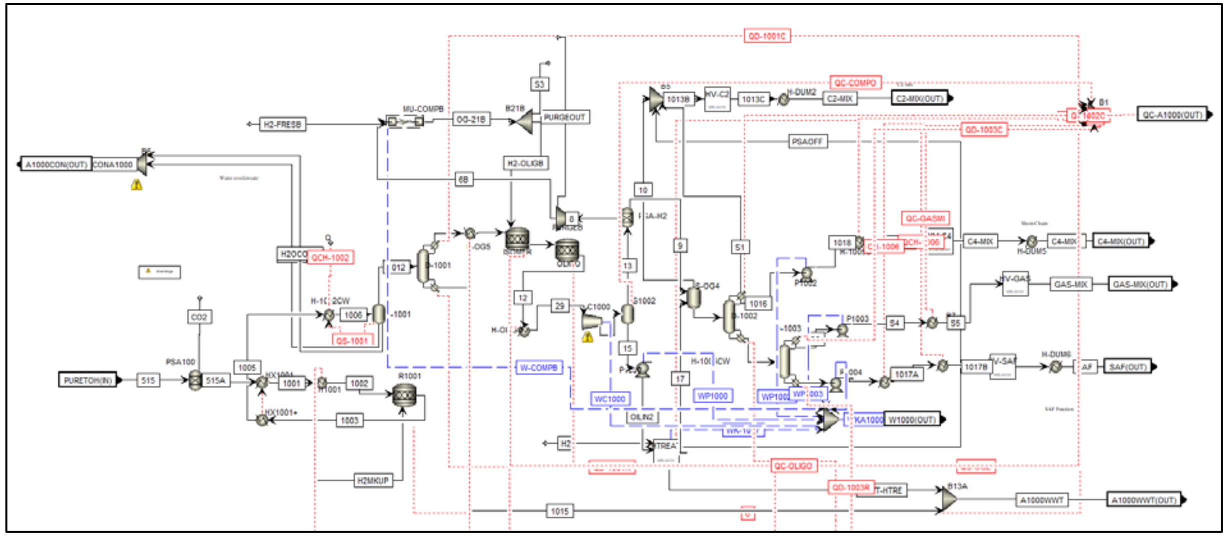


*representative values; can vary from analysis to analysis

MC analysis offers transparent communication of uncertainty associated with economic calculations coupled with assessment of key technical targets (red box)

2. Progress and Outcomes: Analyzing Bolt-on Tech for SAF





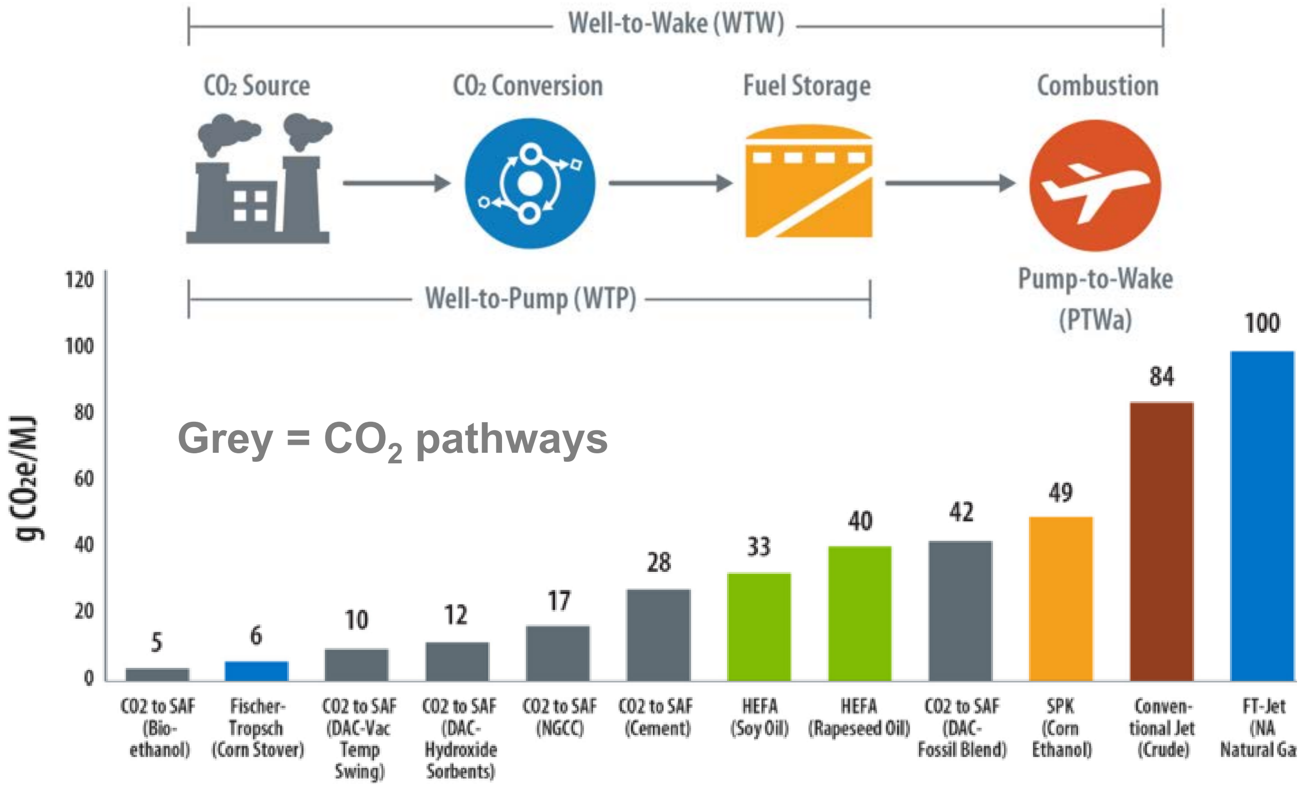
FY22 Pub: *Energy Environ. Sci., 2022, 15, 4798–4812*

- Evaluated promising process design for a bolt-on CO_2 conversion unit for SAF
- Process design leveraging core BETO strategic assets
- Near-term deployable option to reach 2030 decarbonization and SAF targets (3B gal/yr)

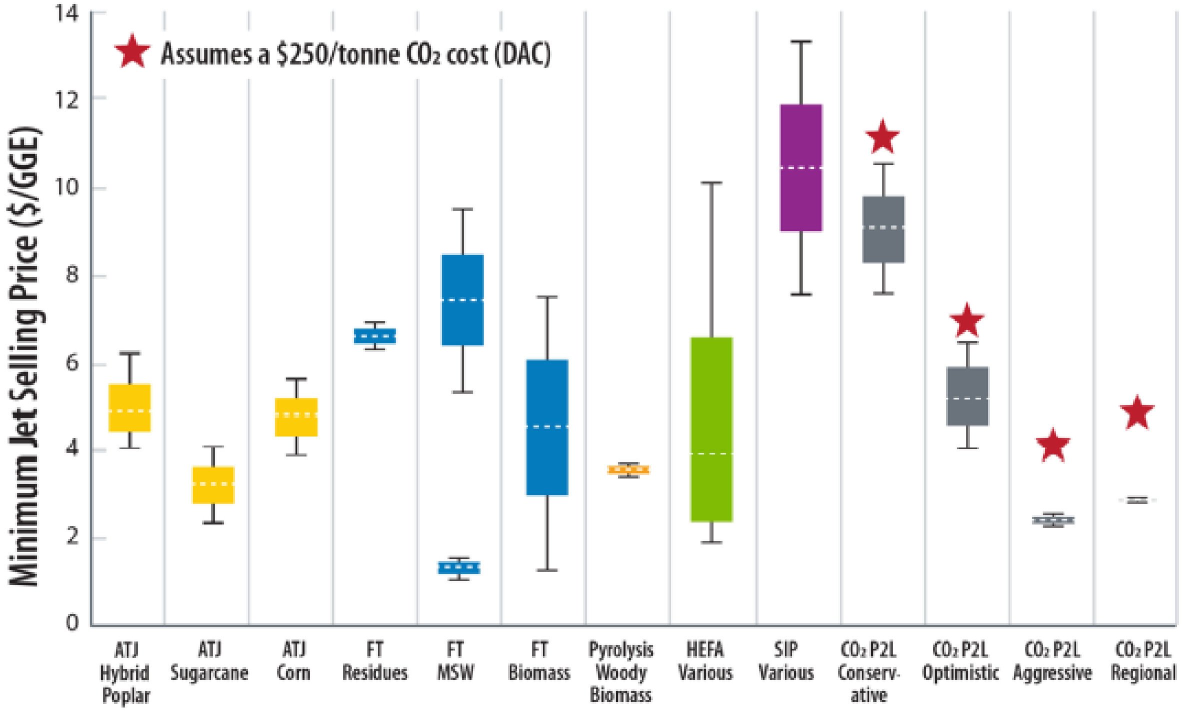
Dioxide Materials The CO2 Recycling Company™ LanzaTech Pacific Northwest NATIONAL LABORATORY

2. Progress and Outcomes: TEA/LCA for Bolt-on SAF Production

Life-cycle Analysis



Techno-economic Analysis



Well-to-wake emissions show opportunities for 50 - 94% CI reduction relative to conventional practices

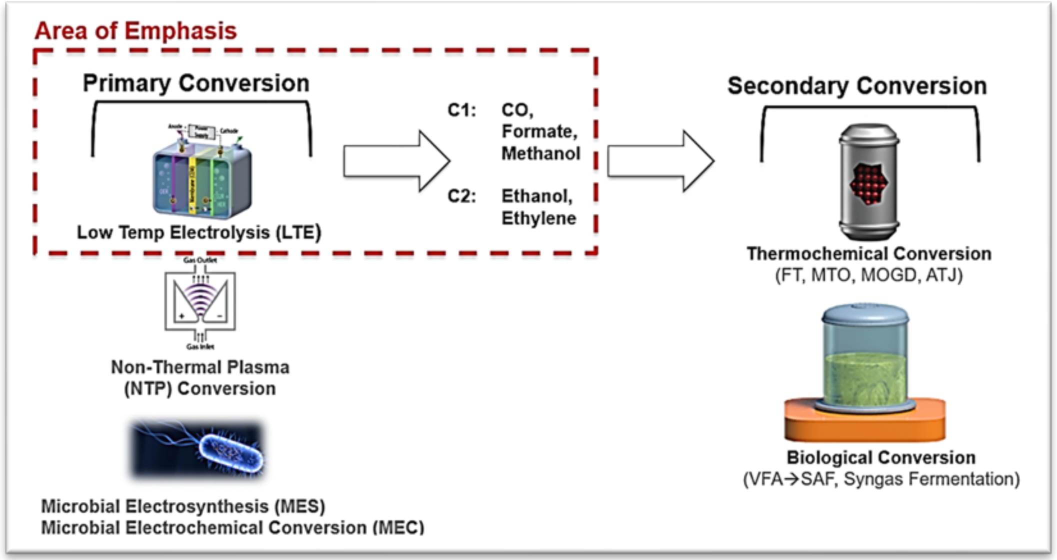
CO_2-derived SAF shows pathways to low cost with aggressive future performance and market assumptions

FY22 Pub: *Energy Environ. Sci., 2022, 15, 4798–4812*

2. Progress and Outcomes: A Strategic Plan for CO_2 Conversion

How to drive decarbonization of fuels and chemicals by 2050?

- *Where is the “white space”?*
- *Where are the opportunities for applied R&D across **low-to-moderate TRL**?*
- *What are the economic and environmental targets that should be achieved?*




Commercializing CO_2-based Fuels and Chemicals by 2050: R&D Gaps and Opportunities in the Direct Electrification of CO_2 Conversion

R. Gary Grim, Jack Ferrell, Zhe Huang, Ling Tao, Mike Resch

National Renewable Energy Laboratory

- *Availability of CO_2*
- *Identification of promising chemicals*
- *Strategic R&D needs*
- *Accelerated testing needs*
- *Commercialization timelines*
- *Technical targets*

2. Progress and Outcomes: Setting Future Targets

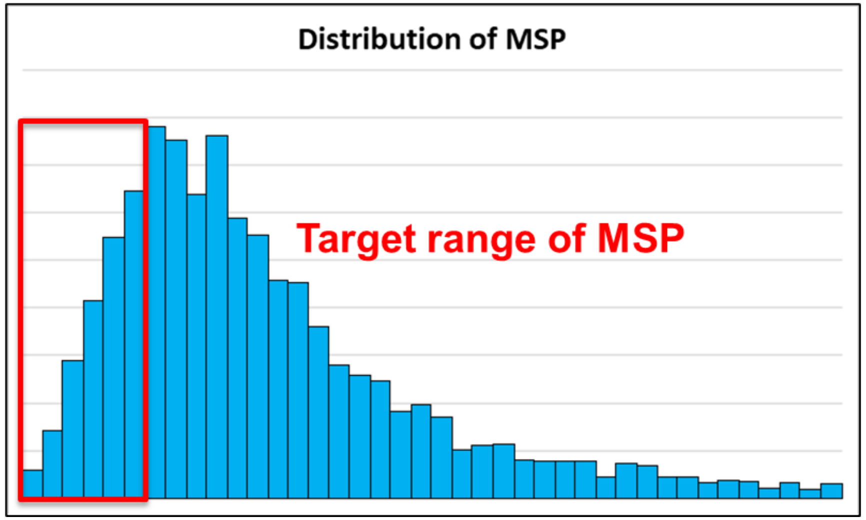
Chemical-specific Technical Targets for LTE CO_2 Conversion

	Faradaic Eff. (SOT, %)*	Faradaic Eff. (Target, %)	Current Density (SOT, mA/cm^2)*	Current Density (Target, mA/cm^2)	Voltage (SOT, V)*	Voltage (Target, V)
CO	98	95	200	1040	3.00	2.56
FA	94	95	140	850	3.50	2.59
MeOH	78	87	41.5	1075	2.67	2.57
C_2H_4	60	95	1550	1045	3.23	2.59
C_2H_5OH	52	81	300	1115	2.20	2.55

General Technical Targets for LTE CO_2 Conversion

Metric	SOT Value*	Target Value
Single Pass Conversion (%)	1 – 43	>67
Electrolyzer Unit Cost (\$/m^2)	> 19,730	< 10,600
Stack Lifetime (hours)	10 – 4,000	> 35,000
Process Capacity Factor (%)	no data	>83

Monte Carlo analysis helps to identify specific metric by metric targets to promote an economically competitive CO_2-derived product

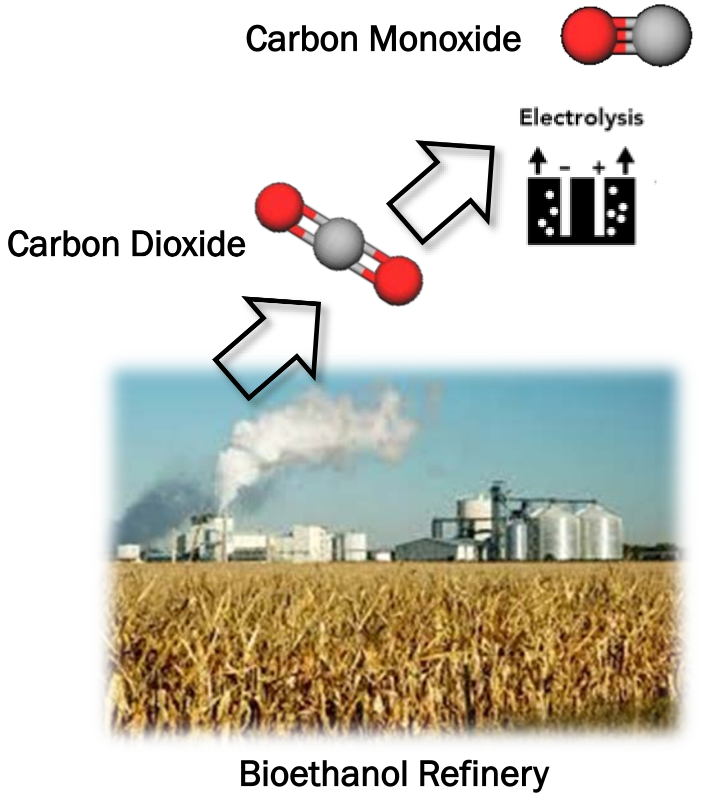


**SOT = State of Technology*
Target data shown assumes target product price of market +50%

2. Progress and Outcomes: Theoretical Timeline for Scale Up

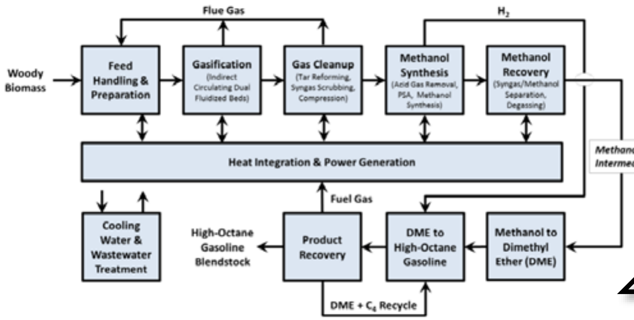
FY23 Pub: *In Prep.*

Stage	Carbon Monoxide at Bioethanol Refineries (2e-)				Technical Metrics							Target	
	Power		CO_2 TpY	MWhe/y	Voltage (V)	FE (%)	CD (mA/cm2)	Conv. (%)	Unit Cost ($/m2)	Stack Lifetime (hr)	Capacity Factor (%)	Year	
	110	MWe	266,500	820,000	2.56	95	1,040	71	$11,175	35,040	83	2050	★
Commercial	20	MWe	53,300	164,000	2.63	95	950	71	$12,092	31,693	77	2047	
	4	MWe	10,660	32,800	2.70	96	860	71	$13,008	28,346	72	2044	
Pilot	1	MWe	2,665	2,050	2.77	96	770	71	$13,925	24,999	66	2041	
	250	kWe	666	410	2.83	96	680	71	$14,841	21,651	60	2038	
Scaling/Reliability	50	kWe	133	82	2.90	97	590	59	$15,758	18,304	55	2035	
	10	kWe	27	8	3.02	97	440	38	$17,286	12,726	45	2030	
	1	kWe	3		3.13	98	290	17	$18,813	7,147	36	2025	
Concept/Research	**100**	**W**			**3.2**	**98**	**200**	**5**	**$19,730**	**3,800**	**30**	**2022**	
	10	W										2020	
	1	W										2014	

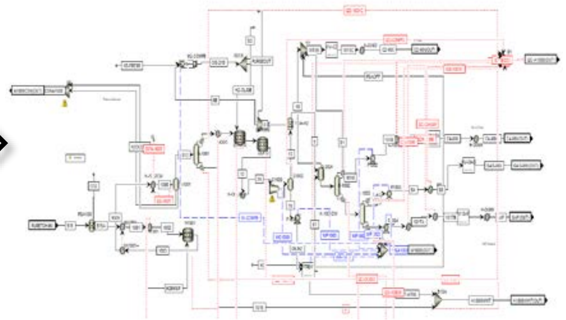


Reaching technical targets and commercializing CO_2-derived products *from direct electrification potentially* achievable by 2050 with sustained gains in metrics as outlined, informed by historical precedents in the PEM H_2O electrolysis industry

2. Progress and Outcomes: Integrated TEA/LCA



1. Block Flow Diagrams

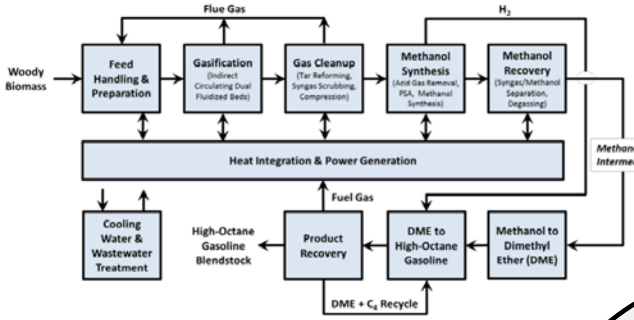


2. Rigorous Process Model

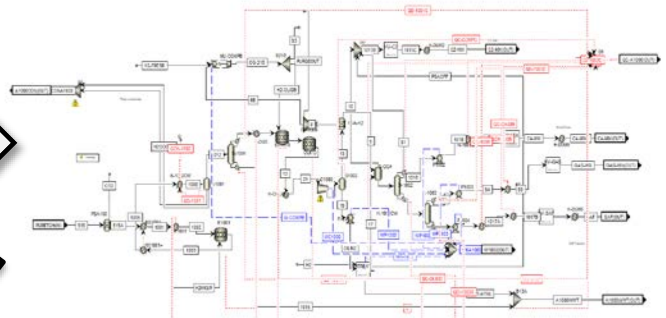
3. TEA

4. LCA

Conventional Workflow
(processes optimized for price)



1. Block Flow Diagrams



2. Rigorous Process Model

3. TEA+LCA

Integrated Workflow
(processes optimized around price and environmental parameters simultaneously)

3. Impact: *Peer-reviewed Publications*

ACS Energy Letters

http://pubs.acs.org/journal/aelccp

REVIEW

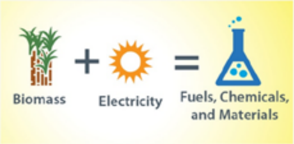
Electrochemical Routes for the Valorization of Biomass-Derived Feedstocks: From Chemistry to Application

Francisco W. S. Lucas, R. Gary Grim, Sean A. Tacey, Courtney A. Downes, Joseph Hasse, Alex M. Roman, Carrie A. Farberow, Joshua A. Schaidle,* and Adam Holewinski*

Cite This: *ACS Energy Lett.* 2021, 6, 1205−1270 Read Online

ACCESS | Metrics & More | Article Recommendations

ABSTRACT: The drive to reduce consumption of fossil resources, coupled with expanding capacity for renewable electricity, invites the exploration of new routes to utilize this energy for the sustainable production of fuels, chemicals, and materials. Biomass represents a possible source of platform precursors for such commodities due to its inherent ability to fix CO_2 in the form of multi-carbon organic molecules. Electrochemical methods for the valorization of biomass are thus intriguing, but there is a need to objectively evaluate this field and define the opportunity space by identifying pathways suited to electrochemistry. In this contribution we offer a comprehensive, critical review of recent advances in low-



ACS Energy Lett. 2021, 6, 4, 1205−1270 **Impact Factor: 23.1**

Energy & Environmental Science

ROYAL SOCIETY OF CHEMISTRY

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Cite this: *Energy Environ. Sci.*, 2021, 14, 3664

The economic outlook for converting CO_2 and electrons to molecules†‡

Zhe Huang, § R. Gary Grim, § Joshua A. Schaidle* and Ling Tao*

Shifting towards a circular carbon economy in the face of rising global population and diminishing natural reserves represents one of the greatest challenges facing mankind. CO_2 reduction reactions powered by renewable electricity offer a possible route to transform our incumbent linear consumption economic model by tapping into the over 10 gigatonnes of carbon emitted globally each year in the form of CO_2. However, many critical questions for CO_2 reduction remain unanswered across the varied pathway-product combinations such as (1) what is the near-term economic viability? (2) what opportunities exist for transformational R&D to reduce cost? (3) what is the impact of CO_2 price? (4) how does renewable electricity intermittency affect the production costs? Herein we perform a comprehensive economic assessment of CO_2 reduction across five major electricity-driven technologies using a scale basis of a 200 million gallon per year bioethanol facility (ca. 600 kilotonnes CO_2 per year) as the CO_2 source. From this framework we address these key issues and report the outlook for the near-, mid-, and long-term production of 11 promising carbonaceous products while providing guidance to the research community on key cost drivers and R&D needs. Our analysis shows that with modest technical advancements and an accompanying reduction in electricity price to \$0.03 kW h^{-1} and CO_2 price to \$20 per tonne, 8 out of 11 CO_2-derived products have the potential to reach production costs at parity with, or even lower than, current market prices.

Received 5th November 2020, Accepted 14th May 2021

DOI: 10.1039/d0ee03525d

rsc.li/ees

Energy Environ. Sci., 2021, **14**, 3664-3678 **Impact Factor: 38.5**

Energy & Environmental Science

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Cite this: *Energy Environ. Sci.*, 2022, 15, 4798

Electrifying the production of sustainable aviation fuel: the risks, economics, and environmental benefits of emerging pathways including CO_2†

R. Gary Grim,*[a] Dwarak Ravikumar,[a] Eric C. D. Tan,[a] Zhe Huang,[a] Jack R. Ferrell III,[a] Michael Resch,[a] Zhenglong Li,[b] Chirag Mevawala,[c] Steven D. Phillips,[c] Lesley Snowden-Swan,[c] Ling Tao[a] and Joshua A. Schaidle*[a]

Due to challenges related to weight and travel distance, the medium to long-haul aviation sector is expected to remain reliant on liquid hydrocarbon fuels into the foreseeable future, representing a persistent source of CO_2 emissions within the anthropogenic carbon cycle. As the world grapples with the environmental fallout from rising CO_2 emissions, a prevailing strategy to mitigate the impact of air travel is through the utilization of sustainable aviation fuels (SAF) produced from biogenic carbon sources such as fats, oils, greases, and biomass. However, with the demand for SAF expected to grow substantially in the coming decades, there is concern around the availability of these feedstocks at scale. Recent studies have proposed that this potential gap in supply could be closed by utilizing CO_2 as a complementary source of carbon combined with renewable electricity to drive the chemical transformation. In this study, a cross-cutting comparison of an emerging CO_2-to-SAF pathway with existing routes to SAF is performed, revealing the potential for CO_2-derived SAF to be competitive both in terms of costs and carbon intensity, further diversifying future options for SAF and providing a complementary option for the conversion of CO_2-to-SAF beyond the decades old methanol to olefins (MTO) and Fischer–Tropsch (FT) technologies. In addition, we discuss potential technical, market, and systems integration risks for the ultimate scale-up and commercialization of the pathway identified herein.

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DOI: 10.1039/d2ee02439j

rsc.li/ees

Energy Environ. Sci., 2022, **15**, 4798-4812 **Impact Factor: 38.5**

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Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

ELSEVIER

A comparative techno-economic analysis of renewable methanol synthesis from biomass and CO_2: Opportunities and barriers to commercialization

Kylee Harris, R. Gary Grim, Zhe Huang, Ling Tao*

Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, 15013 Denver W Pkwy, Golden, CO 80401, United States

HIGHLIGHTS

- Renewable methanol synthesis via biomass gasification and CO_2 electrosynthesis.
- Generated a comprehensive techno-economic assessment addressing four key metrics.
- Biomass-to-methanol technologies are the most economically viable in the near-term.
- Future markets may favor waste-CO_2 utilization pathways.

Appl. Energy. 2021, 303, 117637 **Impact Factor: 9.7**

WILEY-VCH

Edited by Giorgio Graditi and Marialaura Di Somma

Technologies for Integrated Energy Systems and Networks

3

Power Conversion Technologies: The Advent of Power-to-Gas, Power-to-Liquid, and Power-to-Heat

Joshua A. Schaidle, R. Gary Grim, Ling Tao, Mark Ruth, Kevin Harrison, Nancy Dowe, Colin McMillan, Shanti Pless, and Douglas J. Arent

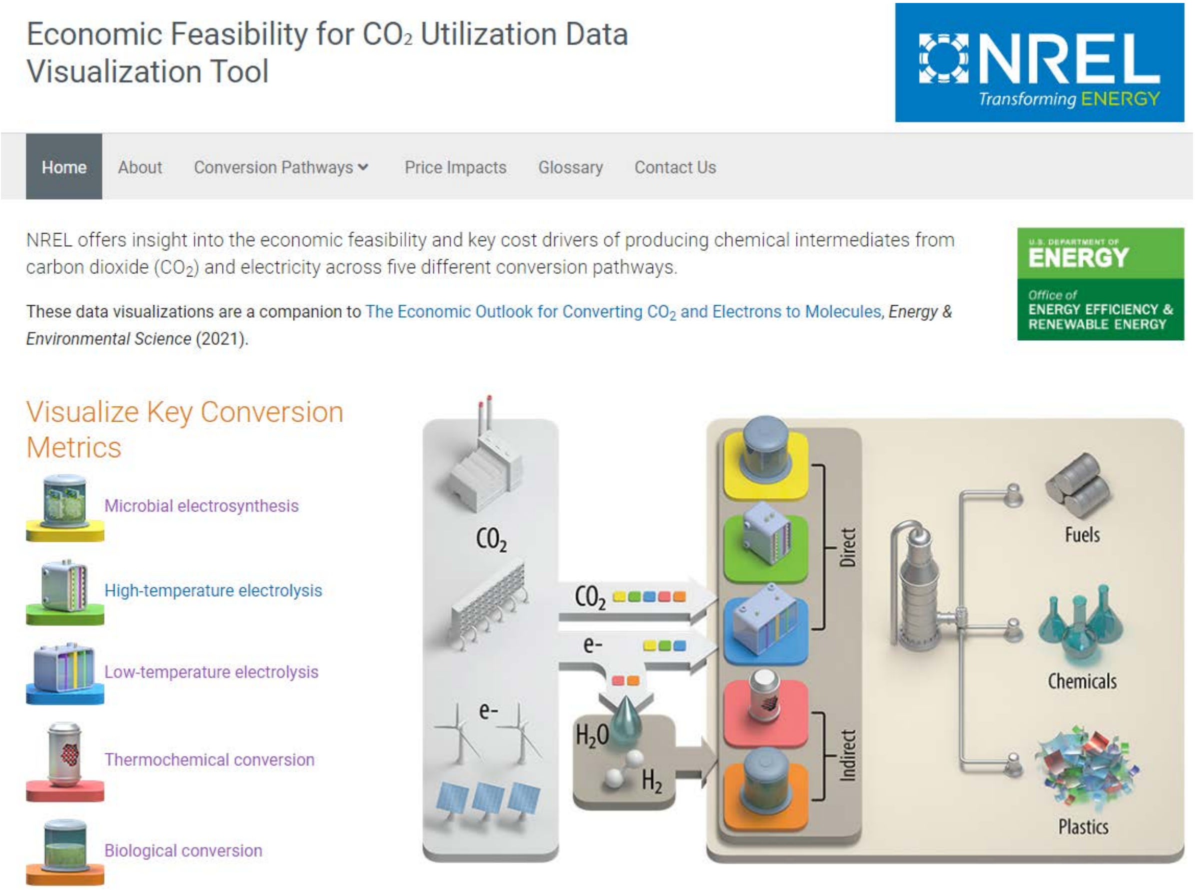
National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO, 80401, USA

March 2022

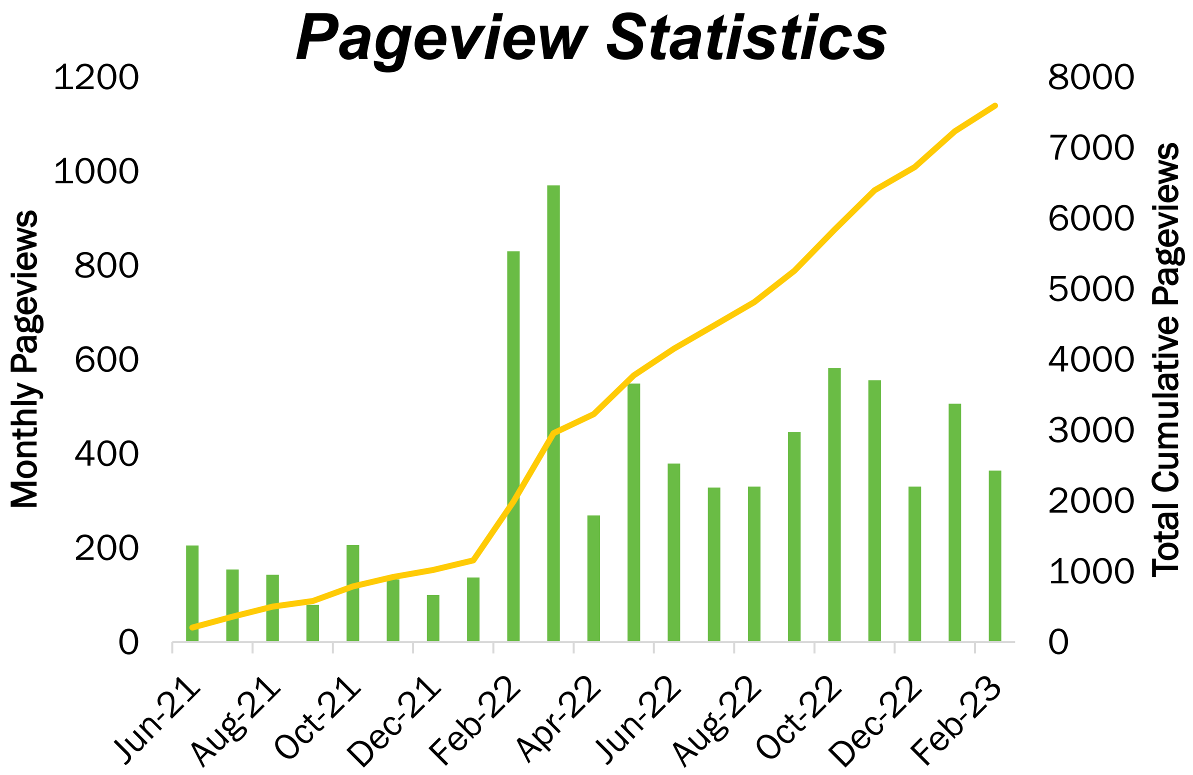
doi.org/10.1002/9783527833634.ch3

5 publications + internal technical reports delivered since previous peer-review meeting

3. Impact: *Interactive Website*



https://www.nrel.gov/bioenergy/co2-utilization-economics/



Positive reactions and increased engagement across a wide variety of users: industry (SpaceX), VC firms, academia, national laboratories

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 accelerate and drive industrial decarbonization and CO_2 conversion

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, the CO_2RUe consortium, and the broader scientific and industrial communities

Outcomes: (1) FY21 – Analyze ***novel bolt-on compatible CO_2 reduction pathways*** to fuels or products from standalone biorefineries and (2) FY22 – Develop and publish a ***comprehensive strategic plan*** for achieving industrial decarbonization goals via CO_2 conversion, with inclusion of outyear technical, cost, and carbon intensity targets

Relevance to Bioenergy Industry: Identify risks and opportunities for leveraging low-cost electricity to improve biorefinery carbon utilization. Identified specific and actionable technical metrics to advance the deployment of technologies

Thank You

NREL/PR-5100-85579

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CO_2 Reduction and Upgrading for e-Fuels Consortium

U.S. DEPARTMENT OF ENERGY