Opportunities and Challenges in Converting CO_2 into Fuels and Chemicals

Josh Schaidle

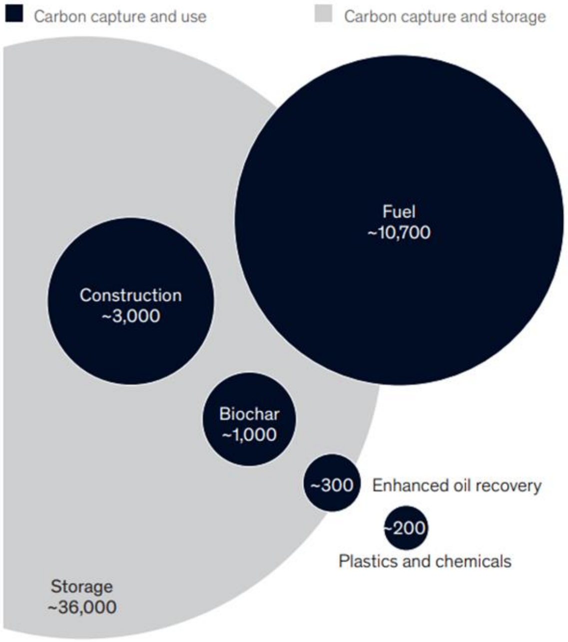
June 27th, 2023

NASEM Committee on Carbon Utilization

Market Size and Value of CO_2 Utilization Products

Market Size

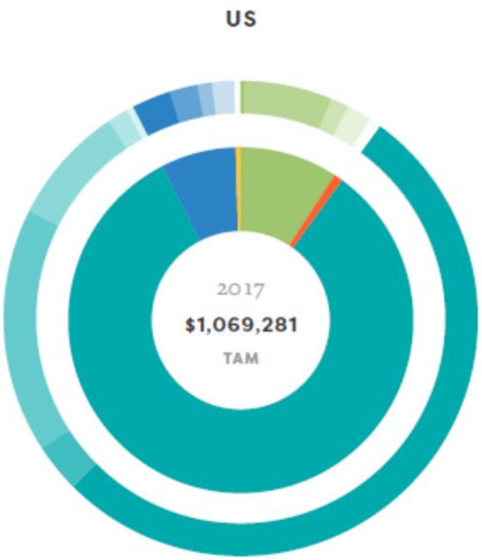
Technical potential of CCUS in 2030, metric megatons of CO_2 per year[1]



Selected examples

Fuel	Synfuel and macro- or microalgae fuel
Enhanced oil recovery (EOR)	Conventional or unconventional CO_2 EOR and CO_2 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



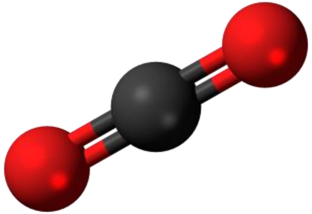
PRODUCT	$ IN MILLIONS
BUILDING MATERIALS	**$101,130**
Cements	$1,240
Concretes	$65,000
Asphalts	$12,190
Aggregates	$22,700
WOOD-BASED PANELS	**$12,508**
FUELS	**$882,149**
Gasoline	$543,400
Jet Fuel	$38,760
Diesel	$186,660
Natural Gas	$83,705
Ethanol	$23,550
Biodiesel	$6,074
PLASTICS	**$71,694**
High density polyethylene	$25,393
Linear Low density polyethylene	$20,502
Low density polyethylene	$11,522
Polypropylene	$14,276
CHEMICALS	**$1,800**
AGRICULTURE AND AQUACULTURE	**N/A**
CONSUMER GOODS	**N/A**
TOTAL	**$1,069,281**

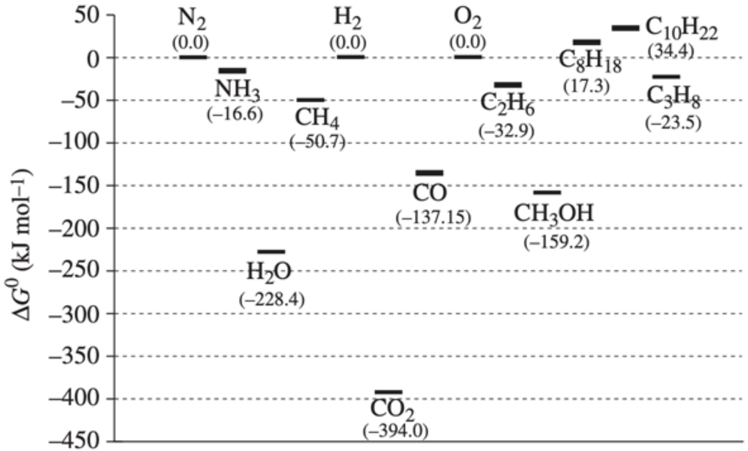
Biniek et al., McKinsey Quarterly, June 2020

Jacobson and Lucas, Carbon180, 2018

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 >40 kWh/kg
  - Ammonia synthesis: ca. 8 kWh/kg*
- 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.

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 CO_2 Utilization?

Technical Feasibility

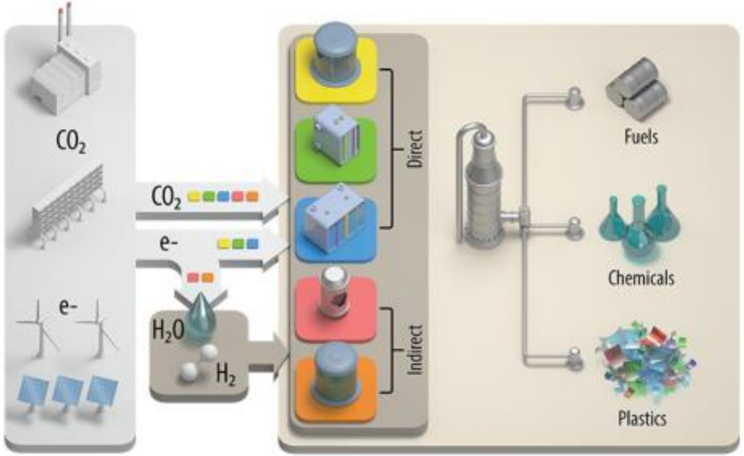
1. *Relative TRL of conversion technologies?*
2. *What kinds of products accessible?*
3. *Unique advantages & disadvantages?*

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*

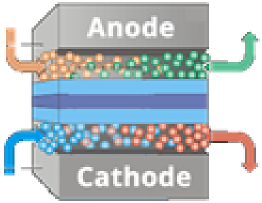


https://www.nrel.gov/bioenergy/co2-utilization-economics/

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

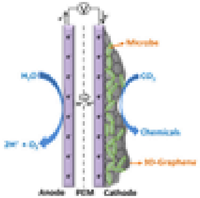
Technology Snapshot

Electrolysis (Alkaline, PEM, SOEC)



- CO
- C_2H_4
- $C(s)$
- $HCOOH$
- C_2H_5OH
- $C_2O_4^-$
- C_3H_7OH
- CH_3COOH
- CH_4
- CH_3OH
- C_3H_6O
- $C_2H_4O_2$
- C_2H_4O
- $C_2H_6O_2$
- CH_3COCH_3
- $C_2H_2O_2$

Microbial Electrosynthesis (MES)

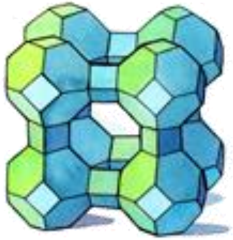


- $HCOOH$
- C_2H_5OH
- C_3H_7OH
- CH_3COOH
- $C_2H_4COO^-$

Fermentation

- C_2H_5OH
- C_3H_7OH
- CH_3COOH
- CH_4

Thermochemistry



- CO
- C_2H_4
- CH_4
- CH_3OH
- C_3H_6

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 CO_2 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

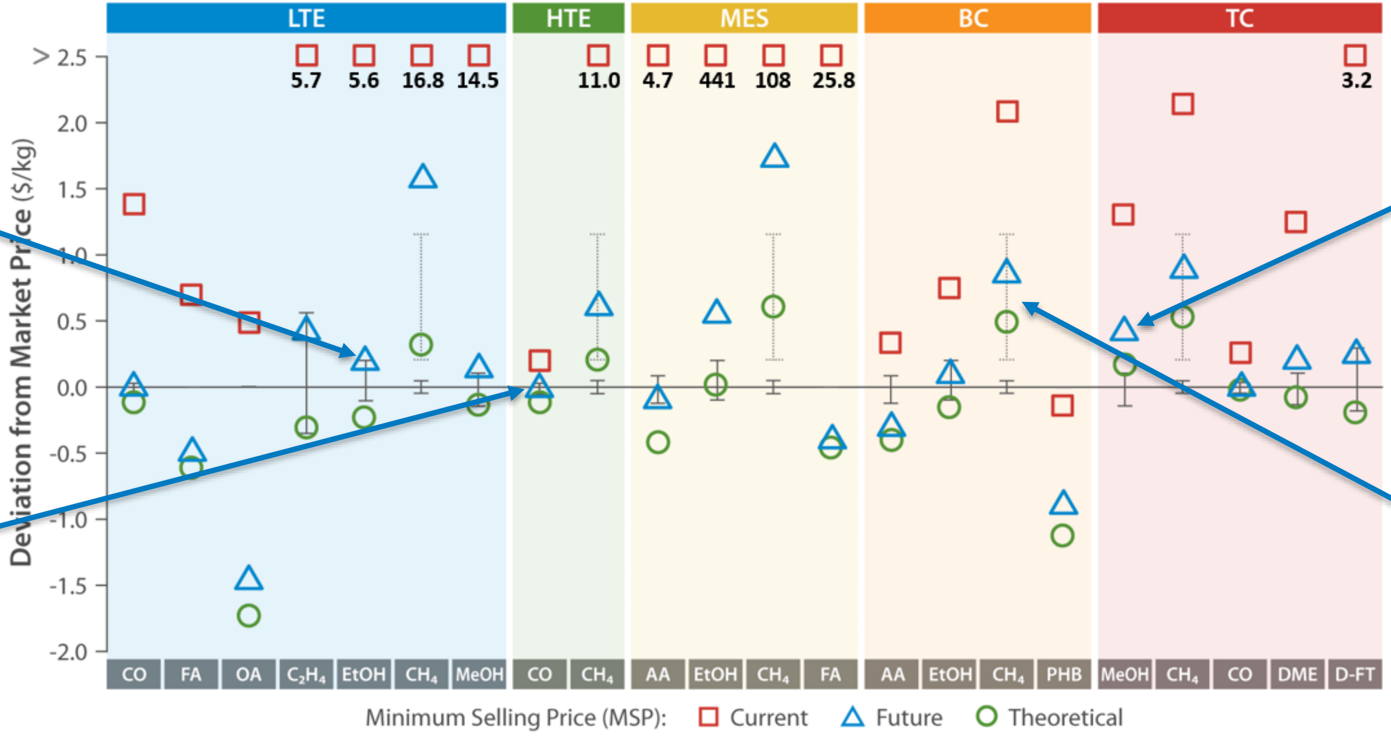
a: High: >200 mA/cm^2 (or commercial TC), Intermediate: 200 > j > 100 mA/cm^2, Low: < 100 mA/m^2
b: High: >80%, Intermediate 80% > FE > 60%, Low: < 60%
c: High: >60%, Intermediate: 60%> EE >40%, Low: <40%
d: High: Operated at TRL > 6, Intermediate: Operated TRL 4-6, Low: Operated TRL 1-3

Economic Perspective

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

Ethanol
$0.74/kg
$27/GJ

CO
$0.15/kg
$15/GJ



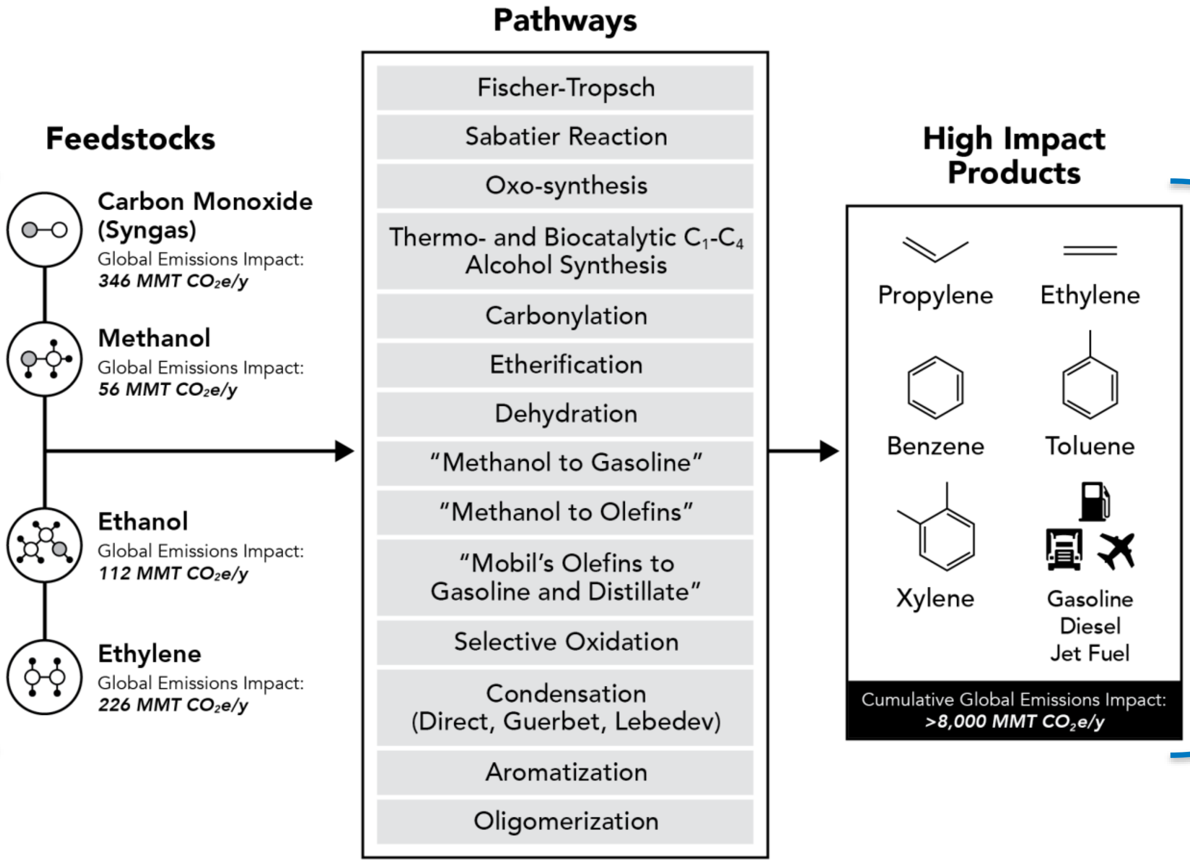
Methanol
$0.8/kg
$40/GJ

Methane

Z. Huang, R. Grim, et al., *Energy & Environ. Sci.*, 2021, **14**, 3664-3678.

Decarbonization Perspective

Potential to Avoid ~0.74 Gt CO_2/year globally

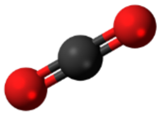


Could scale to multi-Gt avoidance

R. Grim, et al., *Under Review.*

What about Biomass?

CO_2

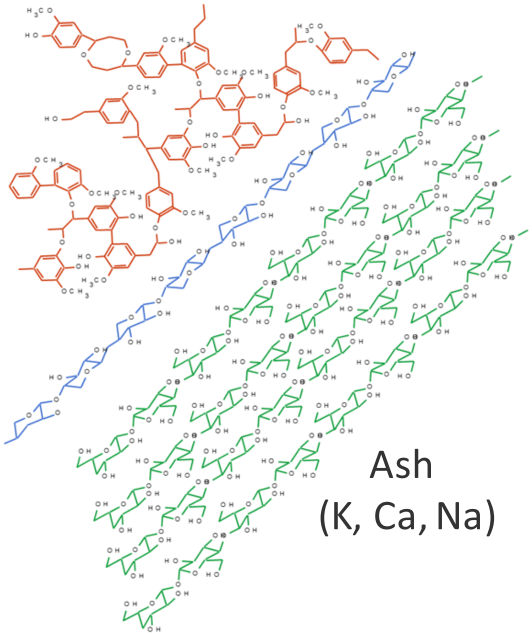


+ Impurities

C_1-C_3 Intermediates

"Build up"

Biomass



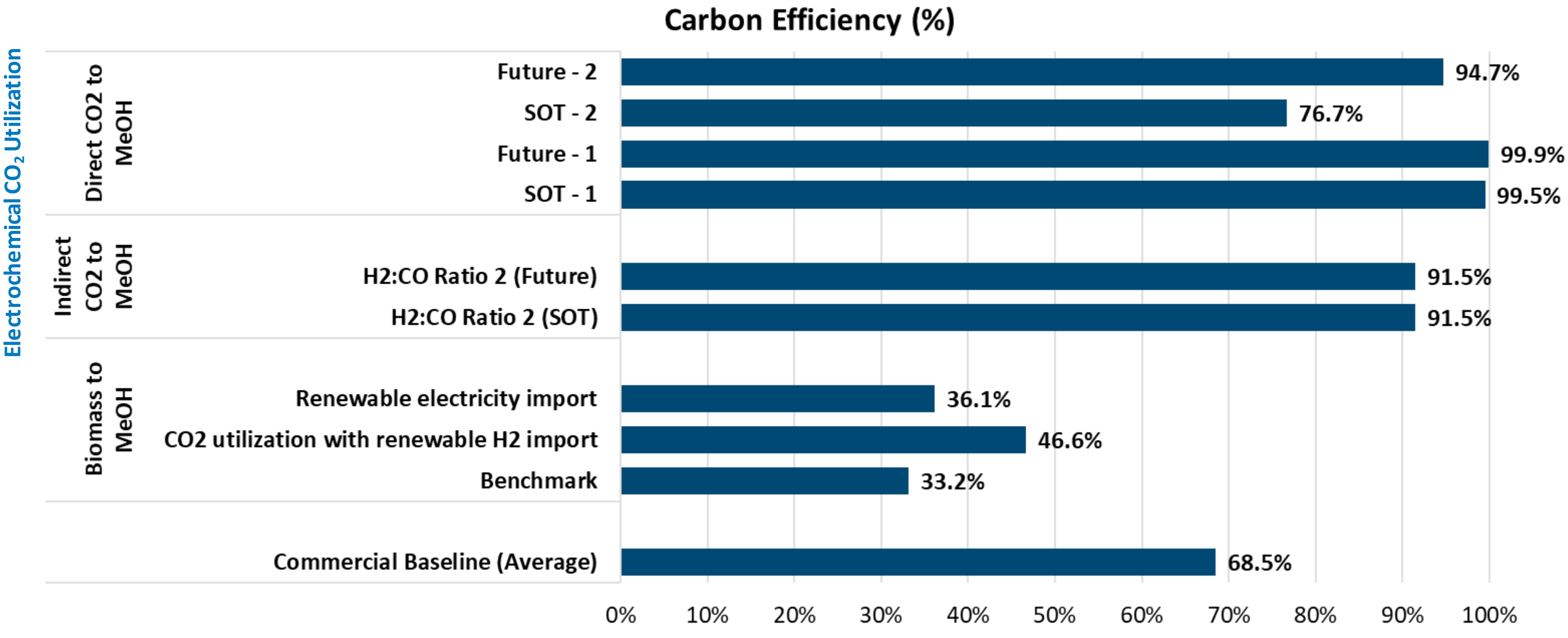
Ash
(K, Ca, Na)

Retain Structure in C_{4+} products

"Break and Reshape"

M. Biddy, et al., NREL/TP-5100-65509, 2016

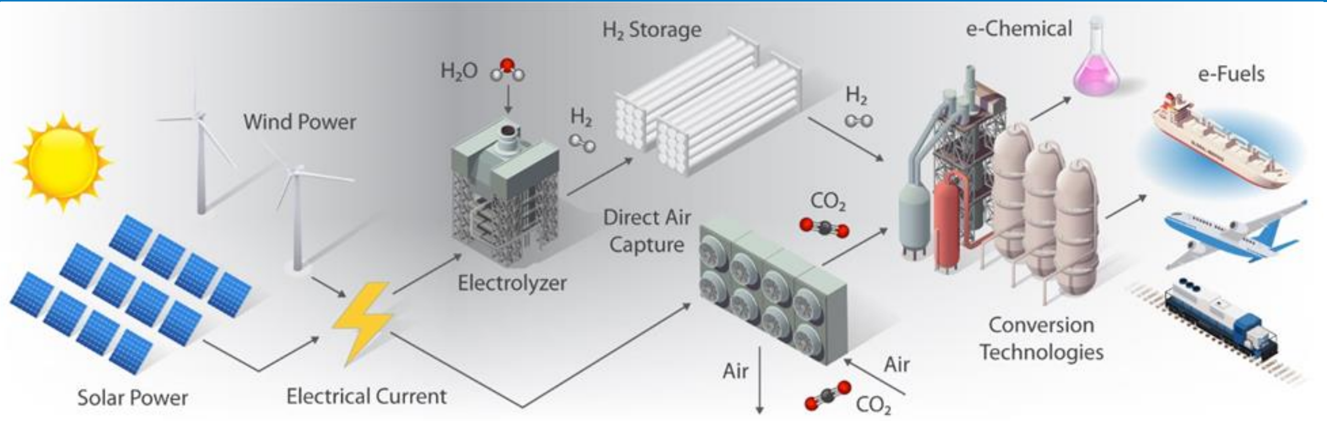
Methanol Production: Biomass vs. CO_2

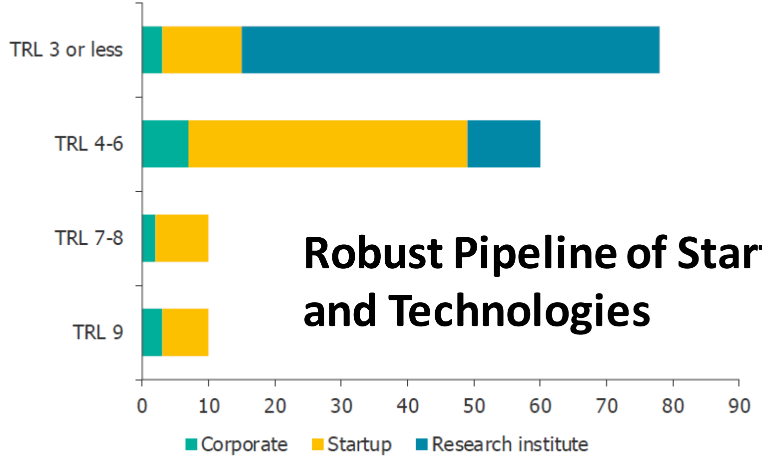


US Drive Net Zero Carbon Fuels Technical Team Analysis Summary Report, 2021

Challenges, Opportunities, and Needs

CO_2 Utilization to Fuels and Chemicals





Robust Pipeline of Startups and Technologies

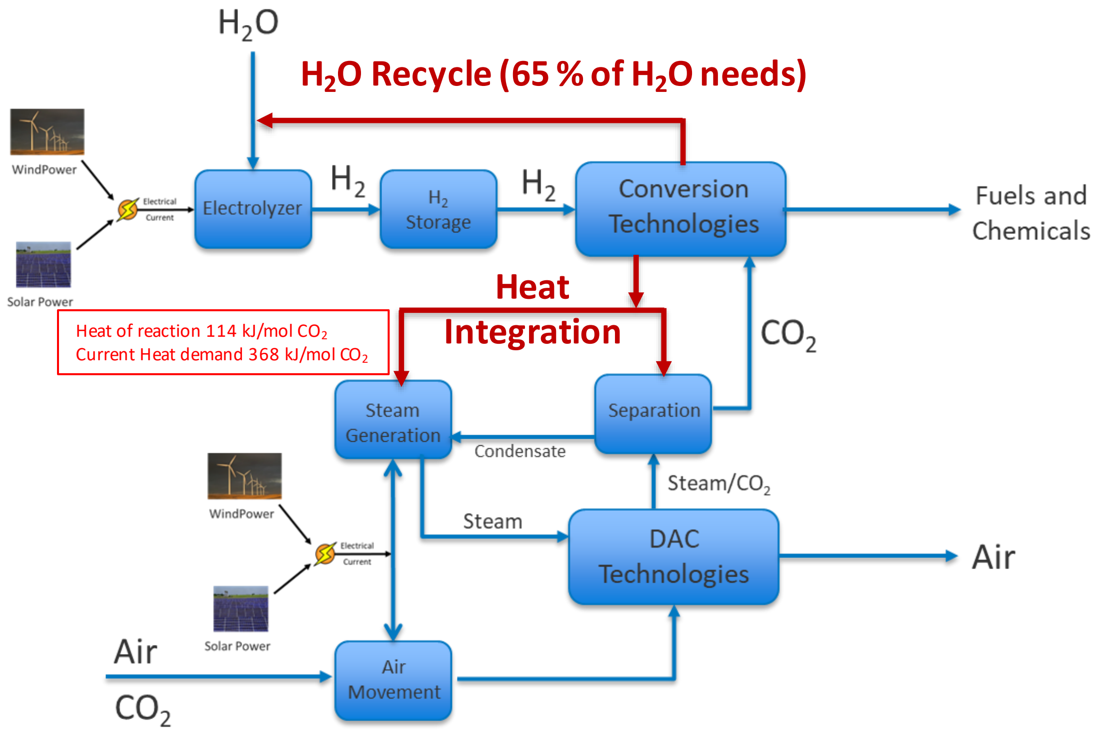
Key Considerations and Challenges:

- Limited integration and diverse unit ops
- Intermittent operation / load following
- Energy intensity and land use
- Cost and market demand
- Scale and rate of CO_2 emissions relative to CO_2 conversion needs

Global CO_2 Initiative, *Implementing CO_2 Capture and Utilization at Scale and Speed*, May 2022

Need for Integration Science

Systems Perspective

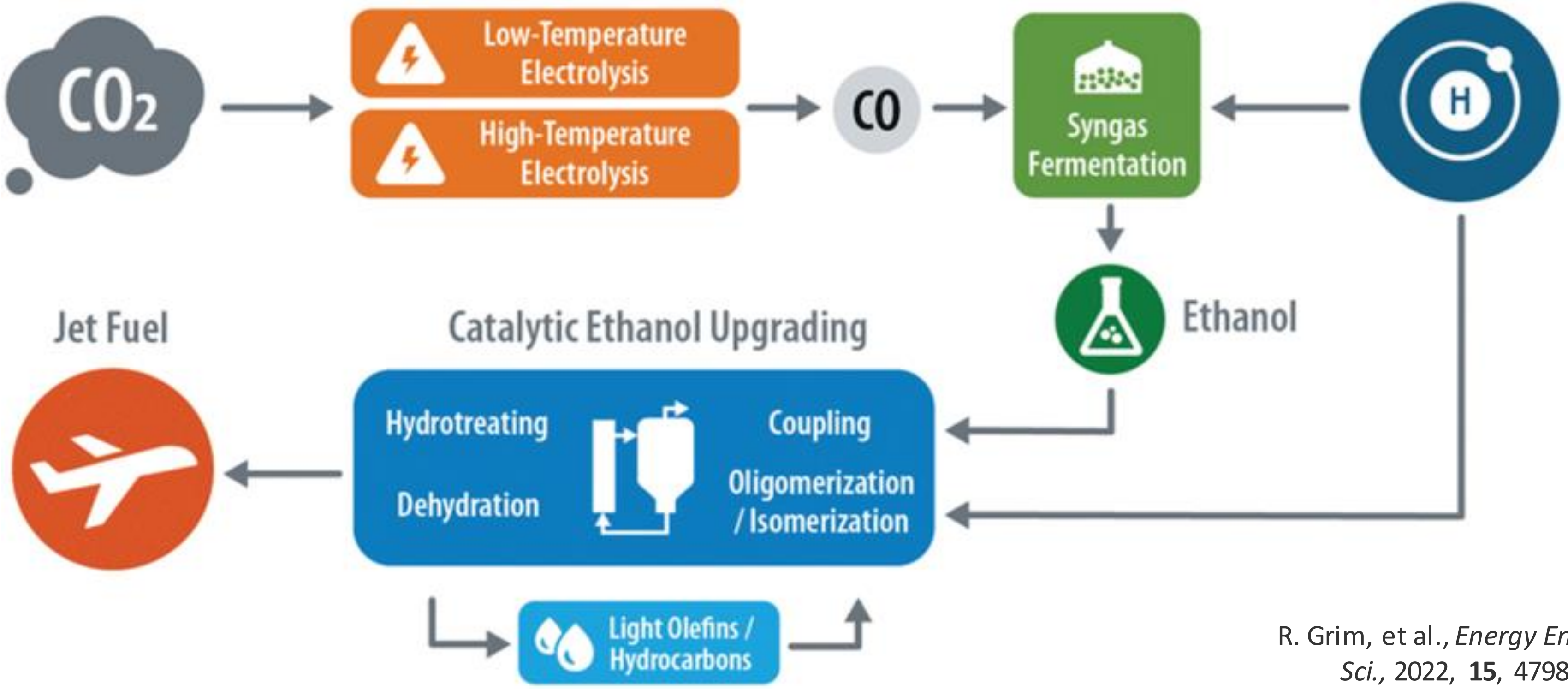


Example Research Questions:

- How can cost be reduced through heat and water integration?
- What are the real cost trade-offs of lower-quality intermediate streams (e.g., CO_2 concentration and impurities)?
- What limits scalability of emerging technologies?
- How can costs be reduced through process intensification?

Producing Sustainable Aviation Fuel (SAF) from CO_2

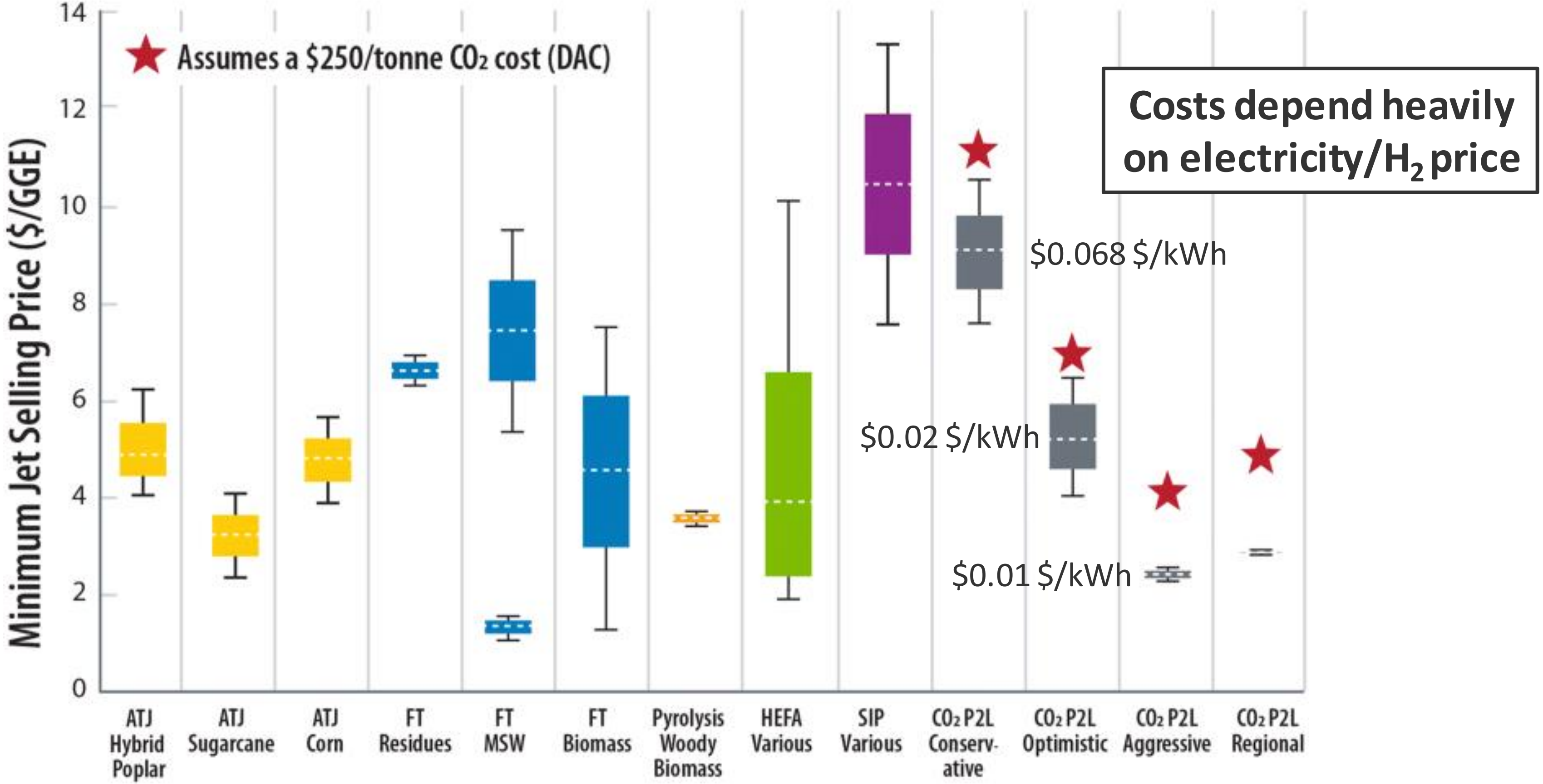
Developed a heat-integrated process model in Aspen Plus



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

**NOTE: This is *one* possible pathway to reach SAF from CO_2 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



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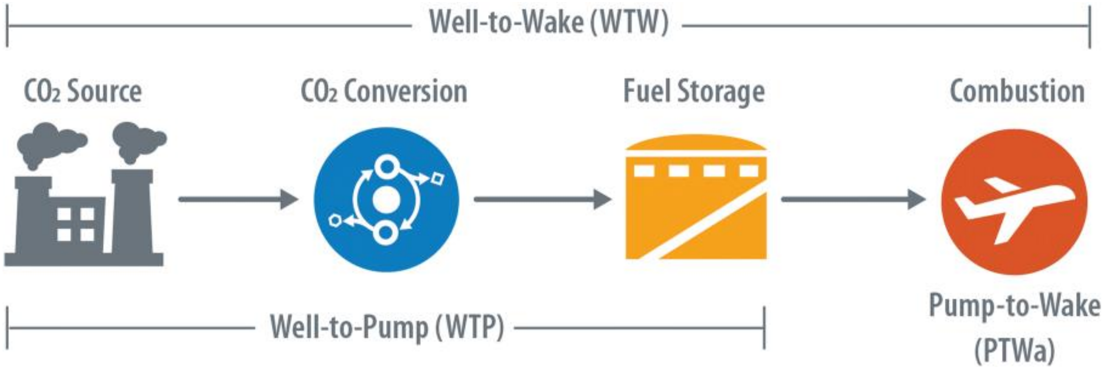
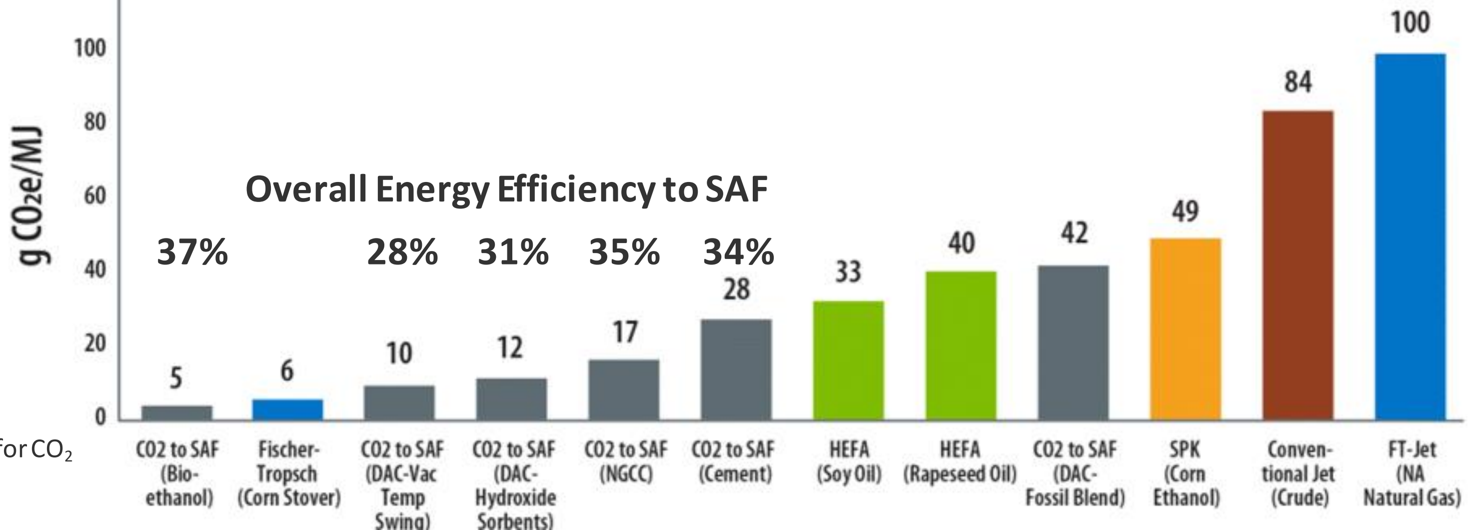
Carbon Intensity of SAF Production

LCA Boundary Conditions



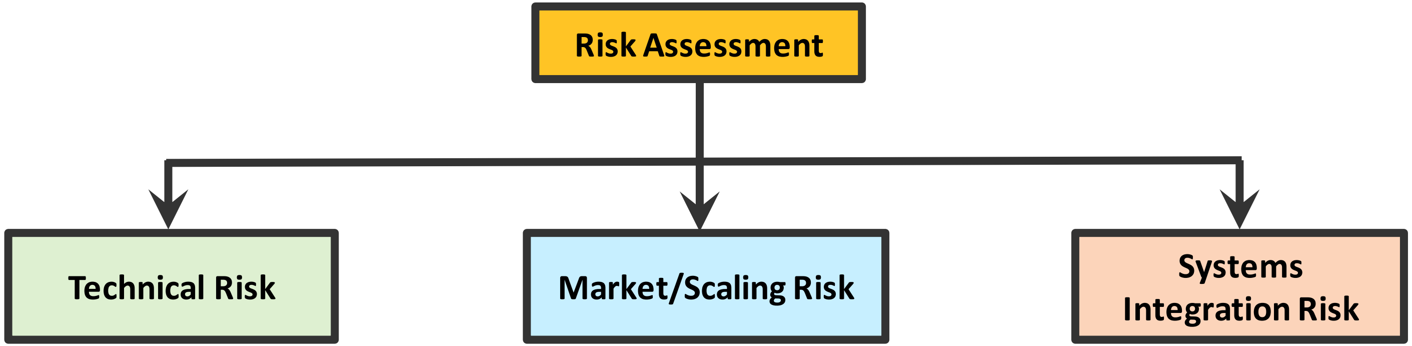
Results



*Assumes use of renewable energy for CO_2 conversion process
**Based on GREET

CO_2-to-SAF Risk Assessment

Identified risks by interviewing subject matter experts



Technical Risk

- Unknown stability of electrolyzers, catalysts, membranes
- Lack of testing with real systems and impact on performance
- Poor performance metrics relative to other technologies

Market/Scaling Risk

- Competition from established markets (i.e., ways to make CO, EtOH)
- Overly complex
- Sourcing rare earths and other materials at the scale needed. Finding suppliers
- High upfront capital costs, loan availability
- Resource allocation preferences

Systems Integration Risk

- Siting risks and requirements
- Integration of multiple complex conversion steps (process intensification)
- Intermittency

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

Opportunity: Reactive Carbon Capture

Emerging Approach: Reactive Capture of CO_2

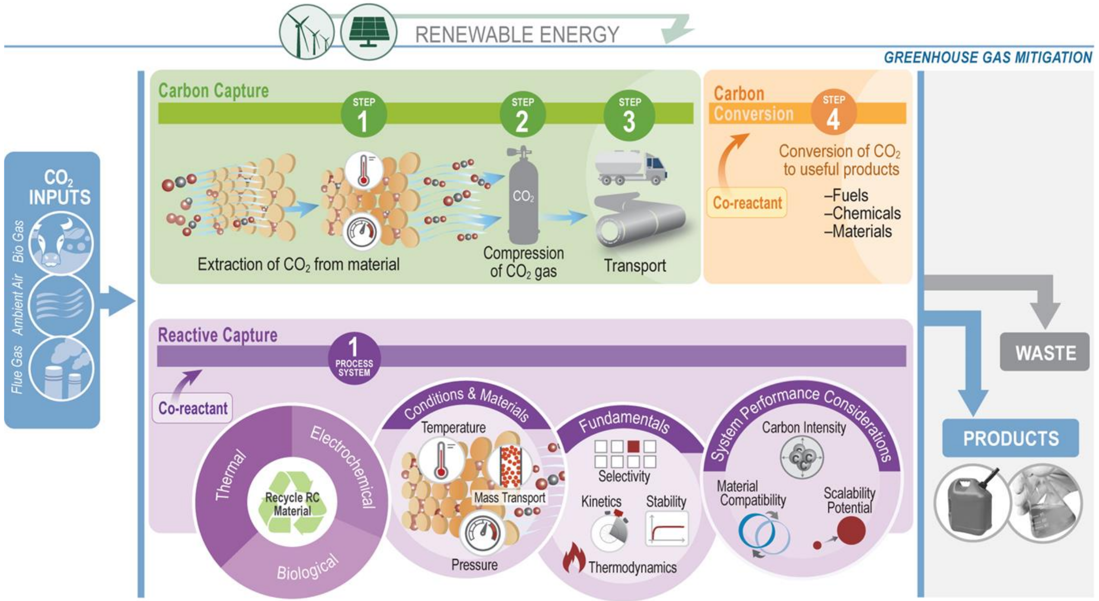
Reactive Capture Definition: The coupled process of capturing CO_2 from a mixed gas stream and converting it into a valuable product *without* going through a purified CO_2 intermediate

Can Include:

- Integration of CO_2 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 CO_2



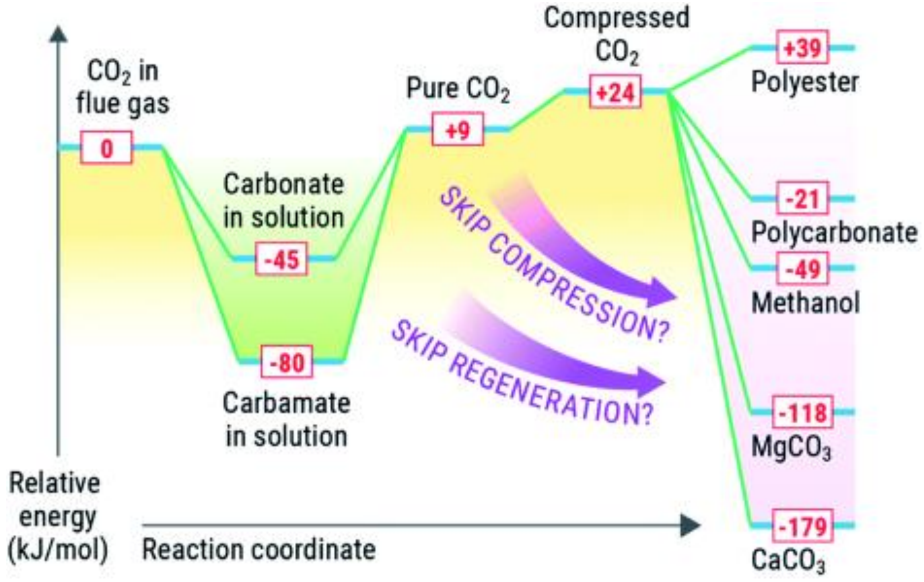
M. Freyman, et al., *Joule* 7 (2023) 631-651.

Proposed Value Proposition

Our proposed value proposition for reactive CO_2 capture is:

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

relative to the separate CO_2 capture and conversion processes that require a purified CO_2 intermediate.

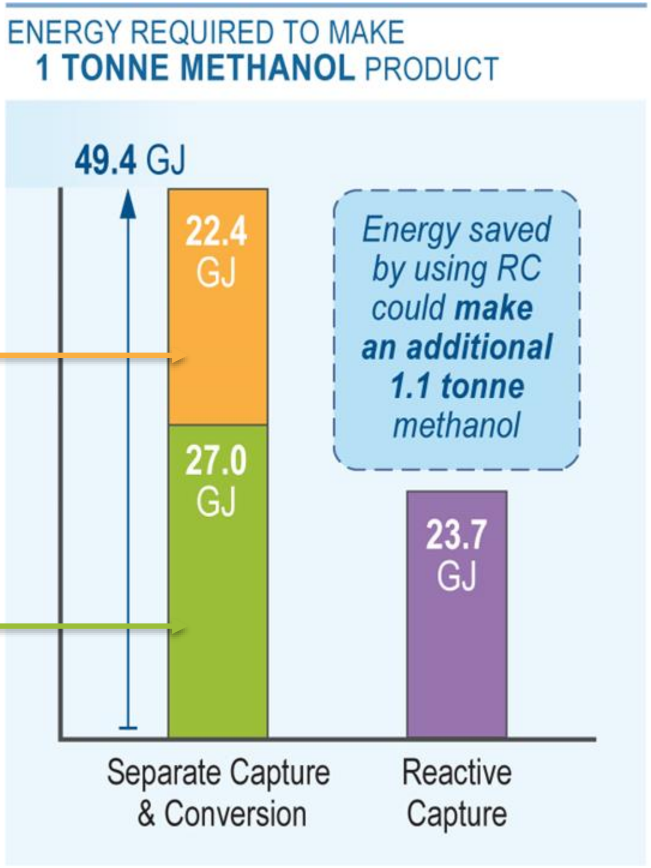


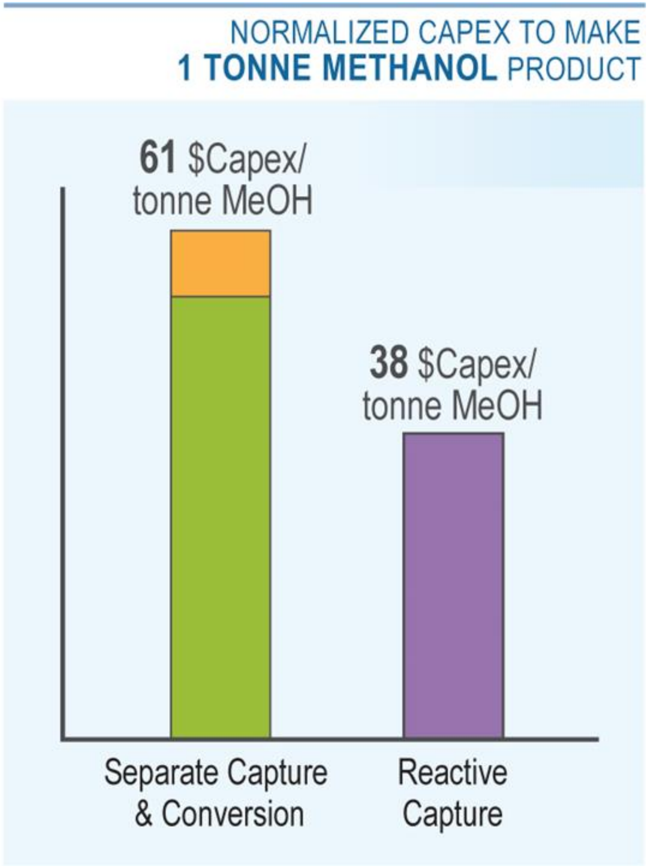
D. Heldebrant, et al., *Chem. Sci.* 13 (2022) 2445-6456

Value Proposition: Potential Savings

Conversion Energy

Capture Energy

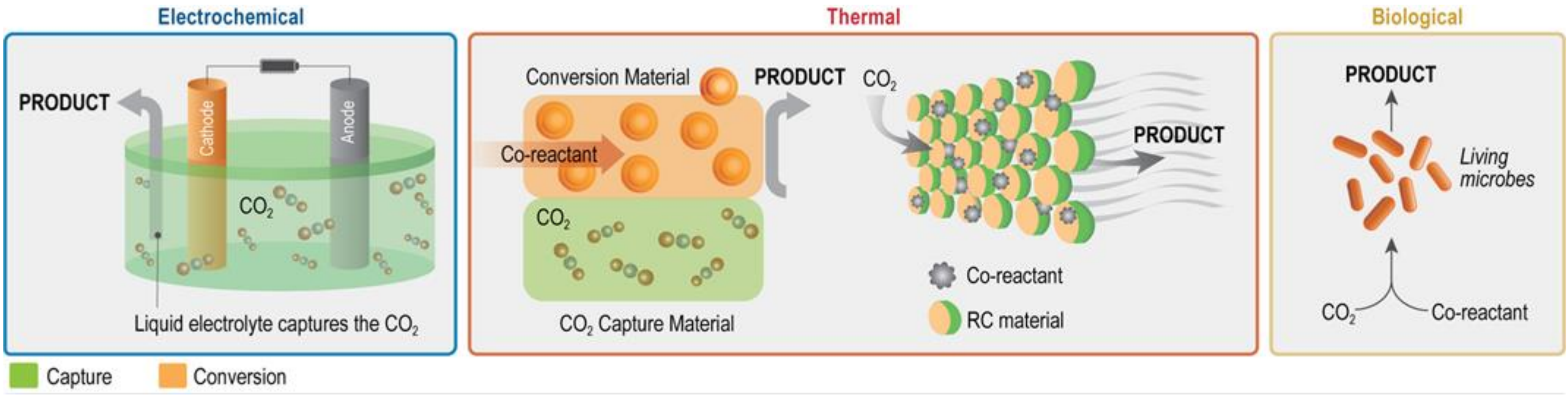




*Calculation assumes same methanol synthesis yield/efficiency regardless of CO_2 purity/captured state

Reactive Capture Technology Categories

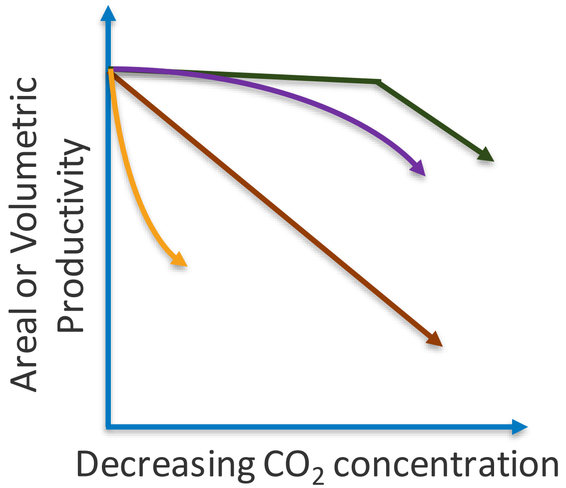
Diverse slate of technologies under development, most of which are at the proof-of-concept stage



M. Freyman, et al., *Joule* 7 (2023) 631-651.

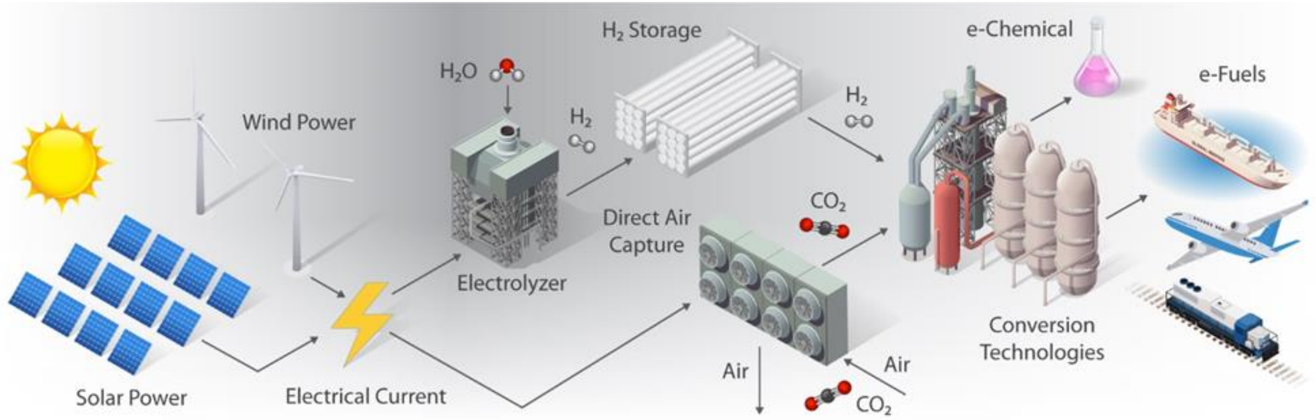
Overarching Challenges and Needs

- 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

- CO_2 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 C_1-C_3 intermediates creates near-term CO_2 conversion opportunities when coupled with renewable energy



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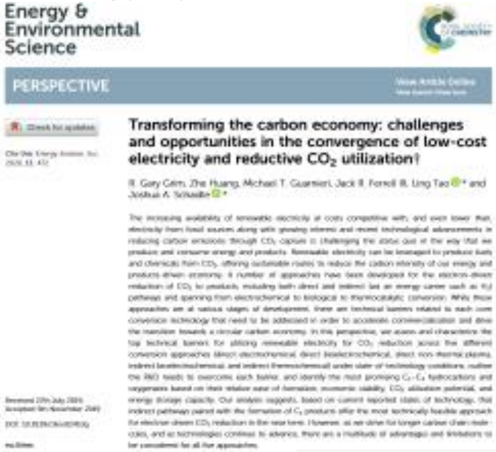
Technology Options and Challenges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Transforming the carbon economy: challenges and opportunities in the convergence of low-cost electricity and reductive CO_2 utilization†

R. Gary Grim, Zhe Huang, Michael T. Guarnieri, Jack R. Ferrell III, Ling Tao and Joshua A. Schaidle

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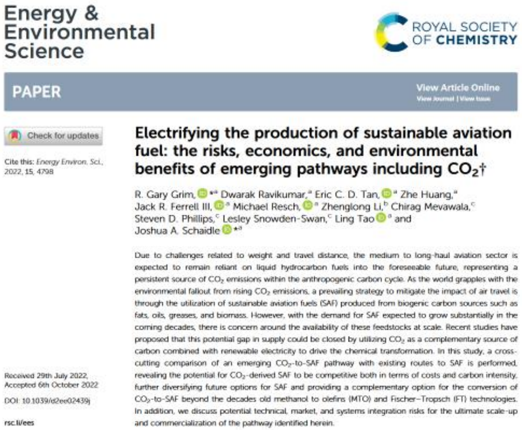
The economic outlook for converting CO_2 and electrons to molecules†‡

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

CO_2-to-SAF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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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rsc.li/ees

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