

Opportunities and Challenges in Converting CO₂ into Fuels and Chemicals

Josh Schaidle

June 27th, 2023

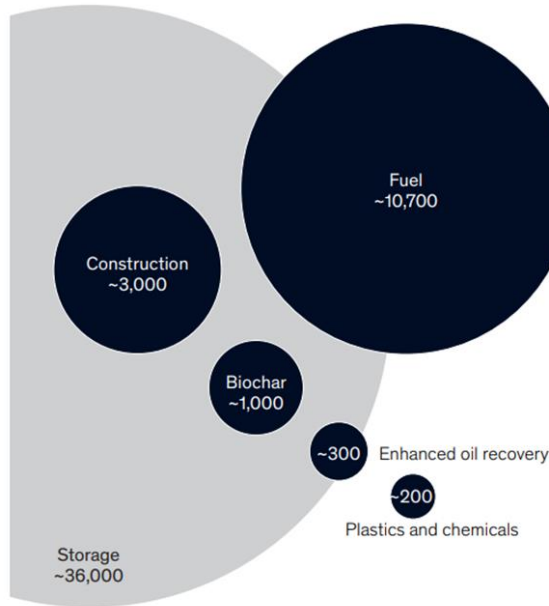
NASEM Committee on Carbon Utilization

Market Size and Value of CO₂ Utilization Products

Market Size

Technical potential of CCUS in 2030, metric megatons of CO₂ per year¹

■ Carbon capture and use ■ Carbon capture and storage



Selected examples

Fuel

Synfuel and macro- or microalgae fuel

Enhanced oil recovery (EOR)

Conventional or unconventional CO₂ EOR and CO₂ EOR in residual oil zones

Construction materials

Cement and aggregates

Plastics and chemicals

Polyethylene, polypropylene, carbon fiber, and methanol

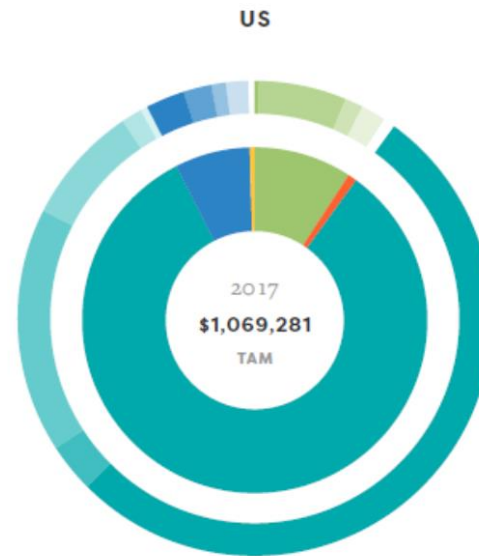
Biochar

A charcoal derived from burning organic agriculture- and forestry -waste products

Storage

Saline aquifers and depleted oil and gas reservoirs

Market Value



PRODUCT

\$ IN MILLIONS

BUILDING MATERIALS

\$101,130

- Cements
- Concretes
- Asphalts
- Aggregates

\$1,240
\$65,000
\$12,190
\$22,700

WOOD-BASED PANELS

\$12,508

FUELS

\$882,149

- Gasoline
- Jet Fuel
- Diesel
- Natural Gas
- Ethanol
- Biodiesel

\$543,400
\$38,760
\$186,660
\$83,705
\$23,550
\$6,074

PLASTICS

\$71,694

- High density polyethylene
- Linear Low density polyethylene
- Low density polyethylene
- Polypropylene

\$25,393
\$20,502
\$11,522
\$4,276

CHEMICALS

\$1,800

AGRICULTURE AND AQUACULTURE

N/A

CONSUMER GOODS

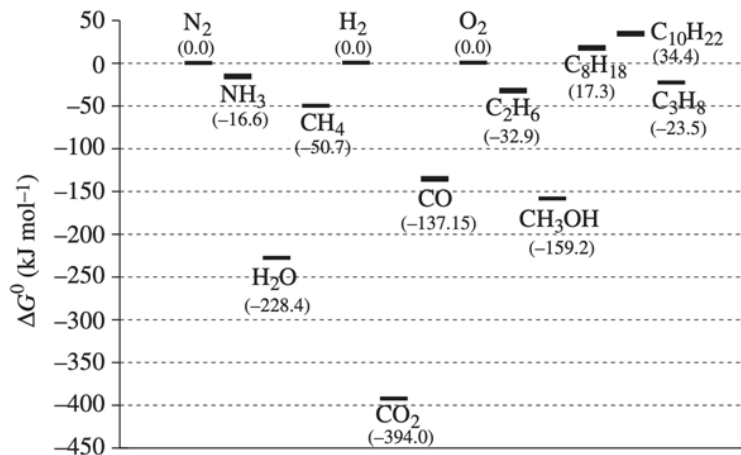
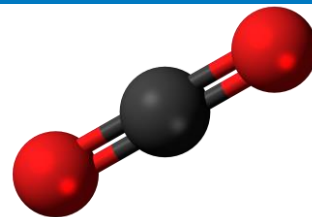
N/A

TOTAL

\$1,069,281

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 >40 kWh/kg
 - Ammonia synthesis: ca. 8 kWh/kg*
- Pipeline availability is limited
- CO₂ as feedstock ≠ lower carbon intensity than the incumbent



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

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

Which Products to Target and Why

What is the Feasibility of CO₂ Utilization?

Technical Feasibility

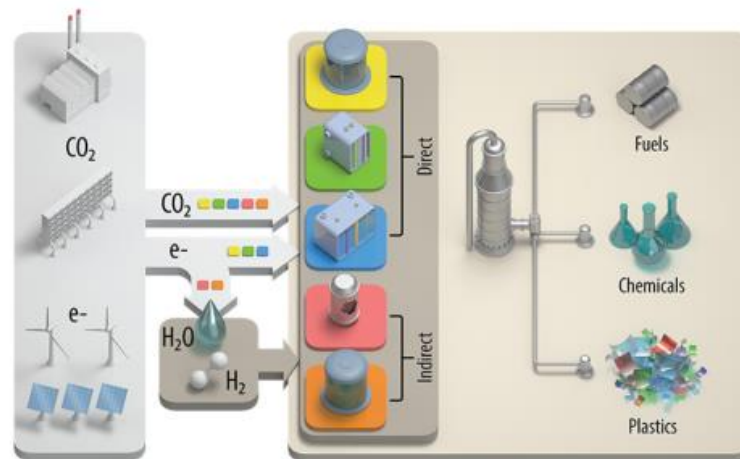
1. *Relative TRL of conversion technologies?*
2. *What kinds of products accessible?*
3. *Unique advantages & disadvantages?*

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*

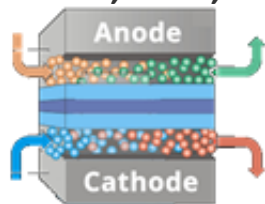


<https://www.nrel.gov/bioenergy/co2-utilization-economics/>

Opportunity: *Use analysis to baseline technologies, products, and identify best practices to accelerate CO₂ utilization deployment*

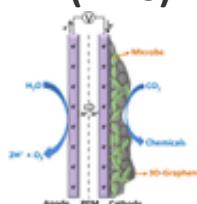
Technology Snapshot

Electrolysis (Alkaline, PEM, SOEC)



CO
C₂H₄
C(s)
HCOOH
C₂H₅OH
C₂O₄⁻
C₃H₇OH
CH₃COOH
CH₄
CH₃OH
C₃H₆O
C₂H₄O₂
C₂H₄O
C₂H₆O₂
CH₃COCH₃
C₂H₂O₂

Microbial Electrosynthesis (MES)



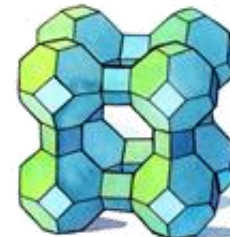
HCOOH
C₂H₅OH
C₃H₇OH
CH₃COOH
C₂H₄COO⁻

Fermentation



C₂H₅OH
C₃H₇OH
CH₃COOH
CH₄

Thermochemistry



CO
C₂H₄
CH₄
CH₃OH
C₃H₆

Aim to answer:

- What are the major technical challenges for each technology?
- What are the most impactful near-term R&D needs?
- What are near- and long-term opportunities?
- Which products should be targeted?

Technical Perspective

Species	Market Price (\$/kg)	\$/e- req. (x10 ³) ^a	Global Prod. (MMT/y)	Equiv. # Coal Plants
Carbon Monoxide	1.20	16.8	~2.5	1.1
Carbon Monoxide (syngas)	0.31	4.3	150.0	66.4
Formic Acid	0.74	17.0	0.6	0.2
Carbon Nanotubes	110.2	331.0	0.003	0.0
Methanol	0.40	2.2	80.5	31.1
Methane	0.18	0.4	250.0	193.2
Acetic Acid	0.59	4.4	14.0	5.8
Ethylene Glycol	0.97	6.0	26.7	10.7
Acetaldehyde	~1.9	8.4	0.9	0.5
Dimethyl Ether	0.64	2.5	3.7	2.0
Ethanol	0.61	2.3	77.0	41.4
Ethylene	0.72	1.7	145	128.1
Acetone	0.93	3.4	6.4	4.1
Propionaldehyde	~1.6	5.8	0.5	0.3
Propylene	1.01	2.4	98.6	84.4
1-Propanol	1.43	4.8	0.2	0.1
Isopropanol	1.32	4.4	1.91	1.2
Oxalate	n.d.	n.d.	n.d.	n.d.
Glyoxal	n.d.	n.d.	n.d.	n.d.
Glycolaldehyde	n.d.	n.d.	n.d.	n.d.
Hydroxyacetone	n.d.	n.d.	n.d.	n.d.
Propionate	n.d.	n.d.	n.d.	n.d.
Allyl Alcohol	n.d.	n.d.	n.d.	n.d.

Evaluated 20+ products across 5 CO₂ reduction technologies to assess ease of formation:

- Metrics: Formation rate, selectivity, energy efficiency and technology readiness level (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/cm² (or commercial TC), Intermediate: 200 > j > 100 mA/cm², Low: < 100 mA/m²

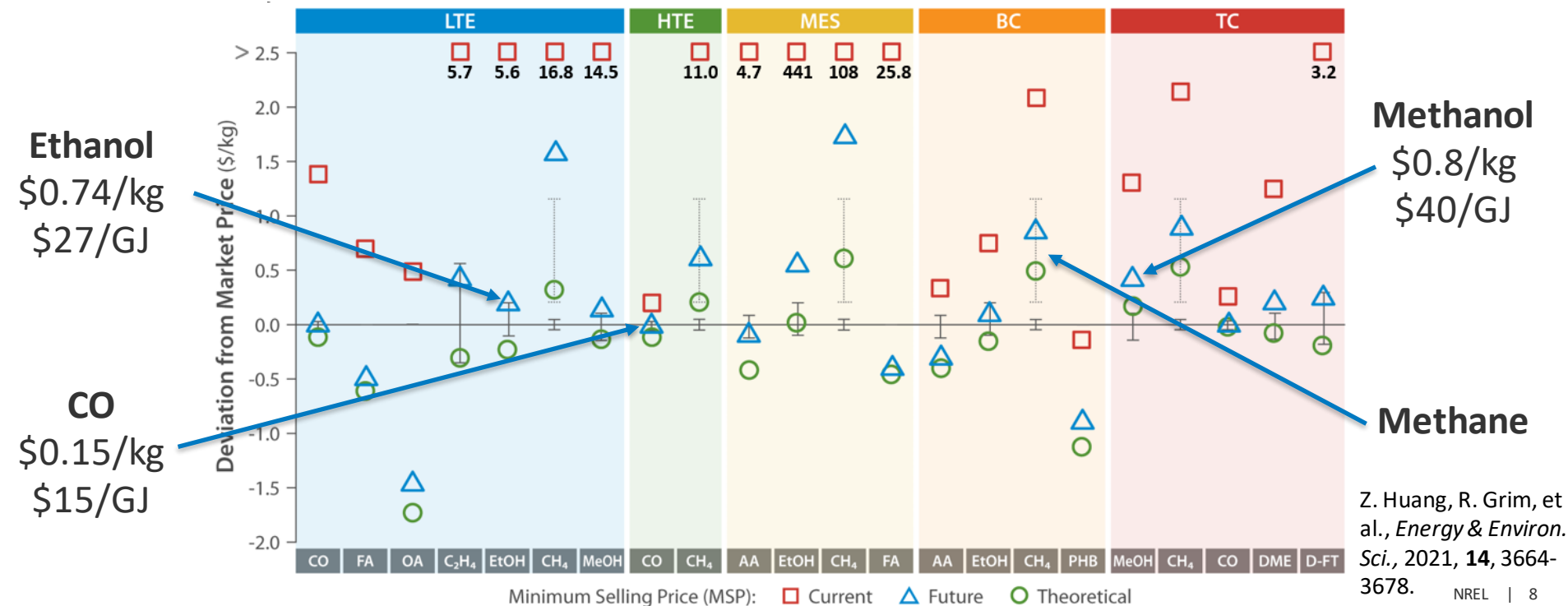
b: High: >80%, Intermediate 80% > FE > 60%, Low: < 60%

c: High: >60%, Intermediate: 60% > EE > 40%, Low: < 40%

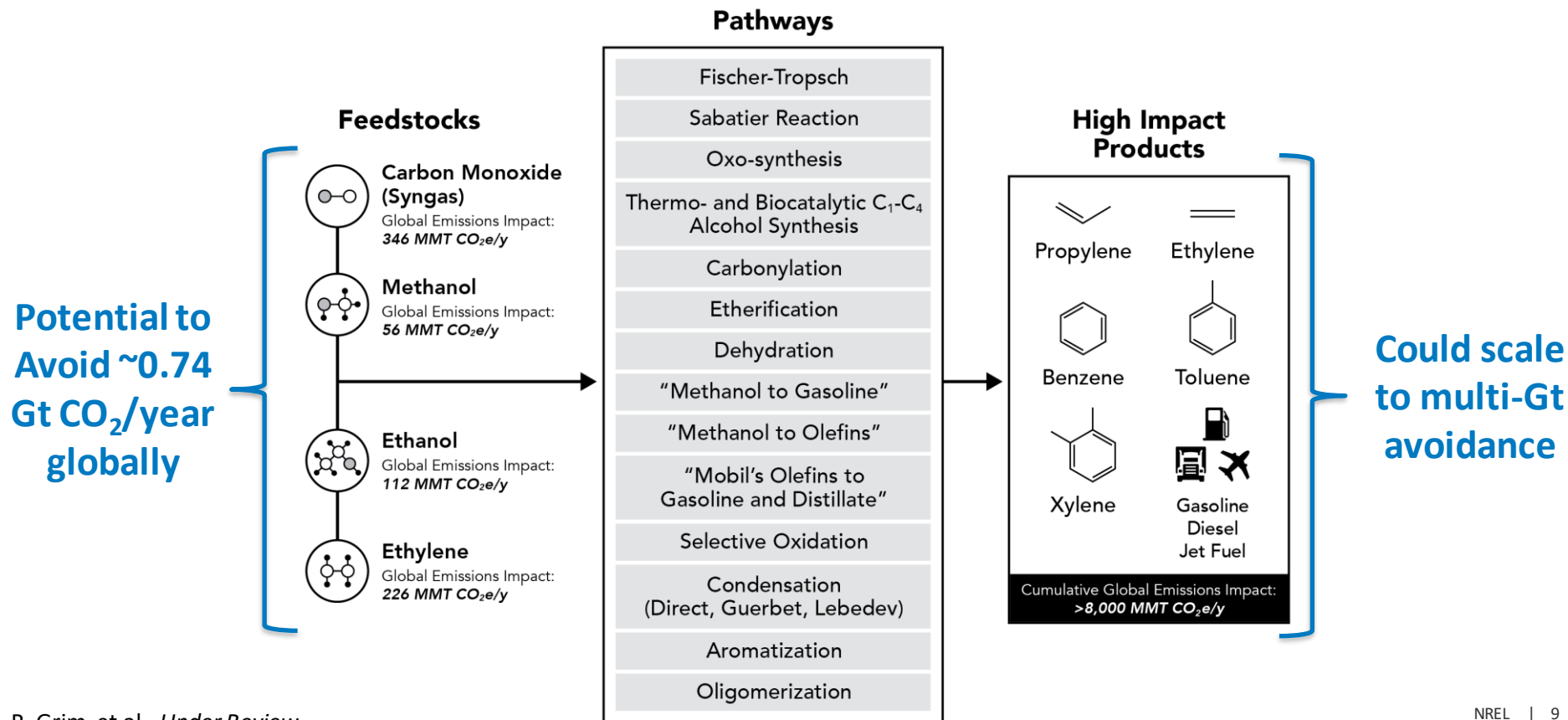
d: High: Operated at TRL > 6, Intermediate: Operated TRL 4-6, Low: Operated TRL 1-3

Economic Perspective

Economics are challenging under current conditions, but 8 of 11 products can reach market parity in future scenario

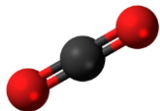


Decarbonization Perspective



What about Biomass?

CO₂

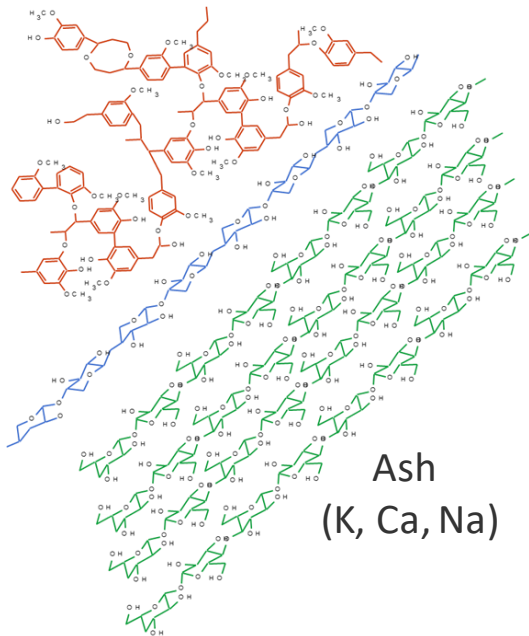


+ Impurities



C₁-C₃ Intermediates
“Build up”

Biomass

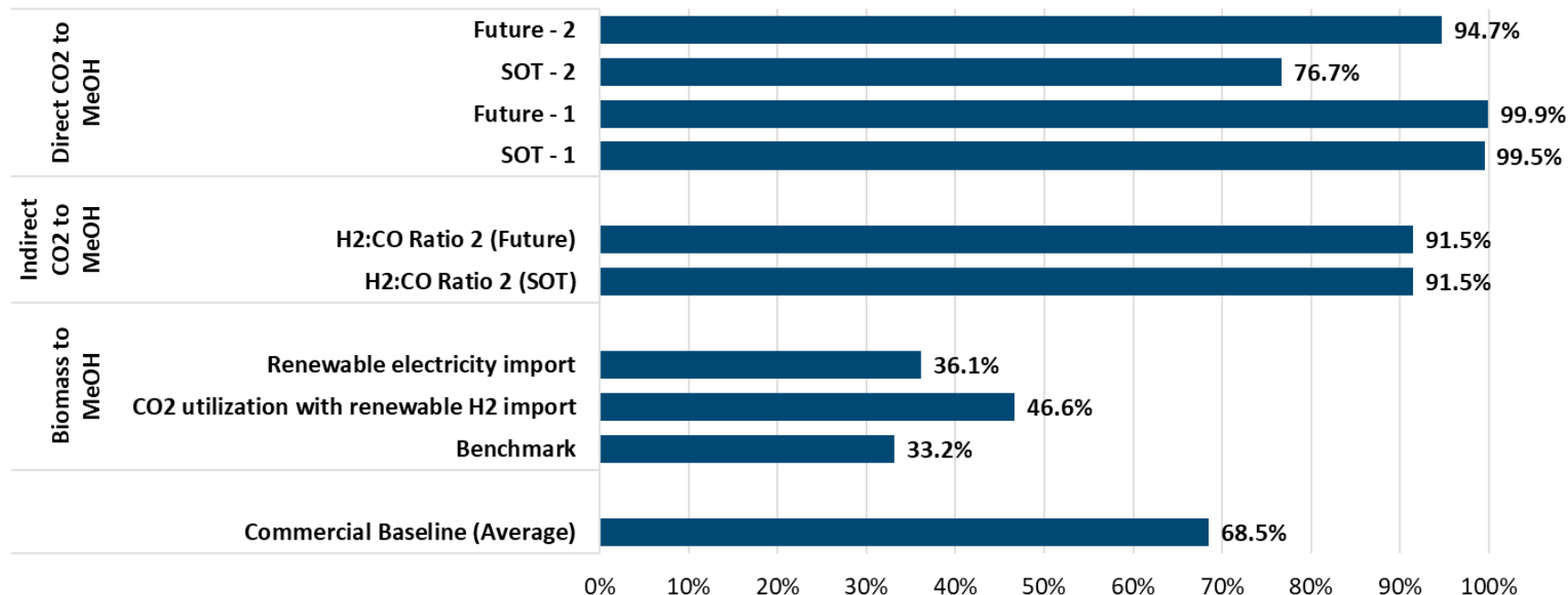


Retain Structure in C₄₊ products
“Break and Reshape”

Methanol Production: Biomass vs. CO₂

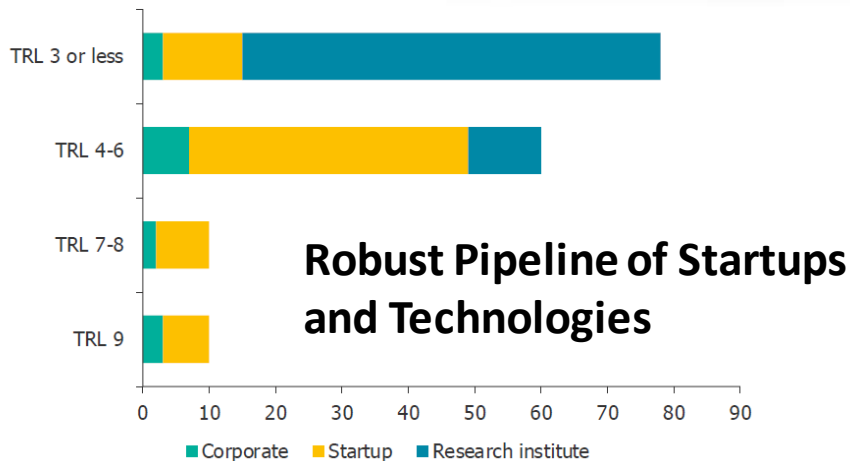
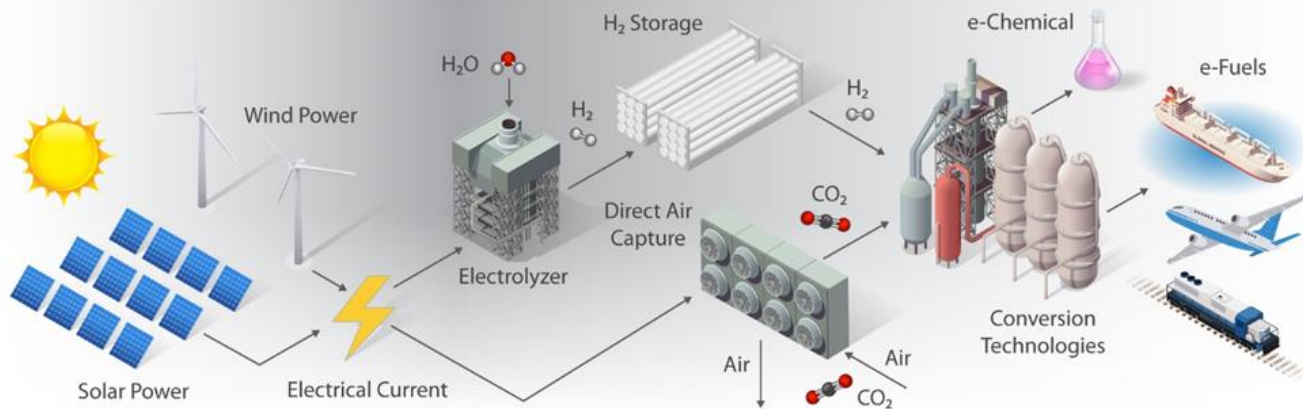
Electrochemical CO₂ Utilization

Carbon Efficiency (%)



Challenges, Opportunities, and Needs

CO₂ Utilization to Fuels and Chemicals

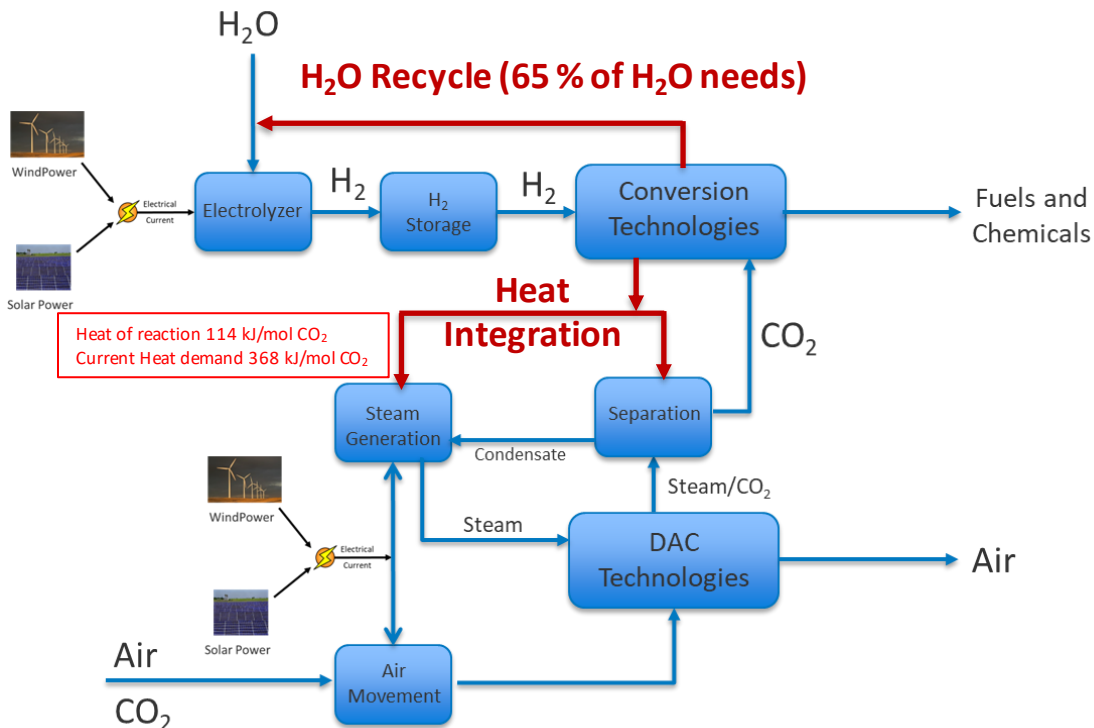


Key Considerations and Challenges:

- Limited integration and diverse unit ops
- Intermittent operation / load following
- Energy intensity and land use
- Cost and market demand
- Scale and rate of CO₂ emissions relative to CO₂ conversion needs

Need for Integration Science

Systems Perspective

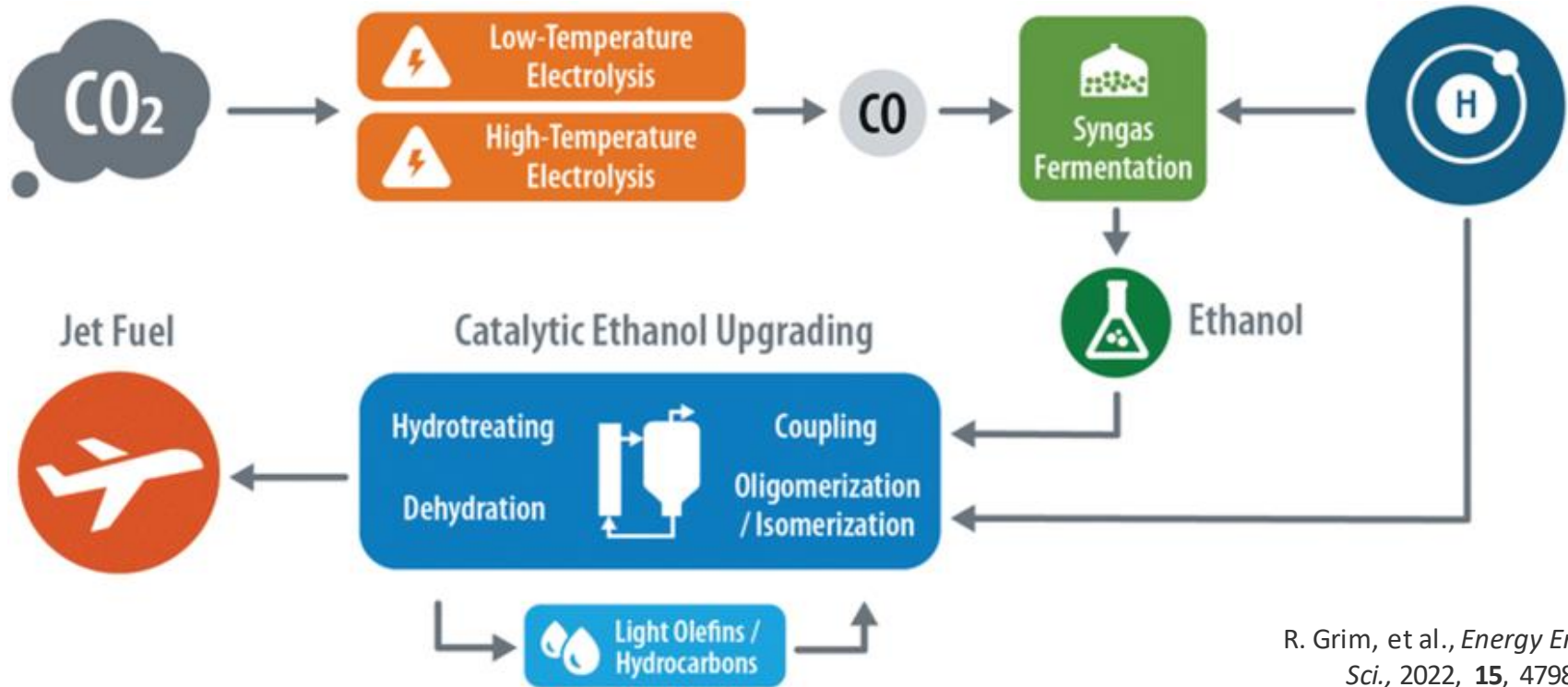


Example Research Questions:

- How can cost be reduced through heat and water integration?
- What are the real cost trade-offs of lower-quality intermediate streams (e.g., CO₂ concentration and impurities)?
- What limits scalability of emerging technologies?
- How can costs be reduced through process intensification?

Producing Sustainable Aviation Fuel (SAF) from CO₂

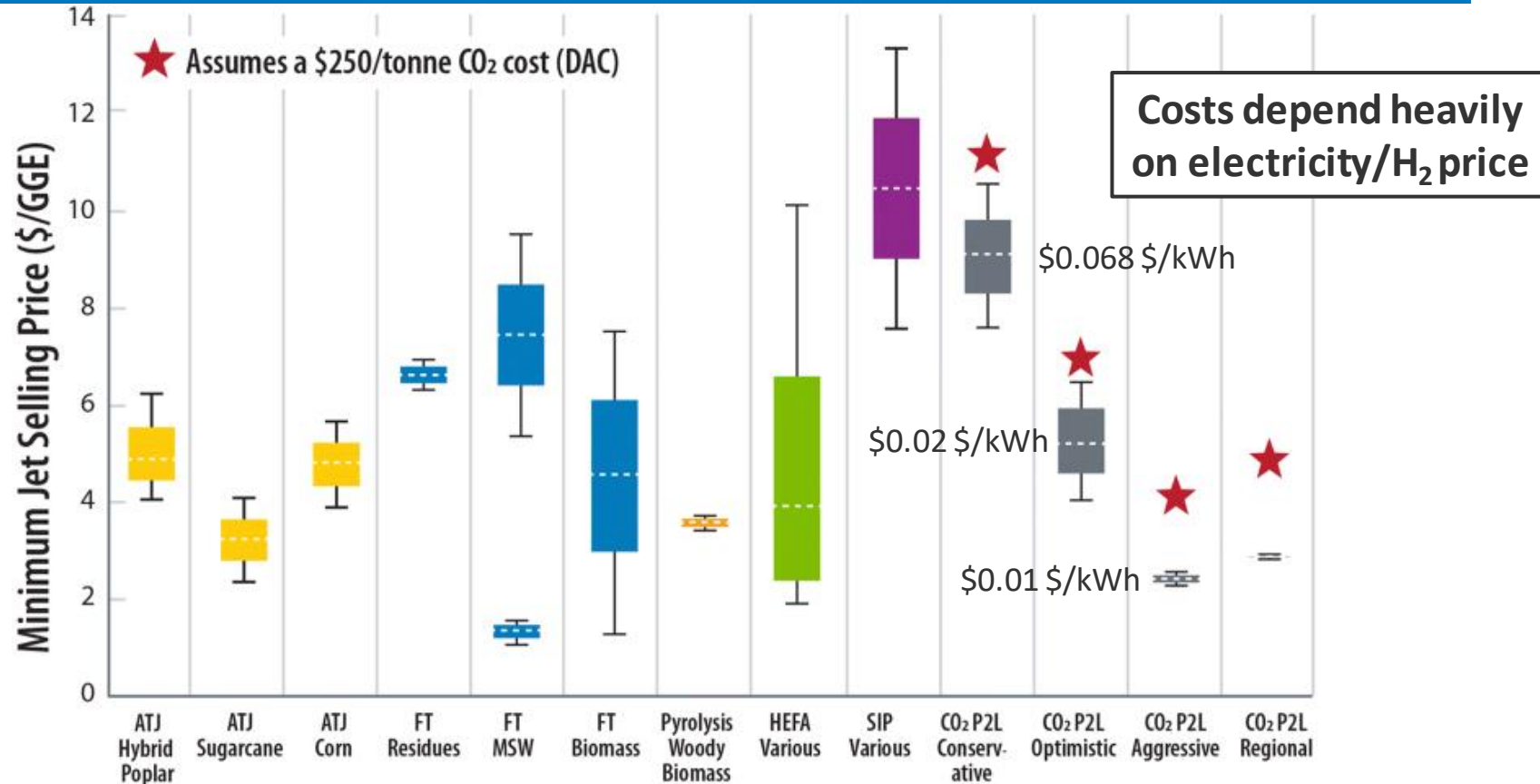
Developed a heat-integrated process model in Aspen Plus



R. Grim, et al., *Energy Environ. Sci.*, 2022, **15**, 4798-4812.

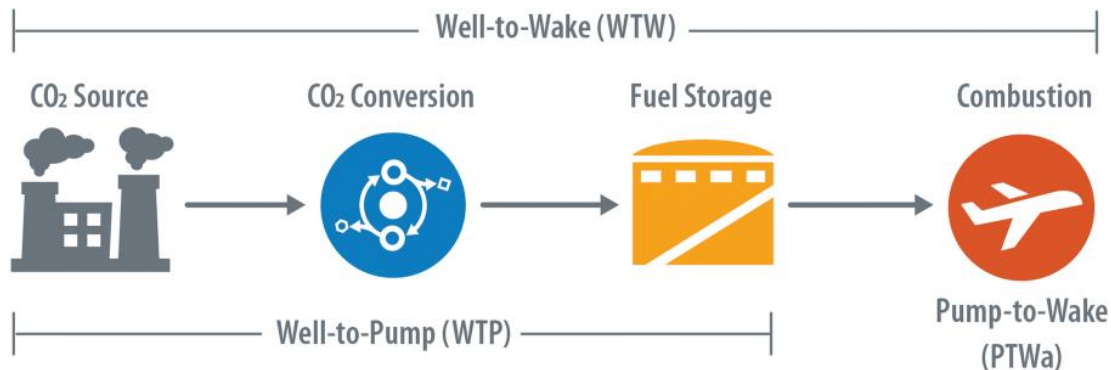
****NOTE:** This is *one* possible pathway to reach SAF from CO₂ and is not necessarily indicative of the most optimized or “best” design. All results are reflective to this pathway only.

Cost of SAF Production Relative to Alternatives

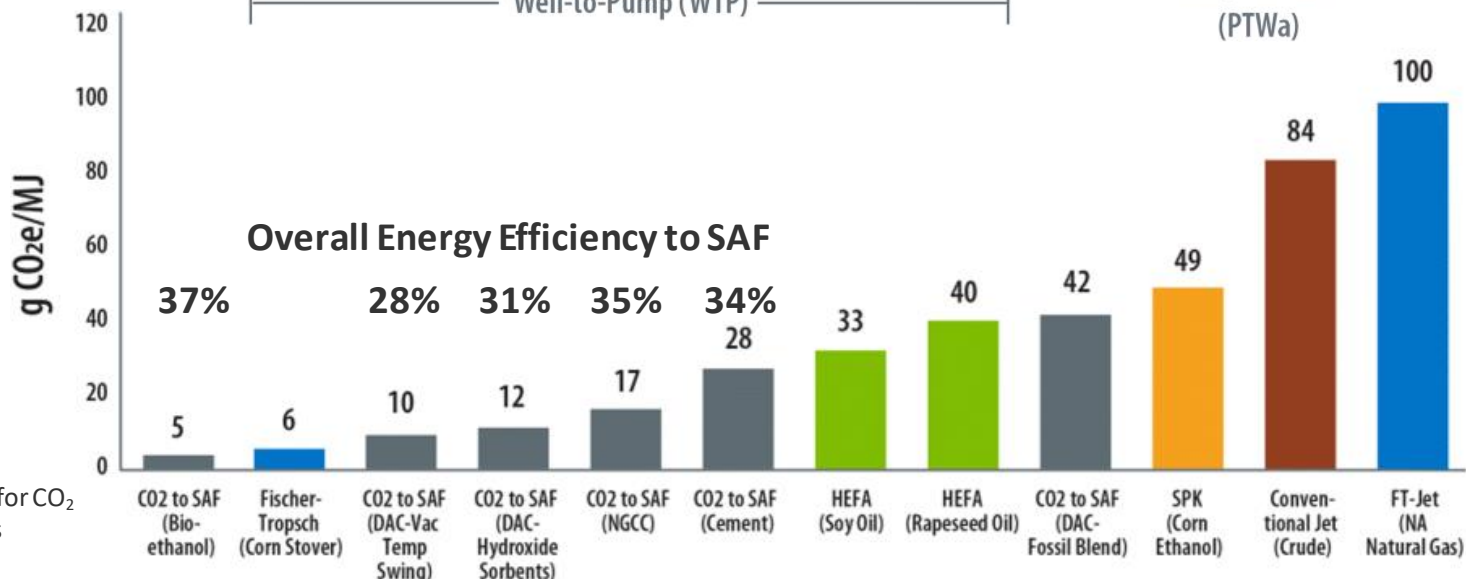


Carbon Intensity of SAF Production

LCA Boundary Conditions



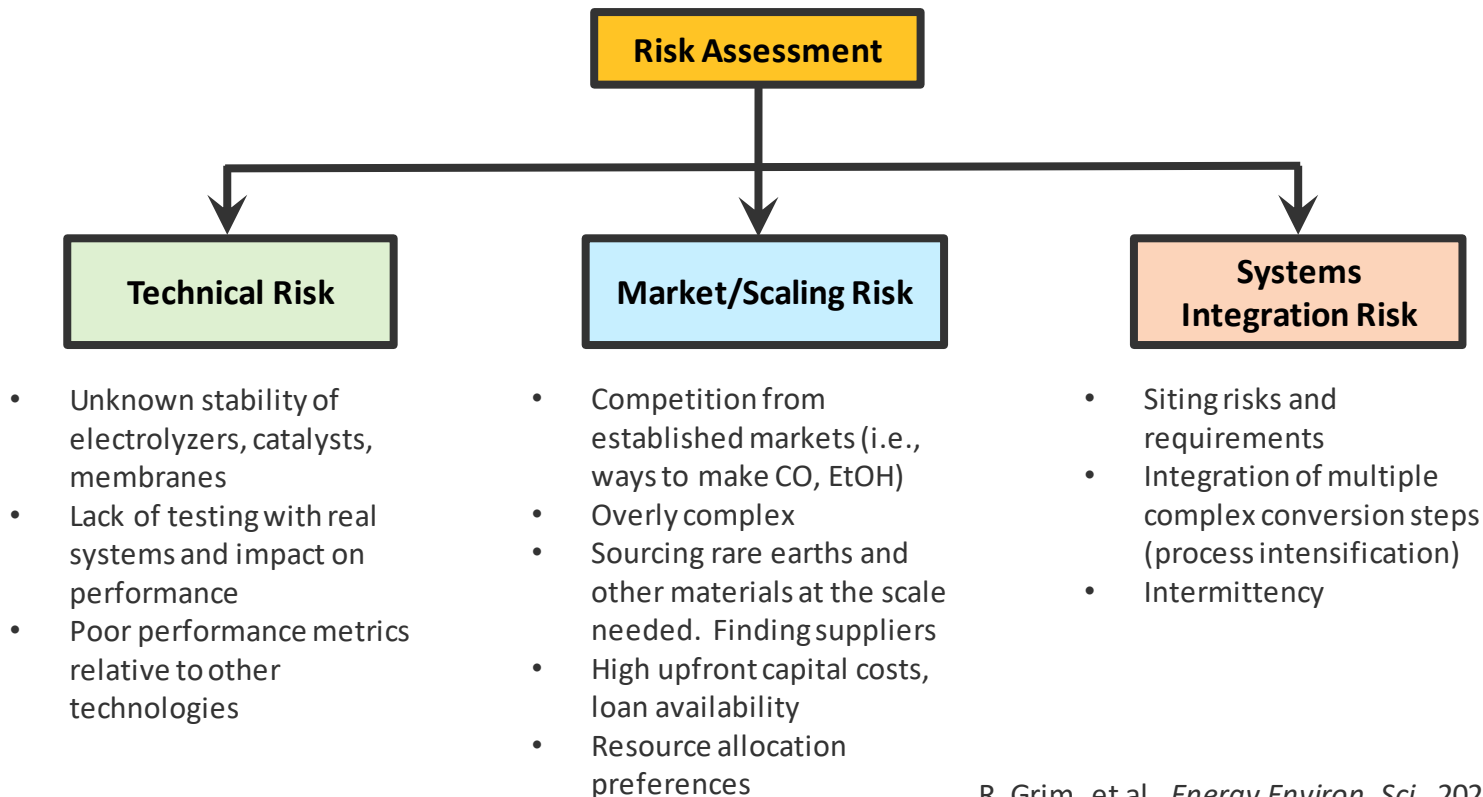
Results



*Assumes use of renewable energy for CO₂ conversion process
 **Based on GREET

CO₂-to-SAF Risk Assessment

Identified risks by interviewing subject matter experts



Opportunity: Reactive Carbon Capture

Emerging Approach: Reactive Capture of CO₂

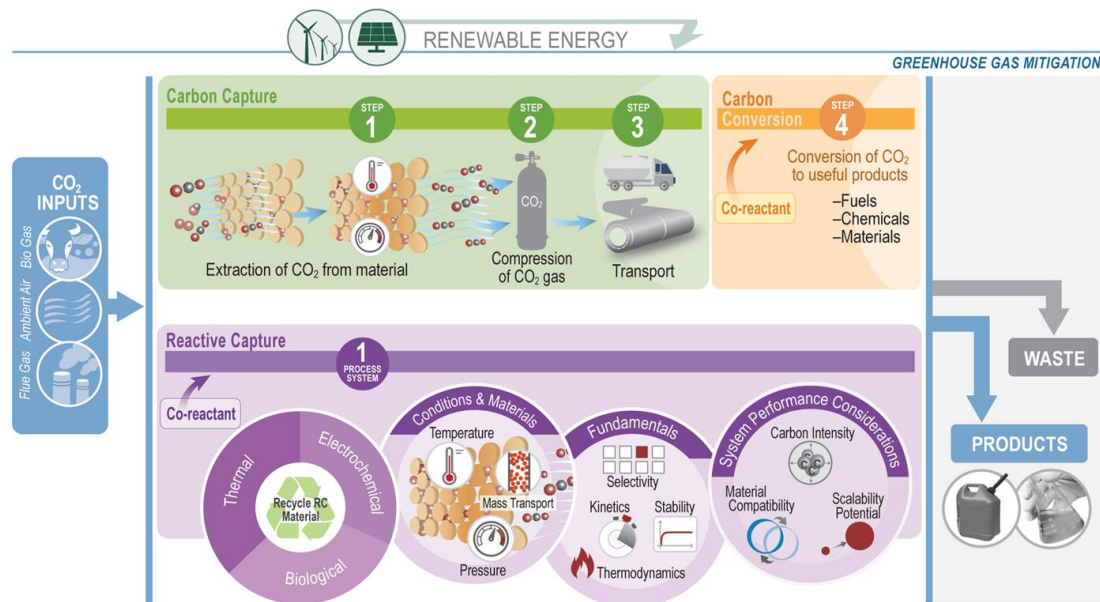
Reactive Capture Definition: The coupled process of capturing CO₂ from a mixed gas stream and converting it into a valuable product *without* going through a purified CO₂ intermediate

Can Include:

- Integration of CO₂ separation and conversion in one step
- Integration of separation and conversion in one unit
- Process intensification

Product Targets:

Form a valuable product, or mixture of products, in a more reduced state than CO₂

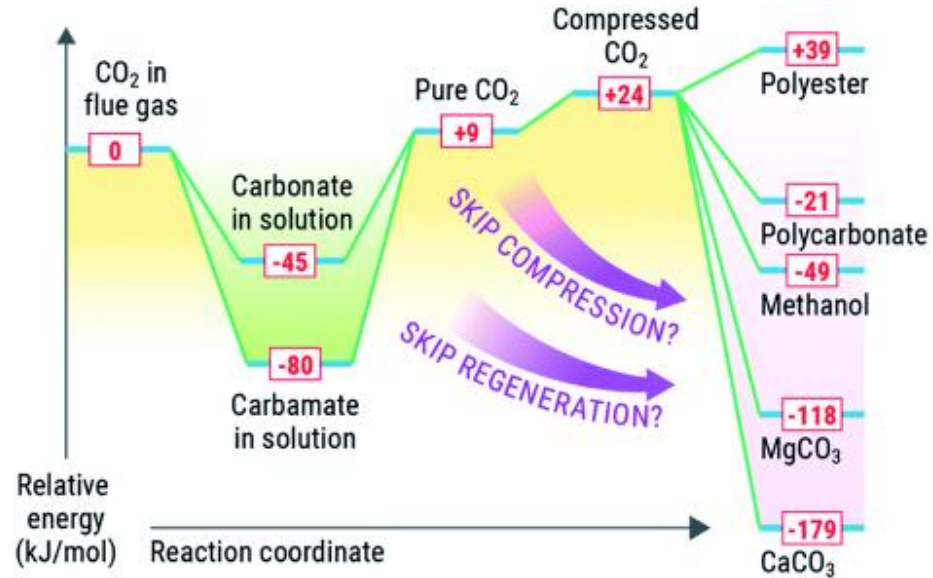


Proposed Value Proposition

Our proposed value proposition for reactive CO₂ capture is:

1. Lower energy intensity
2. Increased capital-expense-normalized productivity (i.e., capital utilization)

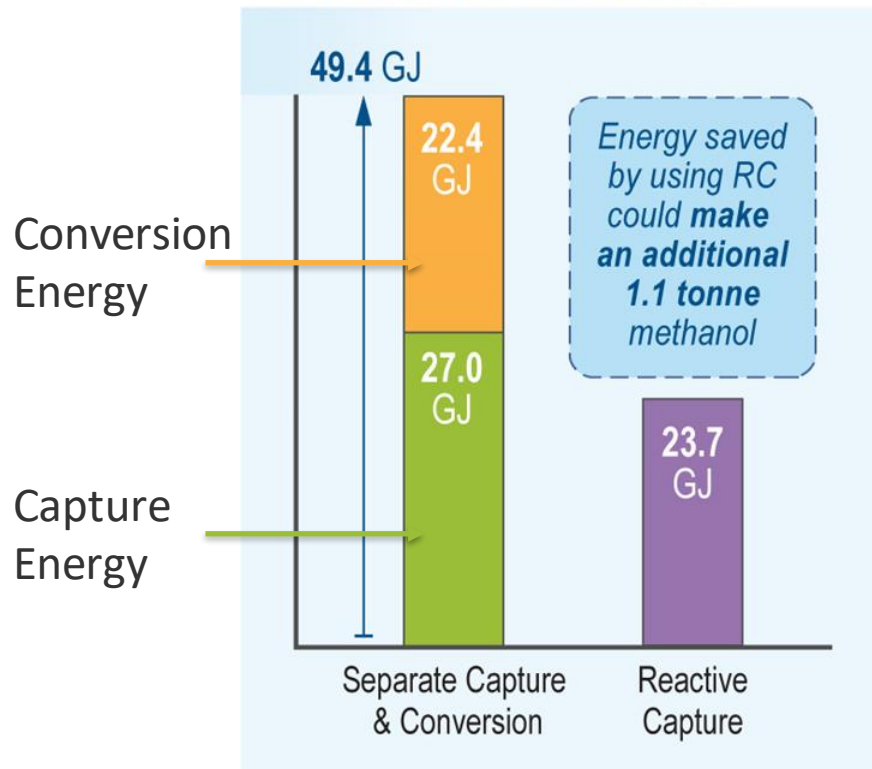
relative to the separate CO₂ capture and conversion processes that require a purified CO₂ intermediate.



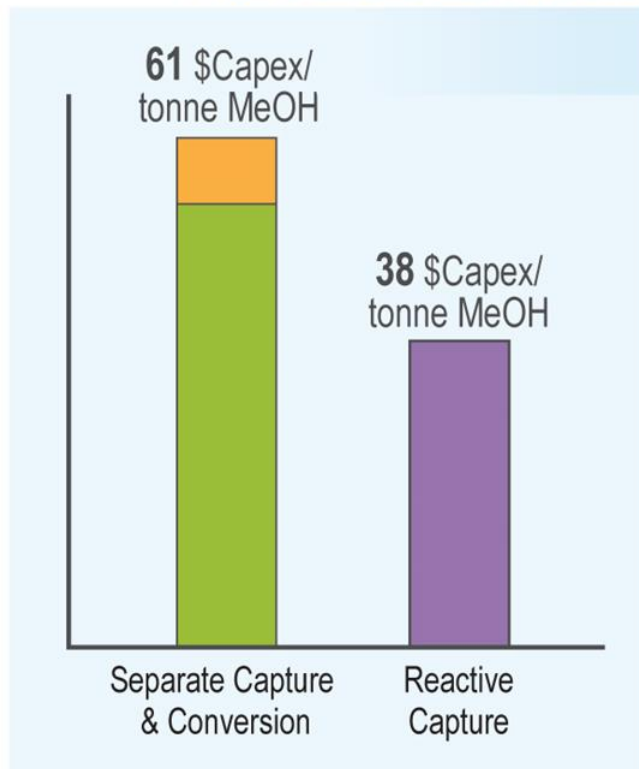
D. Heldebrant, et al., *Chem. Sci.* 13 (2022) 2445-6456

Value Proposition: Potential Savings

ENERGY REQUIRED TO MAKE
1 TONNE METHANOL PRODUCT



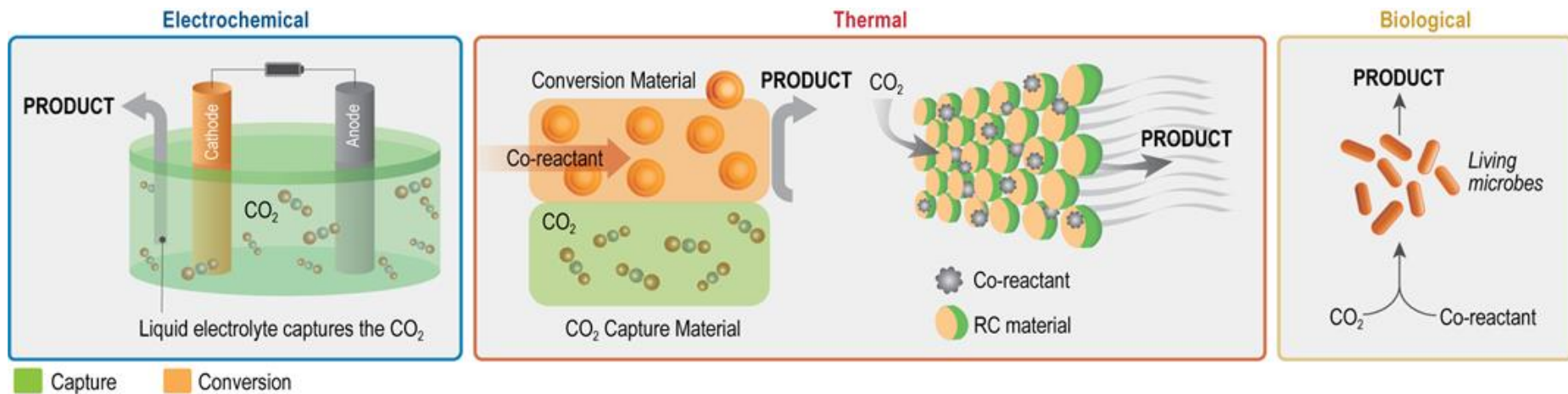
NORMALIZED CAPEX TO MAKE
1 TONNE METHANOL PRODUCT



*Calculation assumes same methanol synthesis yield/efficiency regardless of CO₂ purity/captured state

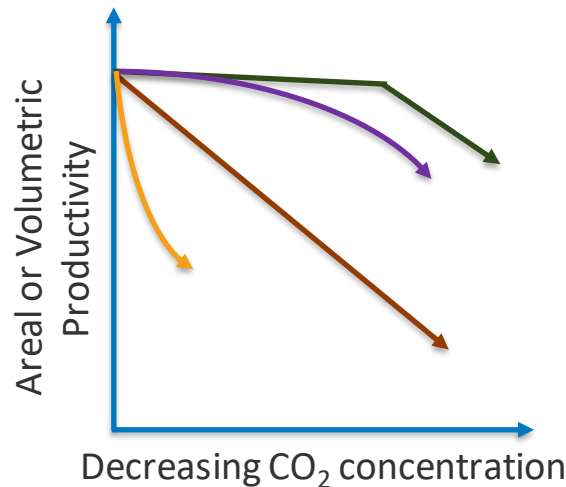
Reactive Capture Technology Categories

Diverse slate of technologies under development, most of which are at the proof-of-concept stage



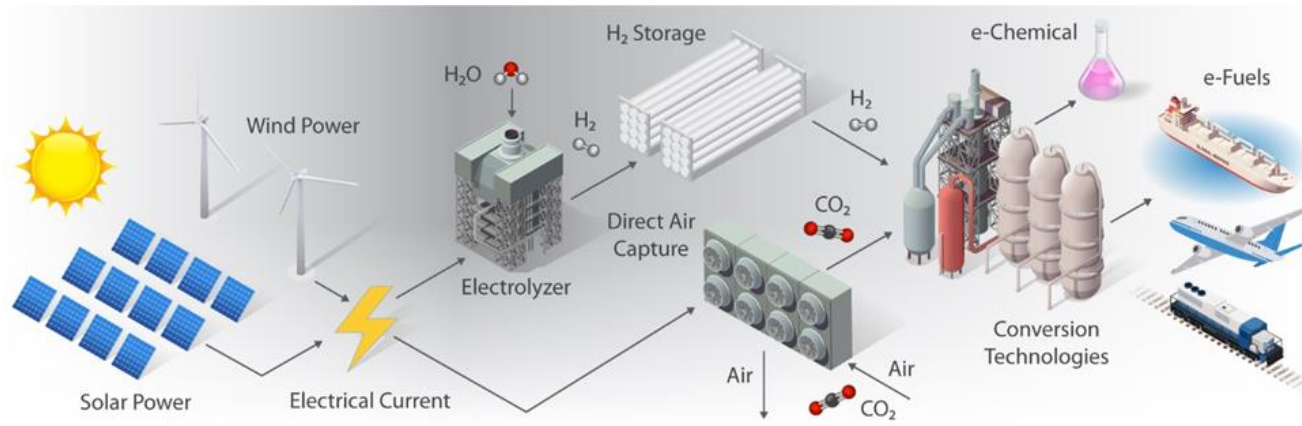
Overarching Challenges and Needs

- Integrating with real process streams
- Transitioning from batch to continuous processing – matching capture and conversion rates
- Understanding and mitigating impacts of impurities
- Quantifying capture media stability, attrition, and cycleability
- Identifying figures of merit
 - Energy intensity
 - Productivity-normalized capex



Summary

- CO₂ conversion to fuels and chemicals has significant opportunity space and can reduce GHG emissions, but is expensive today
- Fundamental to applied R&D is needed to close this cost gap, with an emphasis on integration
- Achieving high energy and carbon efficiency to C₁-C₃ intermediates creates near-term CO₂ conversion opportunities when coupled with renewable energy



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Resources

Technology Options and Challenges

Energy & Environmental Science

PERSPECTIVE

Check for updates

Cite this: *Energy Environ. Sci.* 2023, 16, 432

Transforming the carbon economy: challenges and opportunities in the convergence of low-cost electricity and reductive CO₂ utilization†

R. Gary Grim,¹ Zhe Huang,¹ Michael T. Guarnieri,¹ Jack B. Ferrell III,¹ Ling Tao¹ and Joshua A. Schaidle¹*

The increasing availability of renewable electricity at costs competitive with, and even lower than, electricity from fossil sources along with growing interest and recent technological advancements in reducing carbon emissions through CO₂ capture is challenging the status quo of the way that we produce and consume energy and products. Renewable electricity can be leveraged to produce fuels and chemicals from CO₂, offering sustainable routes to reduce the carbon intensity of our energy and products-driven economy. It is unclear at this time how best to develop for the economic drive reduction of CO₂ to products, including both direct and indirect (via energy carriers such as H₂) pathways and spanning from electrochemical to biological to thermocatalytic pathways. While these approaches are at various stages of development, there are technical barriers related to each: conversion efficiency, process design, and scale-up. This perspective reviews the current state of the art, the challenges that need to be addressed in order to accelerate commercialization and drive the transition towards a circular carbon economy. In this perspective, we define and characterize the top technical barriers for achieving renewable electricity for CO₂ reduction across the different conversion approaches: direct electrochemical, direct biocatalytic, direct non-thermal plasma, indirect biocatalytic, and indirect thermocatalytic under state-of-the-art technology conditions, outline the R&D needs to overcome each barrier, and identify the most promising C₁-C₄ hydrocarbons and oxygenates based on their relative ease of formation, economic viability, CO₂ utilization potential, and energy storage capacity. Our analysis suggests, based on current reported states of technology, that indirect pathways paired with the formation of C₂ products offer the most technically feasible approach to the electro-driven CO₂ reduction in the near term. However, as we strive for longer carbon chain molecules, and as technologies continue to advance, there are a multitude of advantages and limitations to be considered for all the approaches.

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Economics

Energy & Environmental Science

ANALYSIS

Check for updates

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The economic outlook for converting CO₂ and electrons to molecules†‡

Zhe Huang,¹ R. Gary Grim,¹ Joshua A. Schaidle¹ and Ling Tao¹*

Shifting towards a circular carbon economy in the face of rising global population and diminishing natural resources represents one of the greatest challenges facing mankind. CO₂ reduction reactions powered by renewable electricity offer a possible route to transform our incumbent linear consumption economic model by looping into the over 30 gigawatts of carbon emitted globally each year in the form of CO₂. However, many critical questions for CO₂ reduction remain unanswered across the varied pathway-product combinations, such as: (i) what is the near-term economic viability? (ii) what opportunities exist for noncombustional R&D to reduce cost? (iii) what is the impact of CO₂ price? (iv) how does renewable electricity intermittency affect the production cost? Herein, we perform a comprehensive economic assessment of CO₂ reduction across five major electricity-driven technologies using a scale basis of a 200 million gallons per year biorefinery facility for 500 kilowatts CO₂ per year at the CO₂ source. From this framework, we address these key issues and suggest 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 \$0.05 kWh l⁻¹ and CO₂ price to \$20 per tonne, it is not a CO₂-derived products have the potential to reach production costs at parity with, or even lower than, current market prices.

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CO₂-to-SAF

Energy & Environmental Science

PAPER

Check for updates

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Electrifying the production of sustainable aviation fuel: the risks, economics, and environmental benefits of emerging pathways including CO₂†

R. Gary Grim,¹ Dwarak Ravikumar,² Eric C. D. Tan,³ Zhe Huang,¹ Jack R. Ferrell III,¹ Michael Resch,⁴ Zhenglong Li,⁵ Chirag Mevawala,⁶ Steven D. Phillips,⁷ Lesley Snowden-Swan,⁸ Ling Tao¹ and Joshua A. Schaidle¹*

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 CO₂ emissions within the anthropogenic carbon cycle. As the world grapples with the environmental fallout from rising CO₂ 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, grasses, 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 CO₂ 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 CO₂-to-SAF pathway with existing routes to SAF is performed, revealing the potential for CO₂-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 CO₂-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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Economic Feasibility for CO₂ Utilization Data Visualization Tool

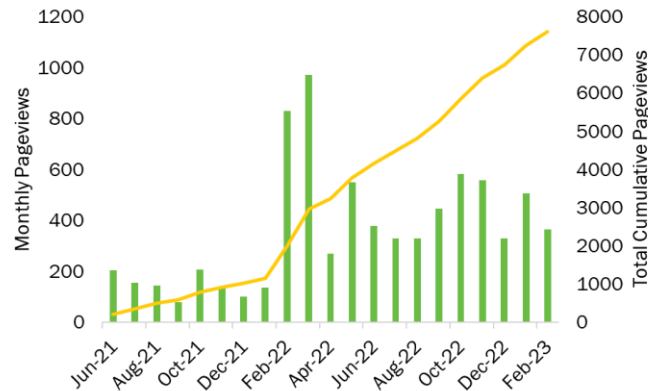
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NREL offers insight into the economic feasibility and key cost drivers of producing chemical intermediates from carbon dioxide (CO₂) and electricity across five different conversion pathways.

These data visualizations are a companion to The Economic Outlook for Converting CO₂ and Electrons to Molecules, *Energy & Environmental Science* (2023).

Visualize Key Conversion Metrics

- Microscale electrocatalysis
- High temperature electrolysis
- Low temperature electrolysis
- Thermocatalytic conversion
- Biological conversion



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