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CO₂ Consortium Overview

Ian Rowe

Division Director, Carbon Dioxide Conversion

Department of Energy | Fossil Energy and Carbon Management



U.S. DEPARTMENT OF
ENERGY

Fossil Energy and
Carbon Management

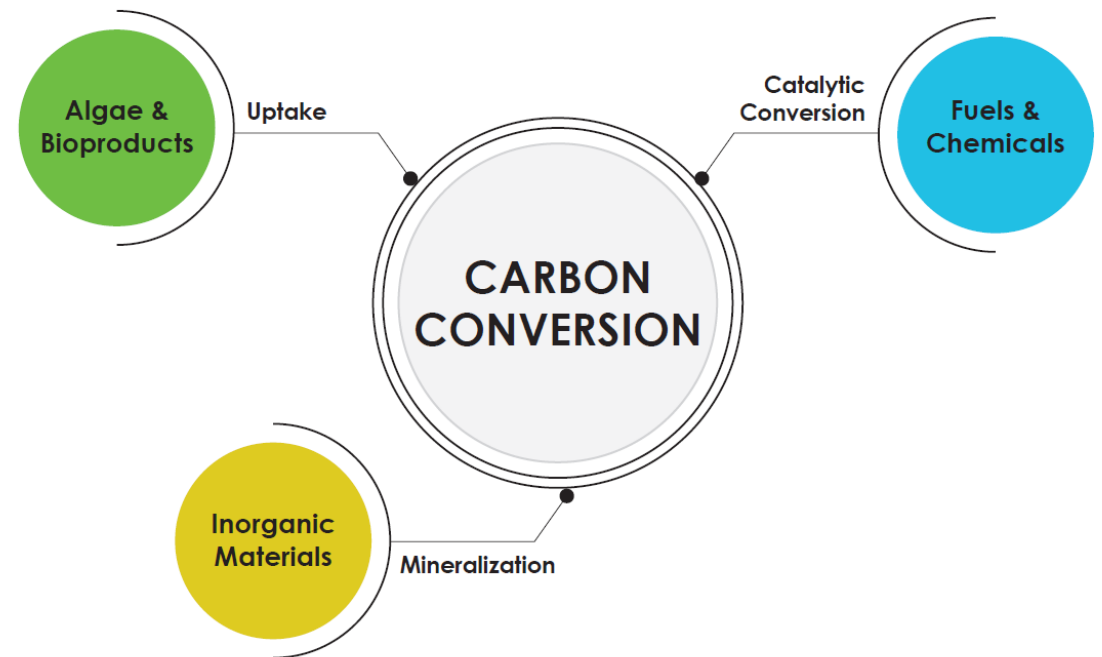
Carbon Dioxide Conversion Program

Research, develop and demonstrate a broad suite of technologies that convert CO₂ into environmentally responsible, equitable and economically valuable products and enable low-carbon supply chains to meet the goal of a decarbonized economy by 2050.

Three major program areas:

- Biological Uptake
- Catalytic Conversion
- Mineralization

FY24 Congressional Budget: \$52M



Alignment with DOE and FECM

- FECM Strategic Vision
- DOE Industrial Decarbonization Roadmap
- SAF Grand Challenge Roadmap
- DOE's Energy Earthshots initiative

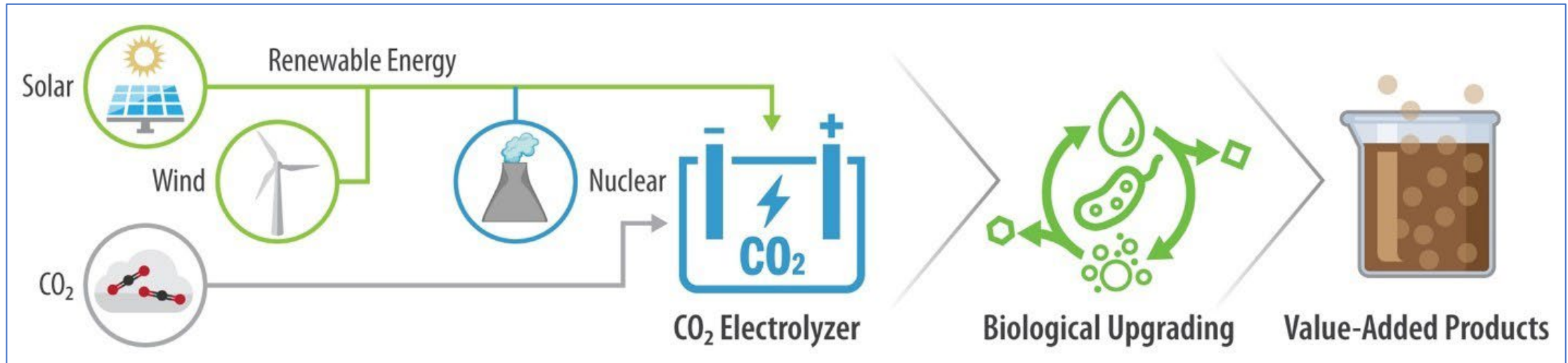


*“a carbon pollution-free power sector by 2035 and ...
a net-zero economy by 2050.”*

CO₂ Catalysis Consortium: FECM and BETO

Two Technology Tracks

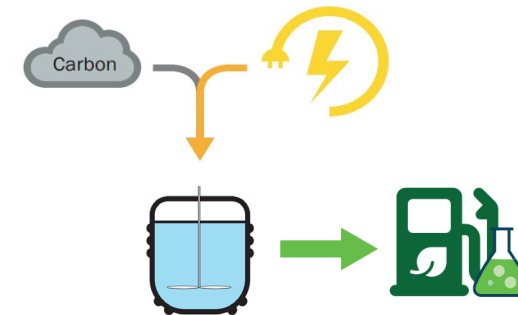
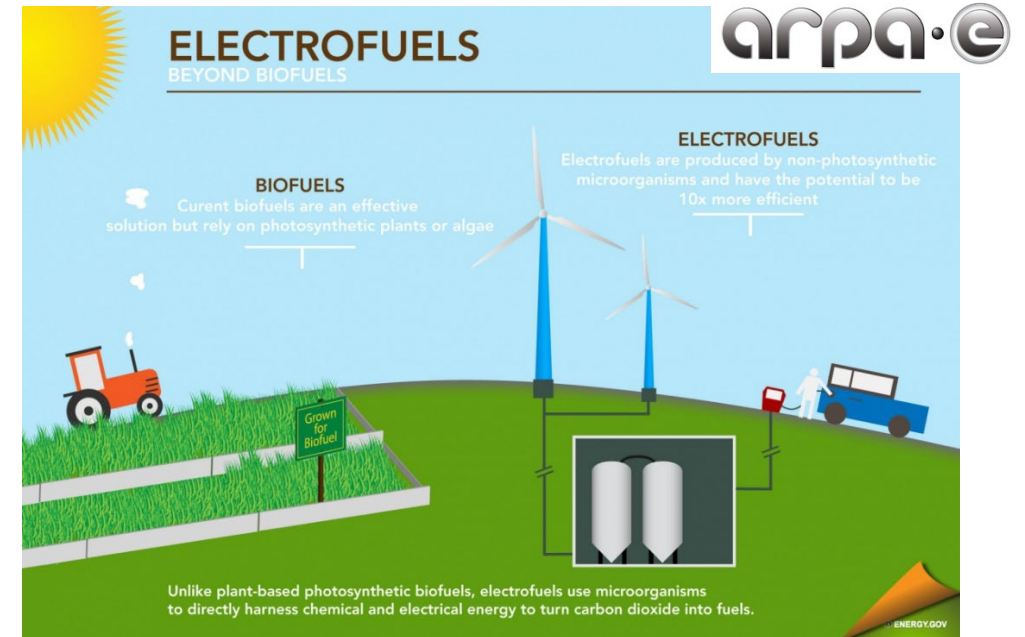
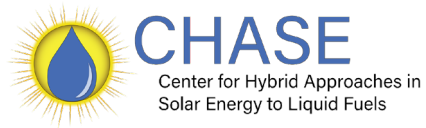
1. CO₂ conversion via **Low Temperature Electrolysis (LTE)**
2. Enabling technologies



Outline

- Overview of previous efforts
- Some up-front questions
- Overview of proposed consortium

Related DOE efforts in catalytic CO₂ conversion



ARPAe "ELECTROFUELS" route



Related DOE efforts in catalytic CO₂ conversion

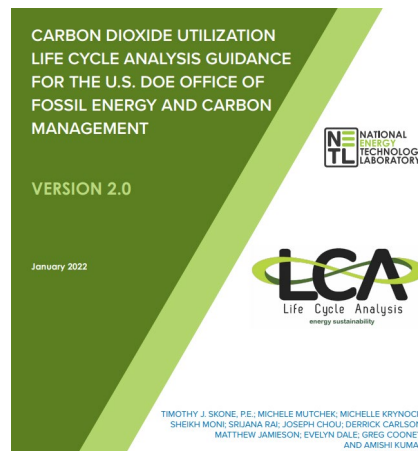
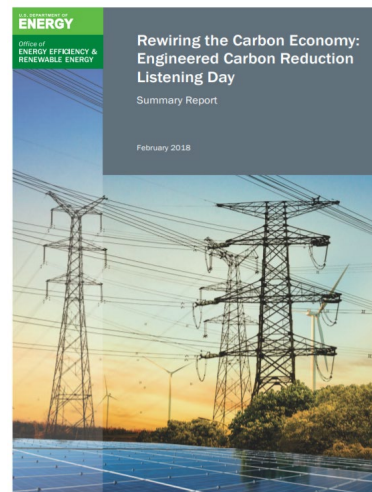
Perspective

The feasibility of direct CO₂ conversion technologies on impacting mid-century climate goals

R. Gary Grim,^{1,*} Jack R. Ferrell III,¹ Zhe Huang,¹ Ling Tao,¹ and Michael G. Resch¹

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

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

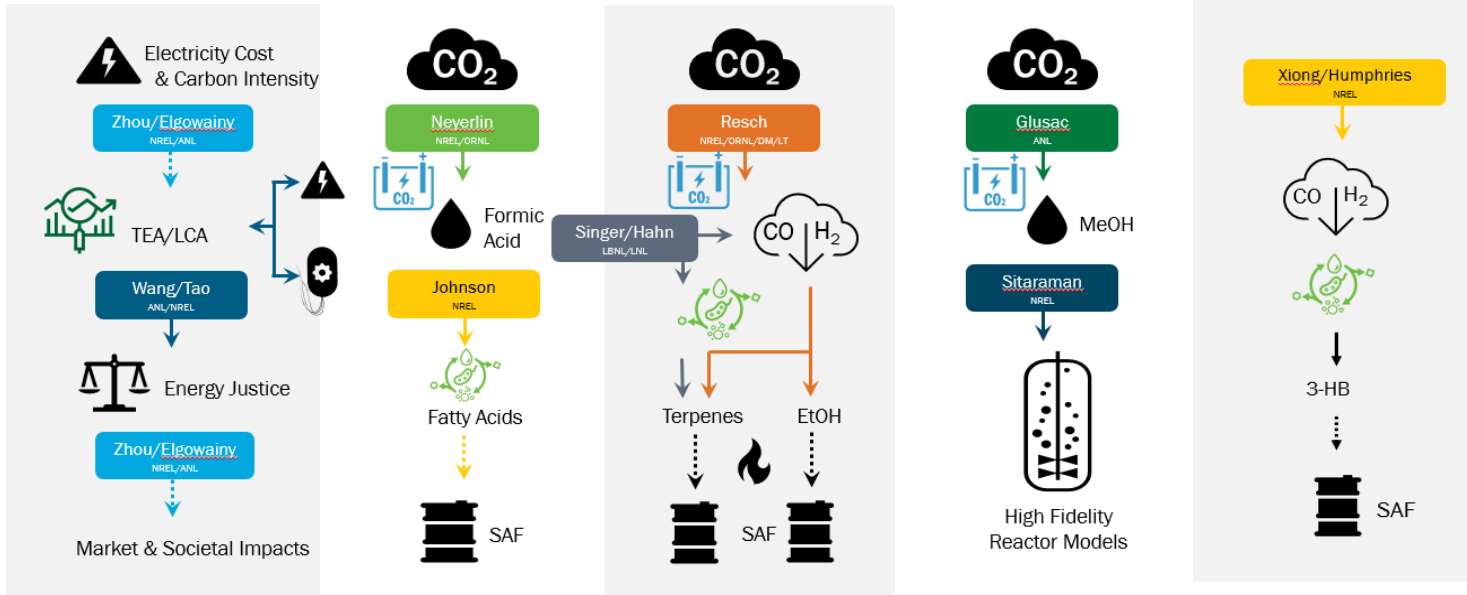


Perspective

What Should We Make with CO₂ and How Can We Make It?

Oleksandr S. Bushuyev,^{1,2,7} Phil De Luna,^{3,7} Cao Thang Dinh,¹ Ling Tao,⁴ Genevieve Saur,⁵ Jao van de Lagemaat,⁶ Shana O. Kelley,² and Edward H. Sargent^{1,*}

CO₂ Reduction and Upgrading for E-fuels consortium

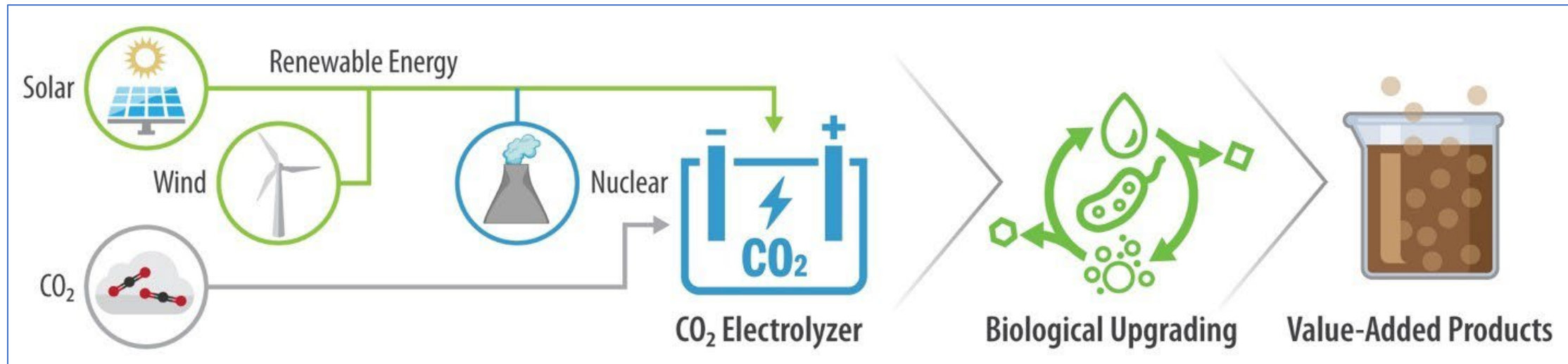


- FY21 – FY24 in EERE
- 10 projects on many different CO₂ conversion routes
- Consolidated into consortium
- **Lesson:** LTE needs less focus on catalyst or new materials discovery; what it needs is a concerted effort into understanding how they would be engineered at scale
- Ending in FY24 and determining next steps

CO₂ Catalysis Consortium: FECM and BETO

Two Technology Tracks

1. CO₂ conversion via **Low Temperature Electrolysis (LTE)**
 - Carbon monoxide and formic acid
2. Enabling technologies
 - Biological upgrading of CO₂ derived intermediates
 - TEA/LCA:



Upfront questions

- Why Low-Temperature Electrocatalysis?
- Why C1 products and not C2+?
- Why not rely on thermocatalysis (i.e., reverse water-gas shift)?
- Why biological upgrading and not more established routes?

CO₂ Consortium structure

Two technology “tracks”

1. CO₂ conversion via low temperature electrolysis (LTE)
 - Approximately 80% CO & 20% formic acid
2. Enabling technologies

Research Thrusts:

1. **Analysis** to identify market scenarios and establish target metrics for deployment
2. **Durability** to lengthen the lifetime of LTE systems
3. **Energy** and carbon efficiency optimization
4. **Scaling** component and system development
5. **Enabling Technologies** (bio) CO₂ Upgrading and process integration

Crosscutting Activities Included in the Research Thrusts:

1. **Modeling** of reactors and systems to improve performance and increase scale
2. **Characterization** of materials and products

Analysis

1) Harmonize baseline TEA and LCA assumptions.

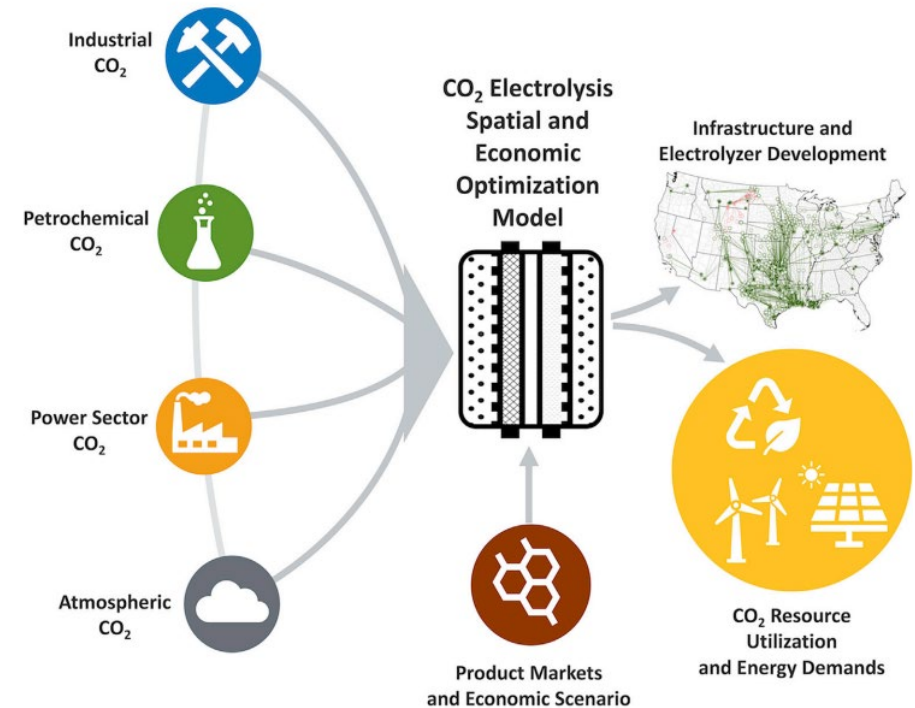
- Publicly available TEA and LCA guidance documents with suggested best practices for market and CO₂ source assumptions, background datasets, and reporting requirements.

2) Deploy user-friendly tools and guidance documents for rapid, high-level TEA and LCA of relevant conversion pathways.

- Rapid feedback so researchers can assess and prioritize how technical improvements ‘move the needle’ across different market and policy scenarios

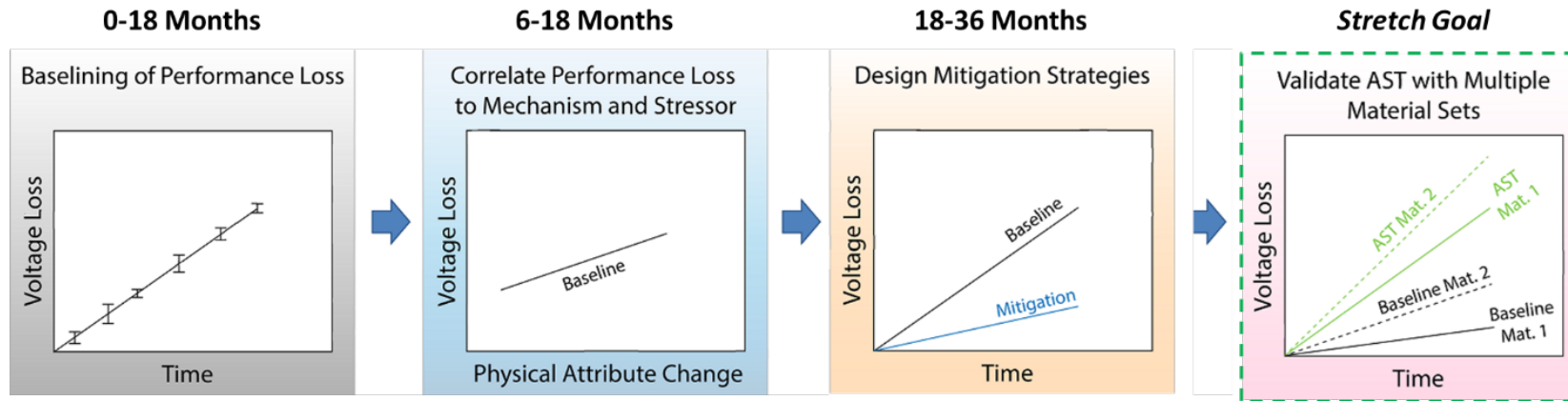
3) Develop regional opportunity maps that link regional resources and markets for LTE CO₂ conversion systems, while considering societal equity and environmental justice.

- Help inform industry and government on potential investment opportunities



Durability

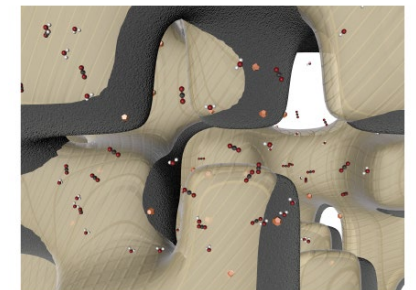
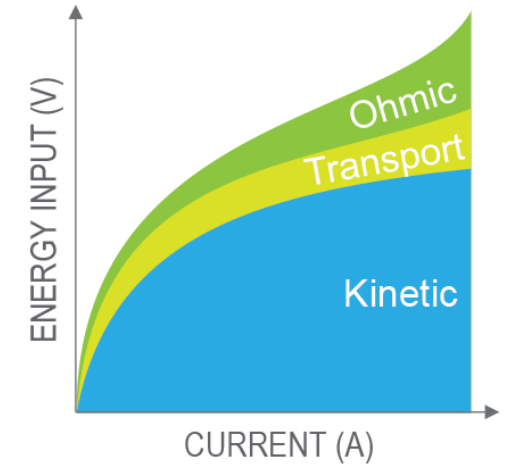
Establish scalable mitigation strategies for degradation modes related to critical operating and environmental conditions



- Identify stack-relevant degradation modes that can be addressed in laboratory scale devices (5-25 cm²)
- Quantify degradation mechanisms and kinetics for relevant conditions.
- Design mitigation strategies for specific degradation modes.
- *Stretch Goal*: develop accelerated stress testing protocols to reduce validation time.

Energy and Carbon Efficiency

- **Delineate the impacts of underpinning phenomena limiting CO₂ electrolyzer energy efficiency and carbon utilization**
 - 1D models and multimodal diagnostics to correlate voltage breakdowns and CO₂ crossover losses with underlying physical processes across a range of operating conditions.
- **Identify design parameters to optimize integration of electrolyzer components and interfaces**
 - Mitigate energy losses from poorly optimized cathode catalyst-ionomer interfaces and electrode structures.
- **Integration strategies that improve energy efficiency and carbon utilization**
 - Predictive modeling and experiment to optimize electrodes, flow fields, and membranes to further improve performance.



● CATALYST
● CATALYST SUPPORT
● POLYMER ELECTROLYTE

Scaling

1. Device scale-up

- Decoupled limitations translating small scale device performance and durability to large scale systems

2. Systems integration

- understand complex degradation mechanisms for integrated systems (contaminants, dynamic operation)

3. Fabrication scale-up

- Enabled translation of electrode fabrication processes from lab level to R2R

4. Modeling scaled devices

- Linearize/parameterize design rules for scale-up supported by predictive modeling

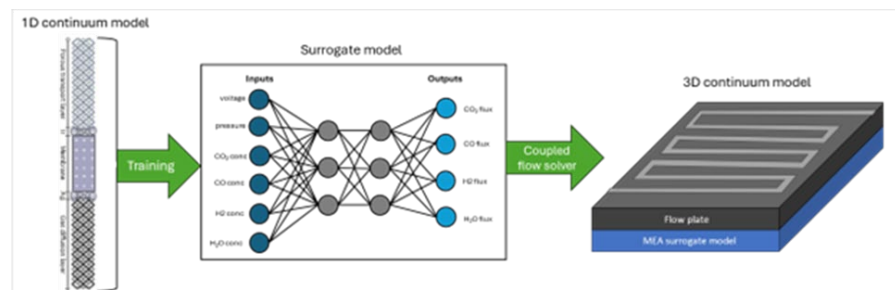
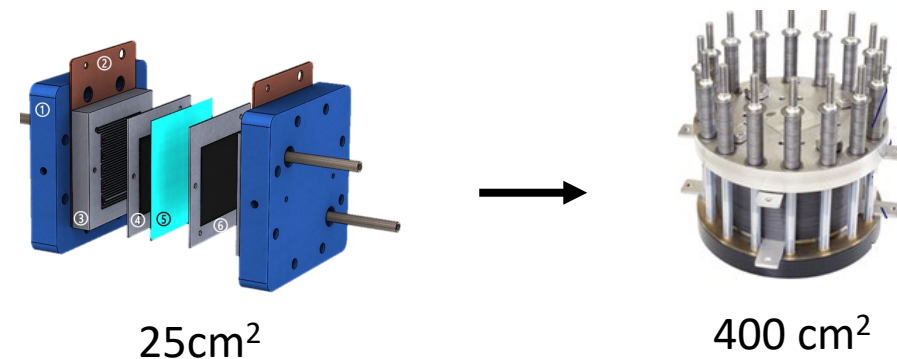


Figure 7. Coupling of surrogate model and physics-based model for the cathode flow field. The surrogate model will be used to calculate the species fluxes, which will be fed to the physics-based model as a boundary condition. Then, the outputs of the physics-based model will be used to determine the inputs for the surrogate model. This will be repeated until convergence is achieved.

Enabling Technologies

1) Anaerobic Strain Development

Production of mevalonic acid (and ultimately, longer-chain isoprenoids) to enable viable process economics

Clostridium autoethanogenum for CO upgrading (from LTE CO₂)
Increase flux from acetyl-CoA into the MVA pathway via rational pathway and protein engineering strategies.

2) Aerobic Strain Development

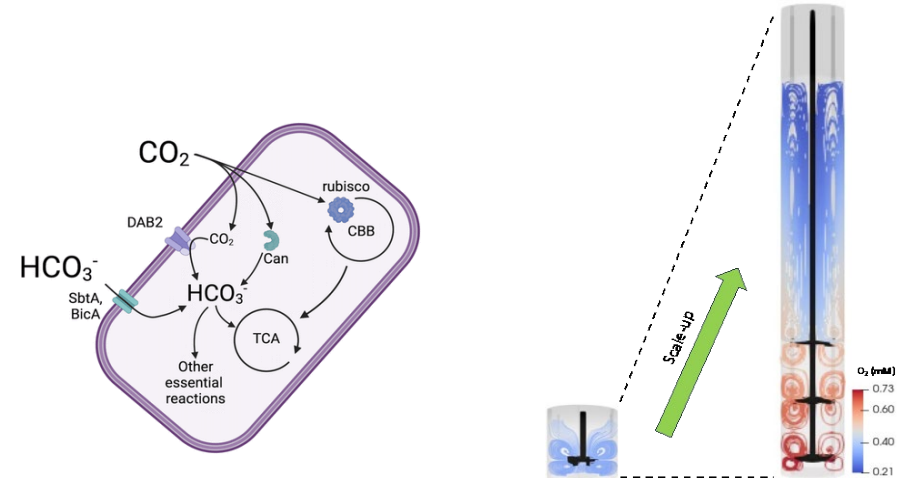
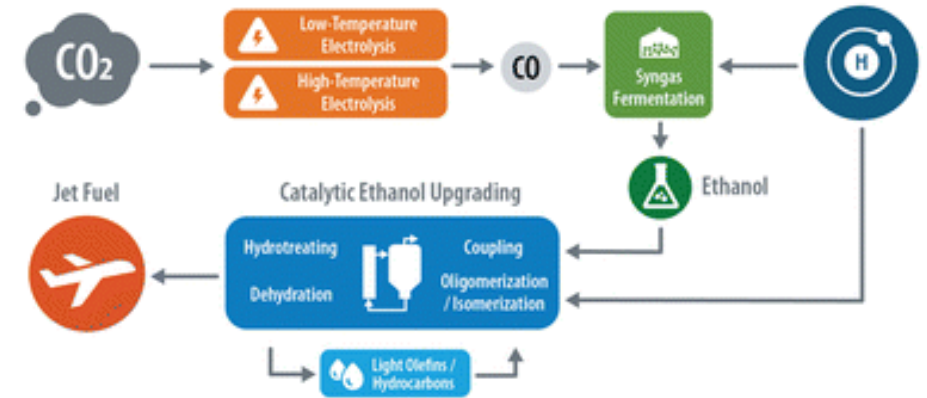
Cupriavidus necator for formic acid upgrading.

Metabolic engineering to increase carbon flux to fatty acids

3) Process Scale-Up and Process Intensification

Immobilized cultivation allows continuous substrate flow and separation of biocatalysts, addressing formic acid delivery issues.

4) Bioreactor modeling CFD will improve reactor designs.



Thursday side event: CO₂ Consortium Industry Day

- 1:30pm in Room 401/402
- Deep dive into the proposed Consortium tasks
- Soliciting industry thoughts on the effort