CO_2 To Methanol With Solid Polymer Electrolytes And Composite Electrodes In Stackable Zero-gap Electrochemical Cells (CO_2eMeOH)

Project Number: DE-FE0032414

Principal Investigator: Ryan Wartena, Aircapture

Co-Principal Investigator: Matt Atwood, Aircapture

Presenter: Dr. Ryan Wartena

U.S. Department of Energy

National Energy Technology Laboratory

Carbon Management Project Review Meeting

August 2024

Project Overview

Funding Opportunity DE-FOA-0002414 AOI-2G

Period of Performance: 12/23/2023 – 12/20/2024

Project Goal: Assess the feasibility of generating carbon-neutral electrochemical methanol for less than $800/tonne.

Administered by Department of Energy – National Energy Technology Laboratory

Total Project Cost: $535,288 Cost Share: $138,292 Federal Share: $396,996

Overall Project Performance Dates: 12/20/23-12/20/24

Project Participants

P.I. Dr. Ryan Wartena & Matthew Atwood

Collaboration with Dr. Jayant Rane & Dr. Thorsten Boger, Corning

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Project Objectives

Objective 1. Conduct a conceptual design and feasibility study with a technology gap analysis on the proposed DACCU integrated process to produce carbon-neutral MeOH from atmospheric CO2.

Objective 2. Perform a cradle-to-gate life-cycle analysis of the DACCU system to determine the environmental sustainability and carbon intensity (CI) of the proposed project and product from the results of the conceptual design study.

Objective 3. Perform a techno-economic analysis (TEA) from results of the LCA and conceptual design study to justify investment to perform laboratory validation of the proposed DACCU system.

Objective 4. Quantify how deployment of the proposed technology will promote and prepare a ready workforce for clean energy and manufacturing jobs and coordinate with community stakeholders to develop a Quality Jobs Plan, a Diversity Equity, Inclusion and Accessibility (DEIA) Plan, a Justice40 Plan Development Proposal, and a Community and Stakeholder Engagement Plan Development Proposal.

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Technology Background

In this project, Aircapture is aiming to produce carbon-neutral electrochemical methanol for less than $800/tonne.

This will be done by integrating electrochemical cell technology with our existing DAC technology to utilize the captured CO_2 as a feedstock for methanol synthesis.

The project will begin with design and development of an integrated electrochemical reduction reaction system that combines our established DAC system with CO_2 electrochemical reduction reactions (CO_2RR).

The project will culminate with the fabrication of a lab-scale system to validate the Direct Air Capture and Carbon Utilization (DACCU) proposed concept.

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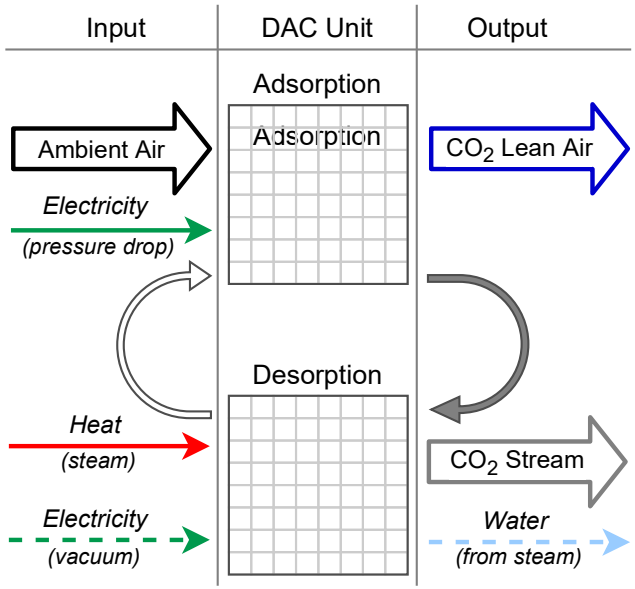
Technology Background – DAC Operation

Step 1 (Capture): CO_2 is collected by moving air or mixtures of air and CO_2 rich gases across a proprietary contactor which adsorbs CO_2.

Step 2 (Regeneration): The contactor is moved into a regeneration box where low-temperature steam flows across the contactor, removing CO_2 from the contactor, and the CO_2 is collected.



Polymeric Amine Sorbent

- Monolithic Contactor
- Low pressure drop
- Low thermal mass
- High geometric surface area
- Compatible with various construction methods

Adsorption

- 900 seconds / monolith in ambient air

Desorption

- Saturated Steam in less than 90 seconds

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Technology Background – Adding Electrochemistry

We are aimed at commercializing modular chemical production systems: modular DAC + Electrochemical plants.

This project proposes to engineer, build, and operate a low-voltage, <1.6V, CO_2RR electrolysis cell to MeOH with PtRu and $PtRuO_2$*(0-xH_2O) electrocatalysts utilizing:

- Flow-optimized ceramic Gas Diffusion Electrodes (GDE) to increase CO2 transport to the composite cathode
- Solid polymer electrolyte membranes with varied thickness for optimal proton conduction

Using this approach, CO_2 enters the GDE cathode, combines with protons generated at the anode, is transported through the polymer membrane and composite cathode materials, and forms liquid products of 1M MeOH in water.

Our goal is to achieve increased current densities, from 1 to 100's mA/cm^2 leading to higher capital efficiency MeOH process with exceptional LCA.

Electrogenerating MeOH at smaller potentials than water electrolysis will lead to a lower energy and economic production cost than traditional reactions with hydrogen produced by water electrolysis.

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Technology Goals

Operational DAC unit at Aircapture's Berkeley, CA headquarters.

The construction and operation of this unit was supported by DE-FE0031961.

Unit has operated over 3,300+ hours at the DOE's National Carbon Capture Center (NCCC).

Yielded key commercial and manufacturing insights for upcoming multi-DAC deployment.

Adding electrochemical methanol generation can enable installation of modular DAC units with small footprints – higher current densities and higher capital efficiency methanol generation.

Potential for improved Lifecycle Analysis (LCA) and more flexibility in installation locations.

DAC-100 SN3 (Berkeley, CA) Apr 24

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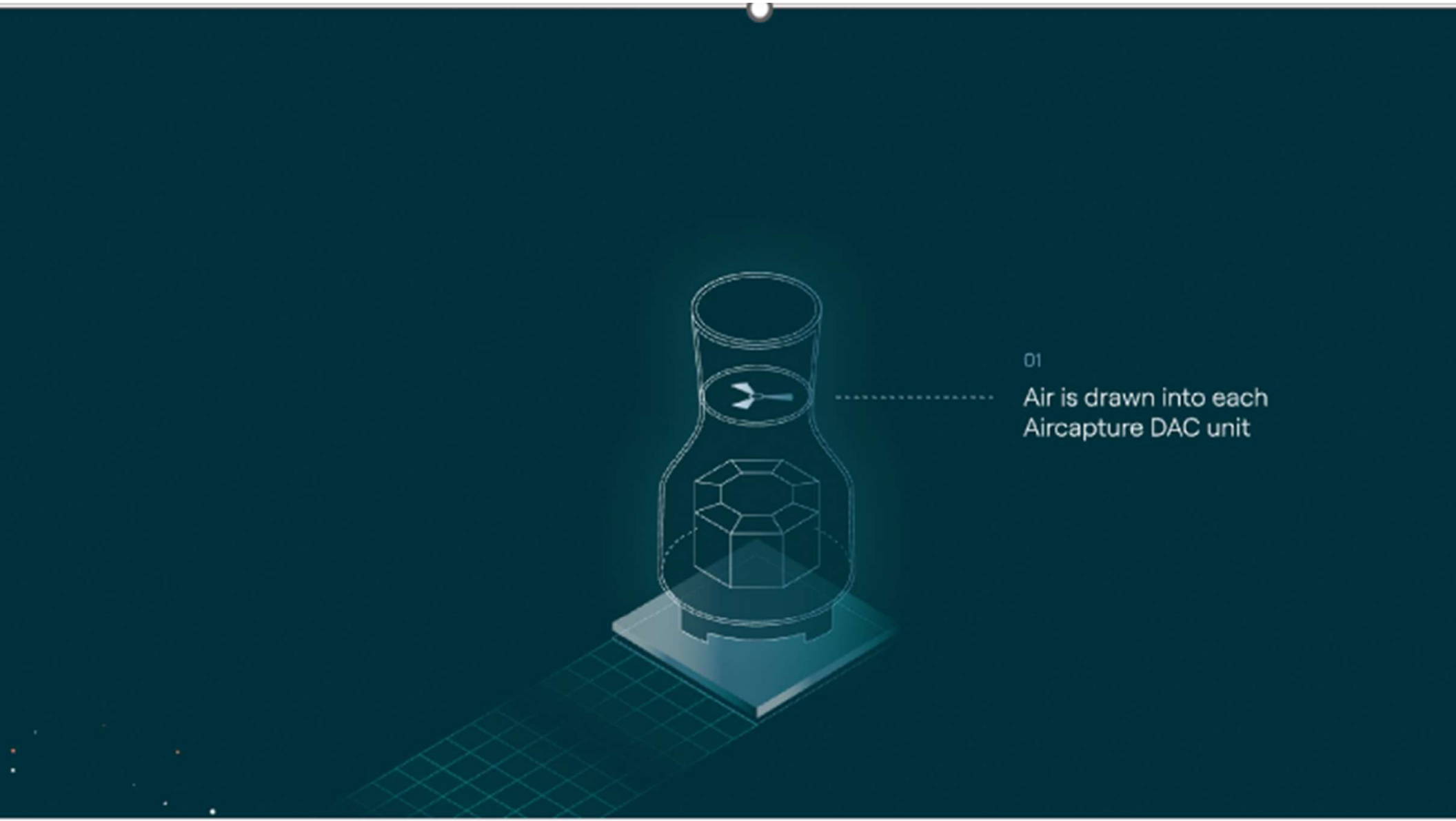
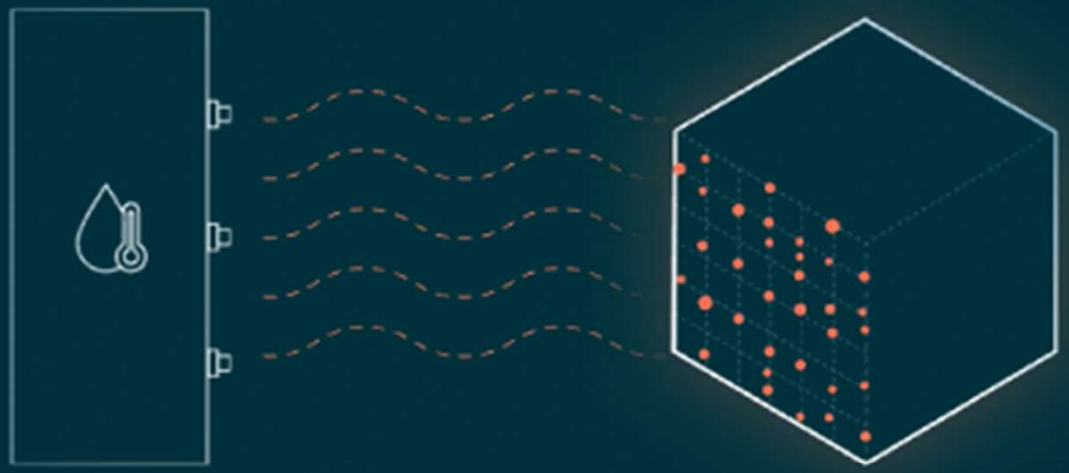

01
Air is drawn into each
Aircapture DAC unit

02

and CO_2 is adsorbed and captured on a series of specialized "contactors"

03

as the now CO_2-depleted air returns back to our atmosphere.



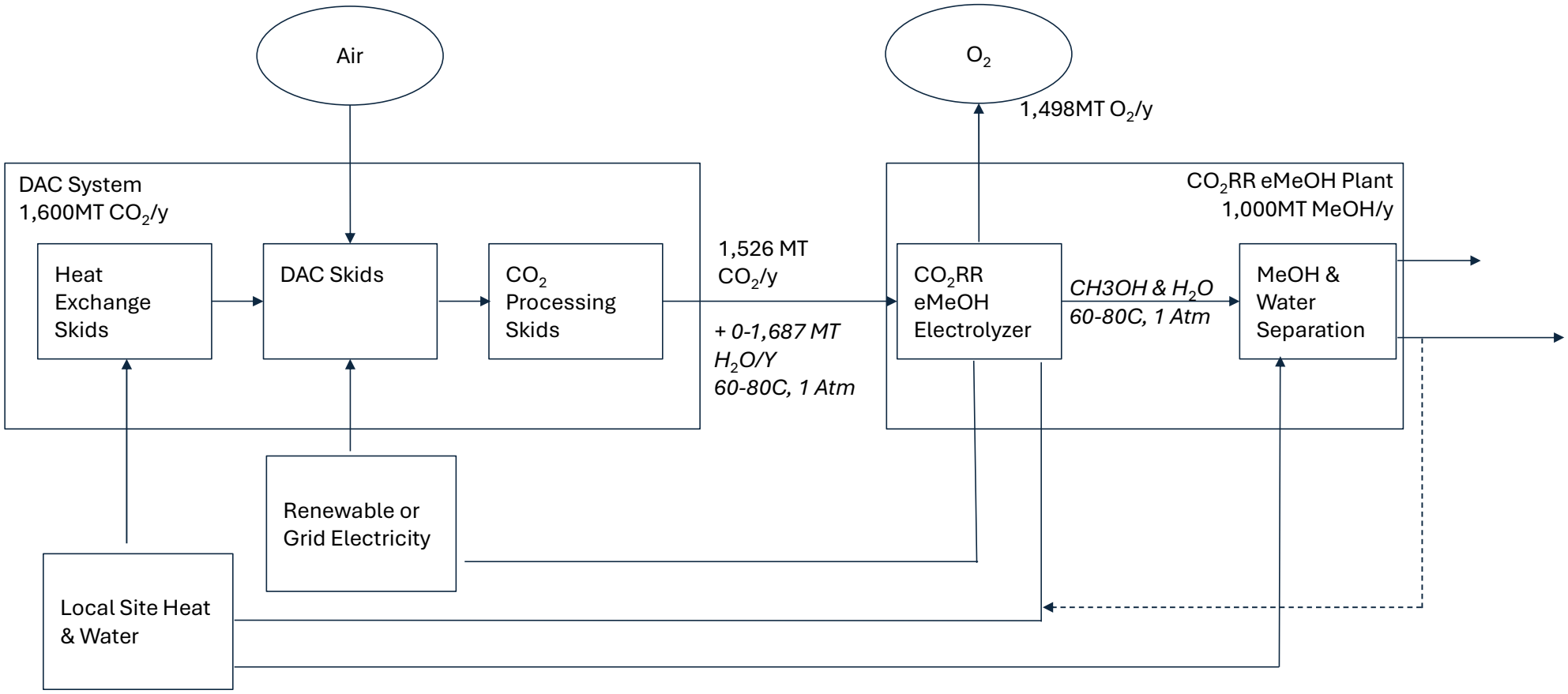
04

Once our contactors are saturated with CO_2, steam releases the pure CO_2

05

as a reliable stream of high quality, gaseous CO_2

DAC + Methanol System Design



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Project Scope

Task 1: Project Management & Planning

- Technological & Economic Feasibility Documents (TEA, LCA, State Point Data Table)
- EH&S Risk Assessment, Tech Maturation Plan, Tech Gap Analysis

Task 2: R&D Community Benefits Plan

- Justice40 & Engagement Project Development Plans
- Quality Jobs Plan, DEIA in Hiring

Task 3: Conceptual Design & Feasibility Study

- Description of DACCU System, Conceptual Design & Process Engineering Package
- Modeling Electrochemistry & Input/Output stream via COMSOL, Constructability & HAZOP Review

Task 4: Experimental Work

- Expandable Electrochemical Methanol Stack Design & Assembly
- Baseline Experiments & Model Validation via Experimental Work

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Technical Approach/Project Scope

$$CO_2 + 6\,H^+ + 6\,e^- \rightarrow CH_3OH + H_2O \qquad E^\circ_{cathode} = 0.04\ V\ vs.\ NHE$$

$$3\,H_2O \rightarrow {}^3/_2\,O_2 + 6\,H^+ + 6\,e^- \qquad E^\circ_{anode} = 1.225\ V\ vs.\ NHE$$

$$CO_2 + 2\,H_2O \rightarrow CH_3OH + {}^3/_2\,O_2 \qquad E^\circ_{cell} = 1.185\ V$$

Xia, X. H., Iwasita, T., Ge, F., & Vielstich, W. (1996). Structural effects and reactivity in methanol oxidation on polycrystalline and single crystal platinum. Electrochimica Acta, 41(5), 711–718. doi:10.1016/0013-4686(95)00360-6

Sebastián, D., Palella, A., Baglio, V., Spadaro, L., Siracusano, S., Negro, P., … Aricò, A. S. (2017). *CO 2 reduction to alcohols in a polymer electrolyte membrane co-electrolysis cell operating at low potentials. Electrochimica Acta, 241, 28–40.*

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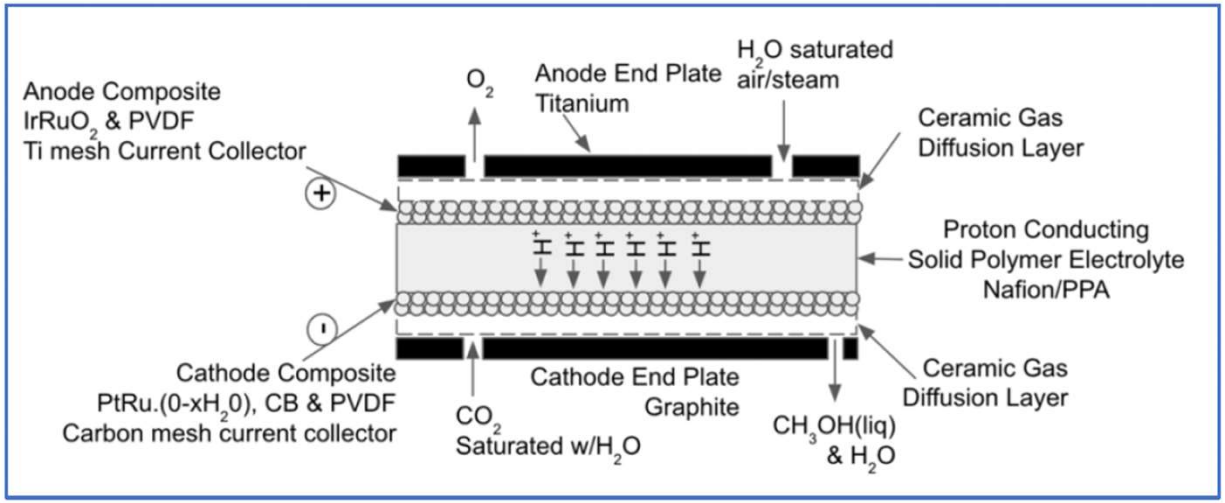
CO2RR Design from a Water Electrolysis Cell

- Initial Piping & Instrumentation Diagram (P&ID) completed
- Selection of water electrolysis cell rather than reverse-direct methanol fuel cell



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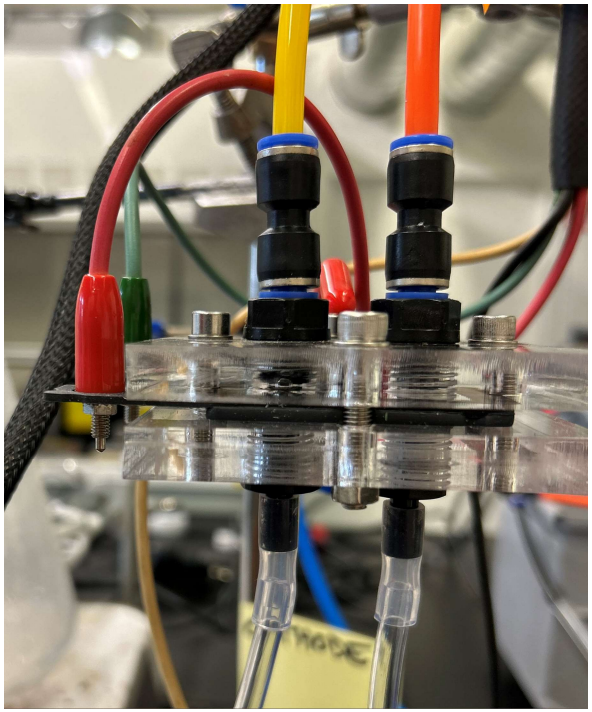
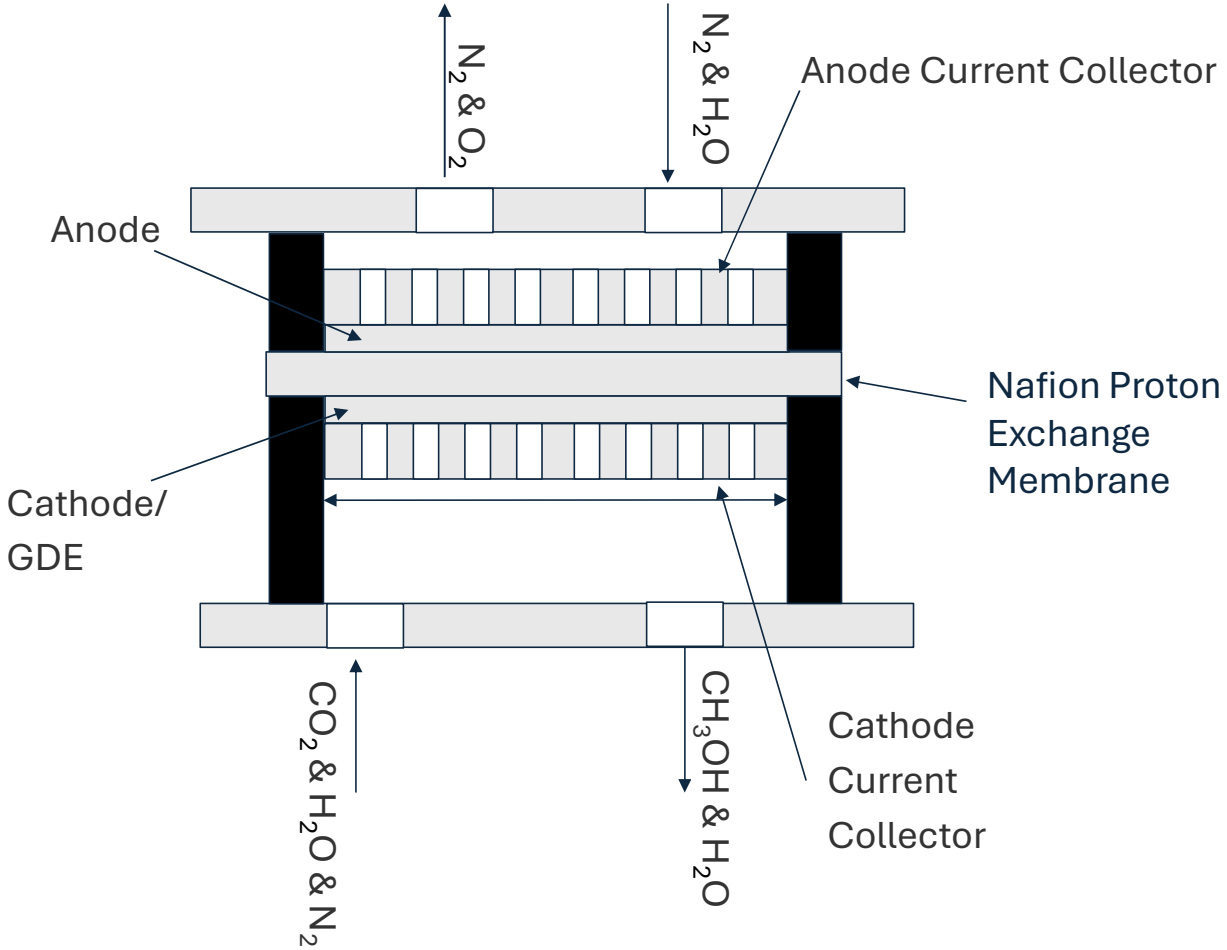
Experimental CO2RR Electrolysis Cell



Electrolysis cell installed in the Aircapture lab.



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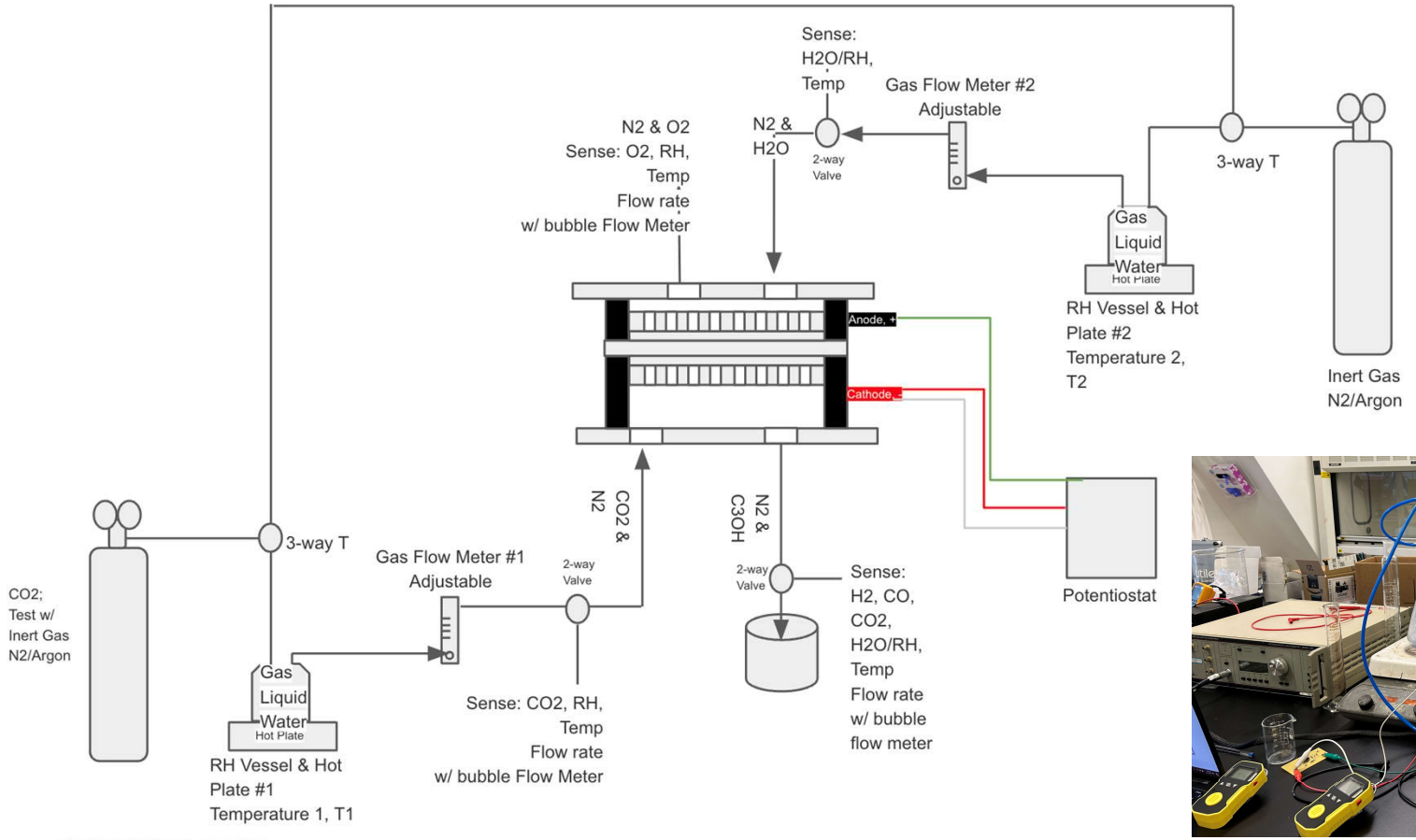
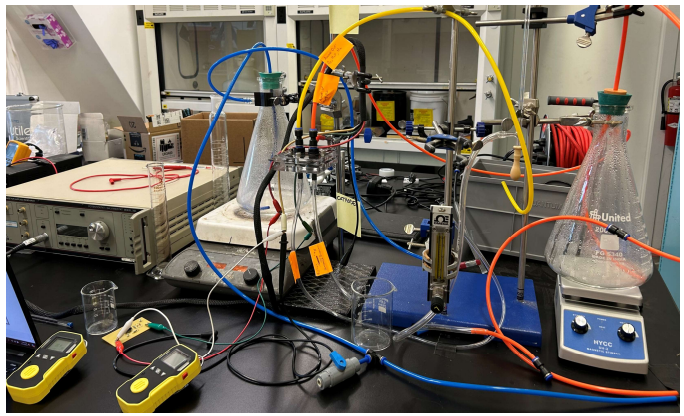
CO2RR Experimental Setup





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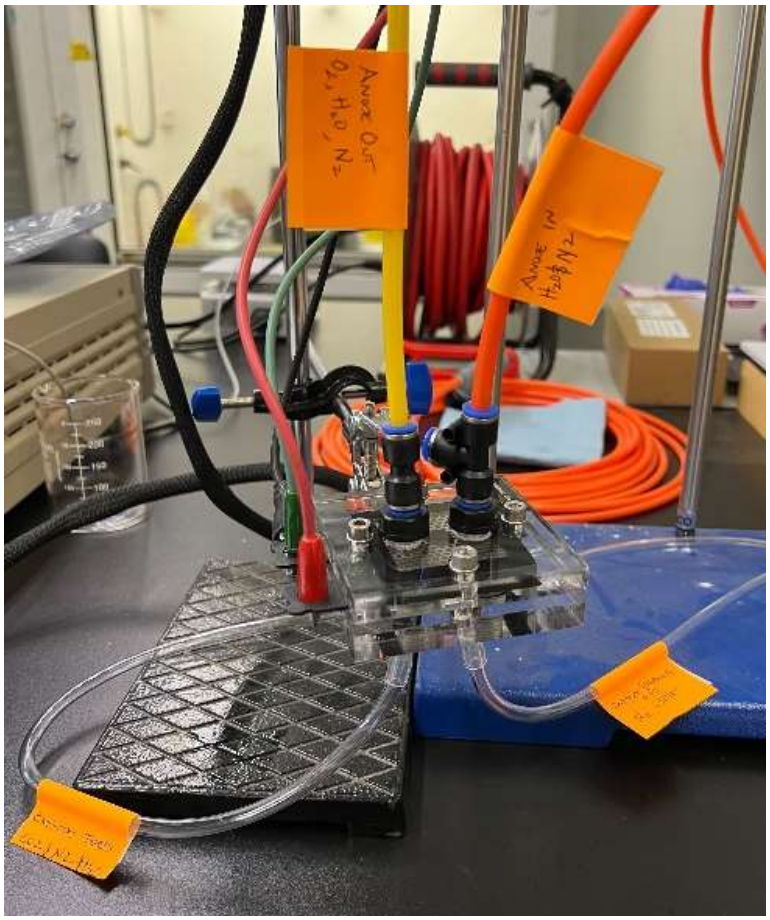
Designing & Assembling Experimental Setup

- System is designed around water electrolysis cell with Nafion membrane.
- Incorporates sensors to monitor temperature, relative humidity, flow rate, gas species, and Potentiostat to control Voltage/current for Chronopotentiometry, Cyclic Voltammetry, and bulk electrolysis.
- Assembled from commercially available components



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Chronopotentiometry Study

- Initial voltage vs. current experiments run with cathode inlet at 5cc/min on 16mm^2 electrodes with (a) 5% CO_2 in N_2 & (b) 0% CO_2 (100% N_2) at consistent temperature, relative humidity and flow rate.
- Hypothesis: observe a higher current at voltages below water electrolysis, indicating that CO_2 is participating in CO_2 reduction reactions.
- Compare these results to the output of the COMSOL model to confirm accuracy.

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Progress

- Applied commercialized water electrolysis cells with Pt-type composite cathode, Ir-type composite anode, proton conducting membrane, and current collectors with diffusion features of perforated plates.
- Low Voltage electrolysis of CO_2 streams shows larger currents than water electrolysis control experiments indicating the reduction of CO_2 to alternate species at low voltages and higher current densities than reported in literature.
- Physics modelling with COMSOL is providing insights towards scaling current density at low voltages and low temperatures.
- Design of Experiments for current density temperature dependance for gas diffusion electrode geometries & materials.

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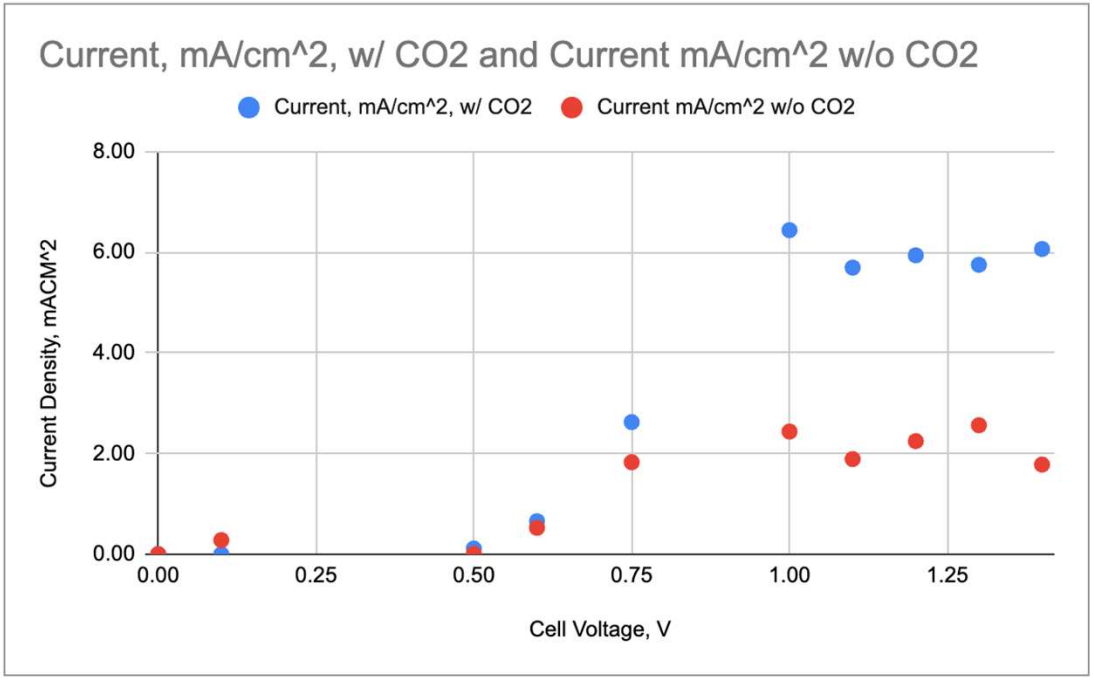
Baseline Experimental Results – Milestone 7

Cathode inlet: 5% CO_2 vs. 0% CO_2 into electrolysis cell at 5 cc/min

Cell Voltage, V	Current, mA/cm^2, w/ CO2	Current mA/cm^2 w/o CO2
0	0.00	0.00
0.1	0.00	0.28
0.5	0.11	0.01
0.6	0.66	0.53
0.75	2.63	1.83
1	6.44	2.44
1.1	5.69	1.89
1.2	5.94	2.25
1.3	5.75	2.56
1.4	6.06	1.78



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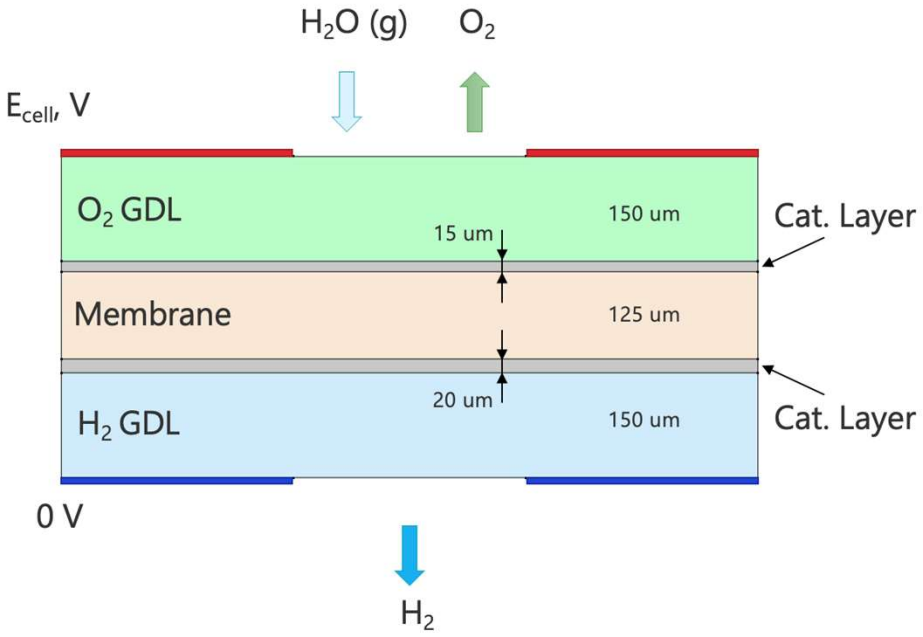
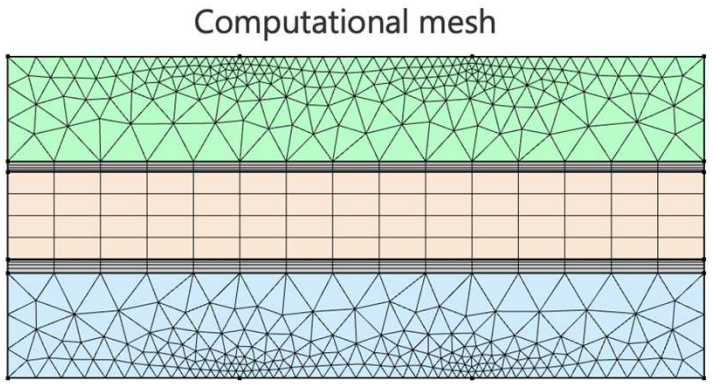
Initial Process Modeling with COMSOL – Milestone 6

Initial model is for water electrolysis for the production of Hydrogen and Oxygen.





- Temperature: 35 – 80 °C
- Pressure: 1.0 – 1.5 bar
- Flowrate (CO2 + N2): 10 cc/min
- Fraction of H2O: 10%

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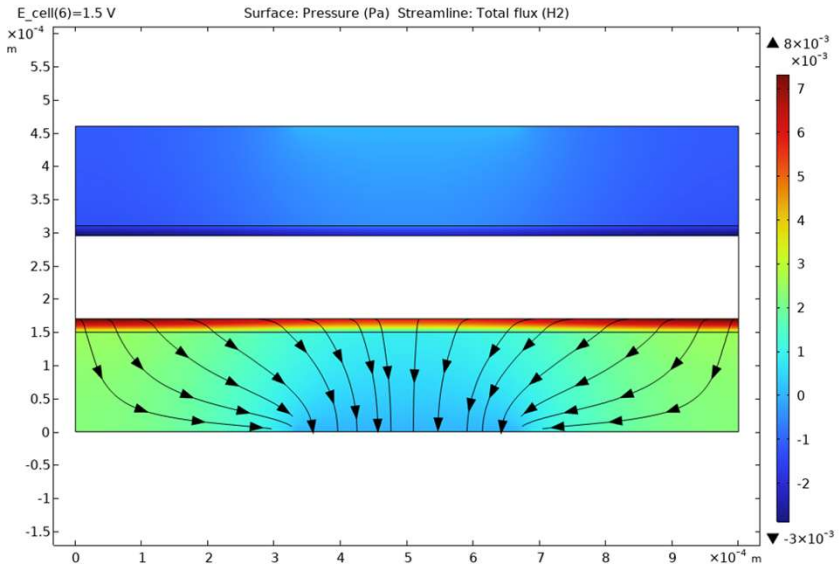
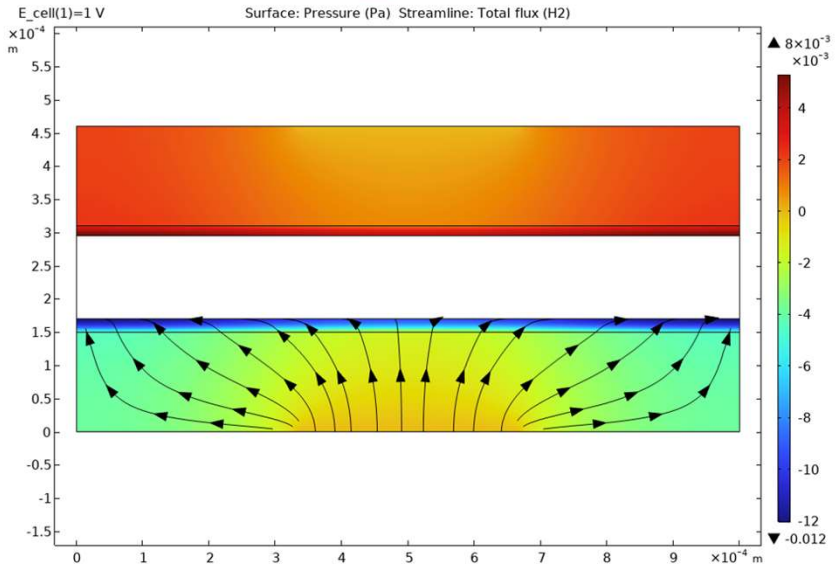
Initial Process Modeling with COMSOL – Milestone 6

Initial H2 flux cell model applied to Electrolyzer regime and Fuel Cell regime.

Electrolyzer (E_{cell} = 1.5 V)



Fuel Cell (E_{cell} = 1.0 V)



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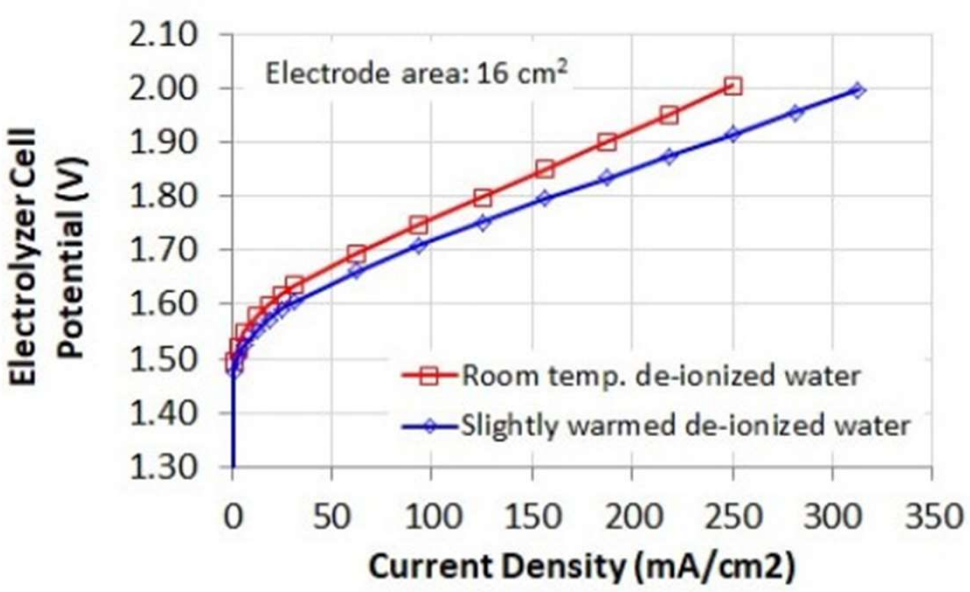
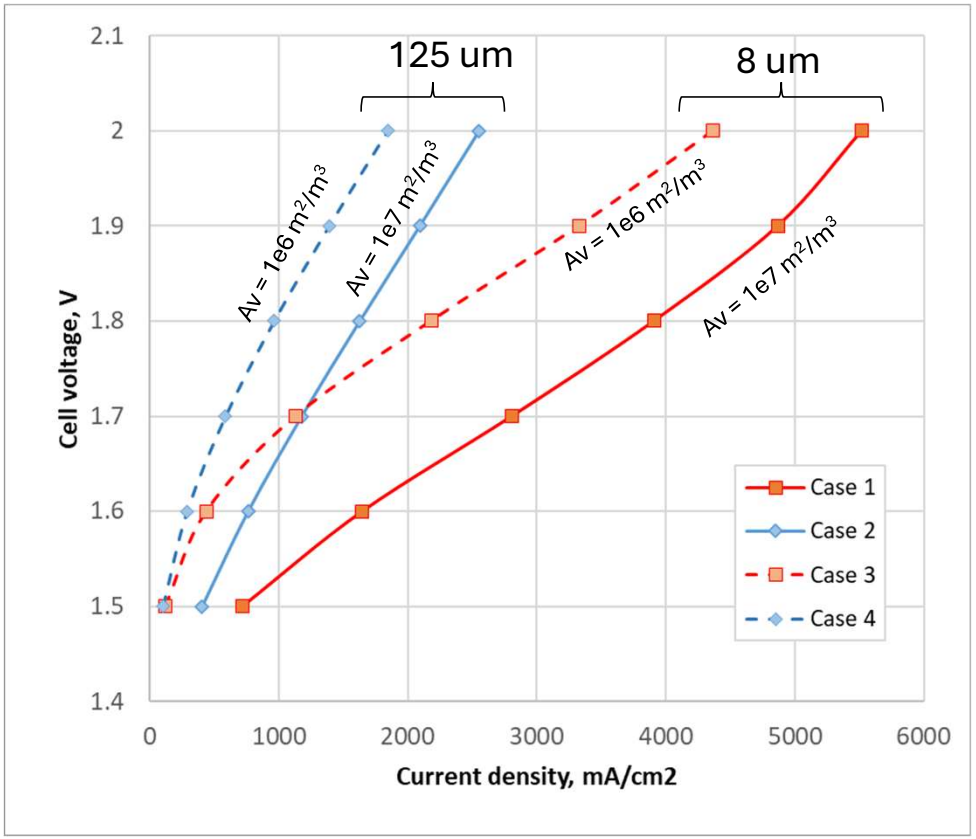
Initial Process Modeling – Milestone 6

Baseline COMSOL Current vs. Voltage Plots for Water Electrolysis





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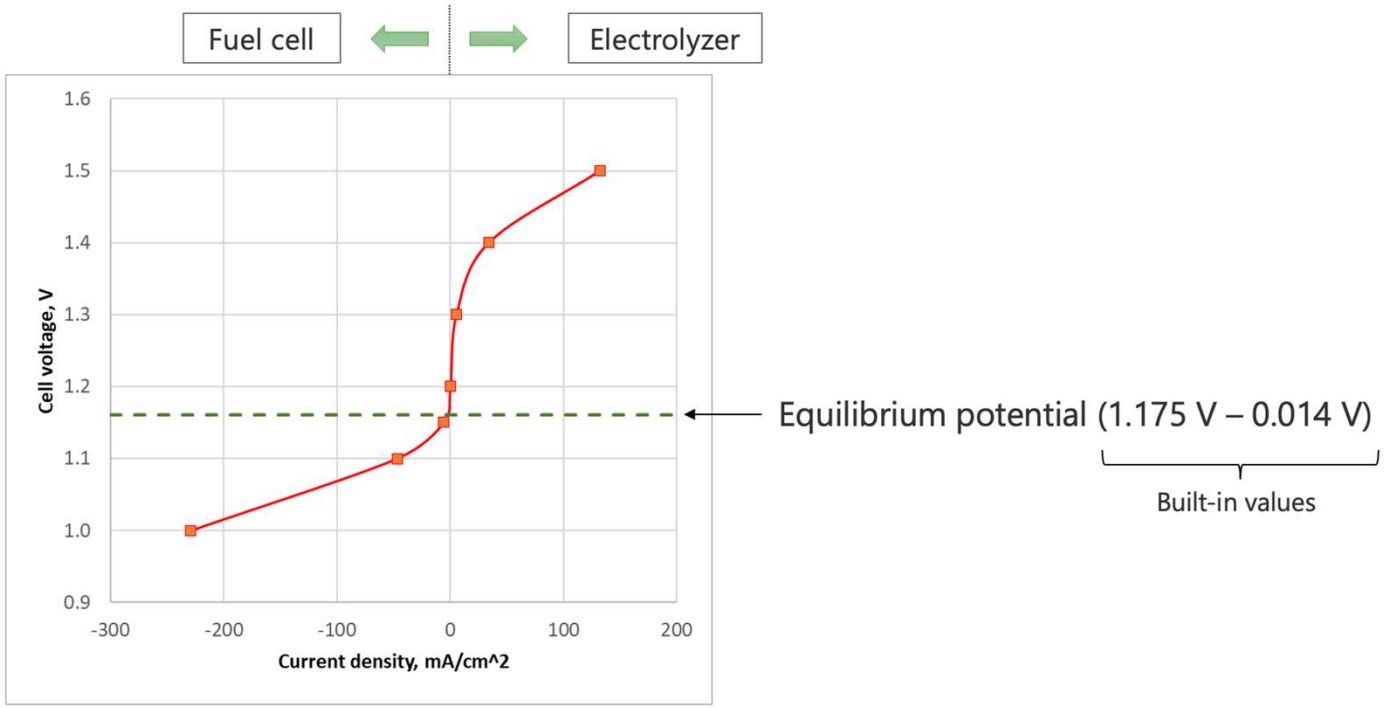
Initial Process Modeling with COMSOL – Milestone 6

Polarization Curve for Electrolyzer and Fuel Cell activity of Hydrogen



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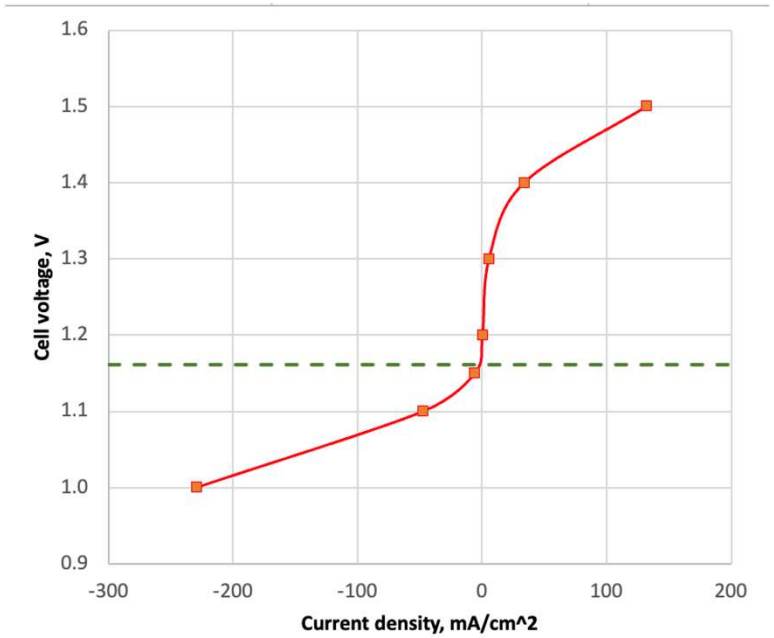
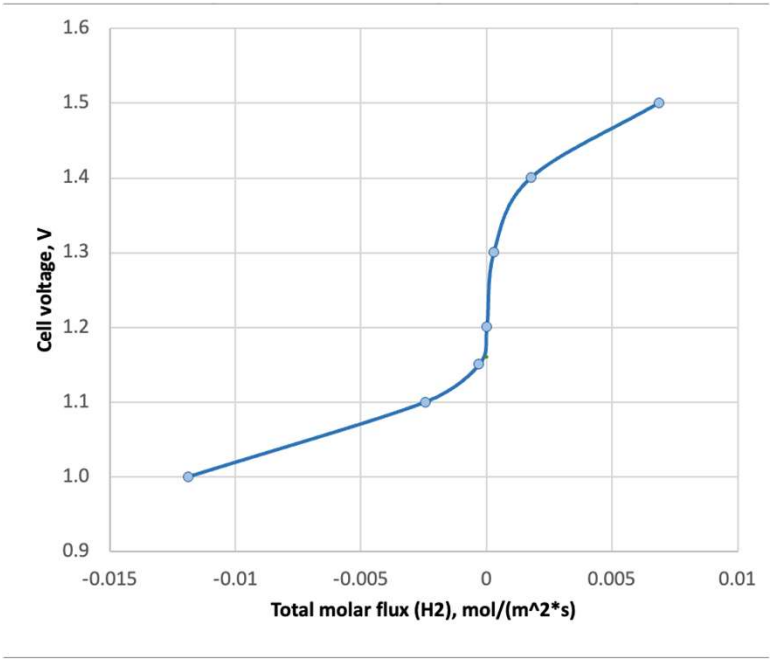
Initial Process Modeling – Milestone 6

Hydrogen Fuel Cell Actions vs. Water Electrolysis Hydrogen Generation





COMSOL Modelling suggests that below 1.16VDC, Protons favor reacting with available species over reducing to hydrogen.

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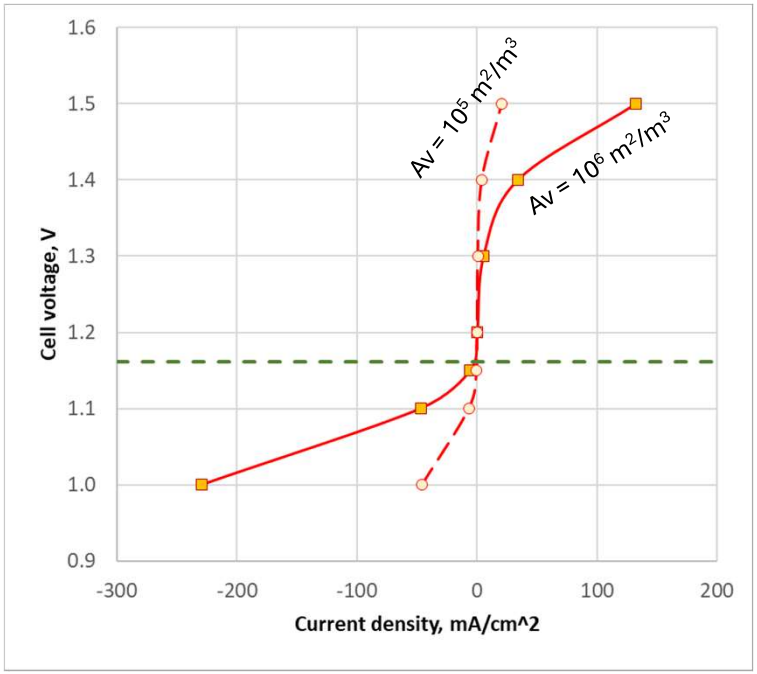
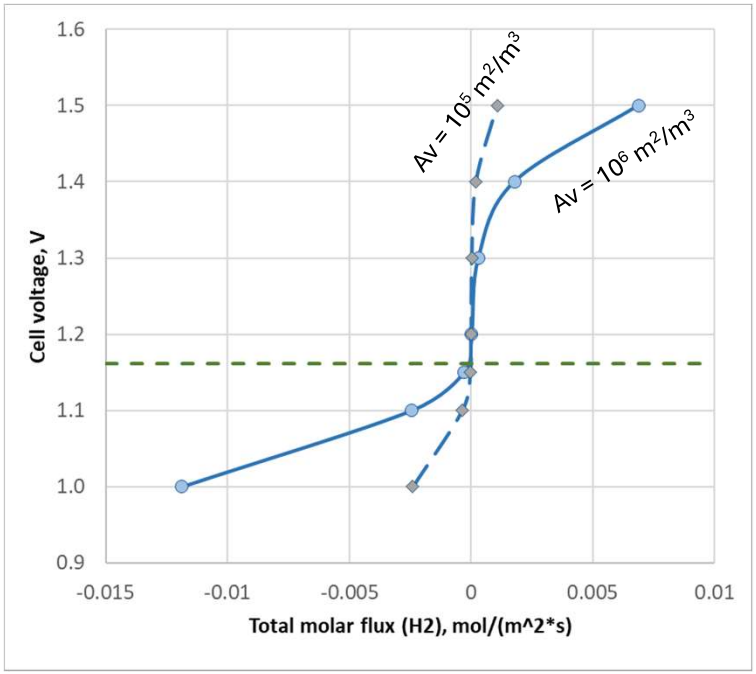
Initial Process Modeling – Milestone 6

Hydrogen Fuel Cell Actions vs. Water Electrolysis Hydrogen Generation





COMSOL Modelling suggests larger active material surface area will lead to higher current densities

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Next Steps

- Bulk electrolysis experiments at low voltage to generate cathodic samples for chemical analysis.
- Design of Experiments for CV, PC, & COMSOL to investigate current density as a function of:
  - CO_2
  - Temperature
  - RH & Flowrates
  - MEA Thickness
  - Flowrates & Diffusion Layer thickness, structure, & porosity

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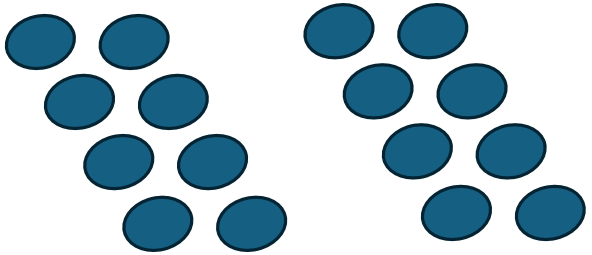
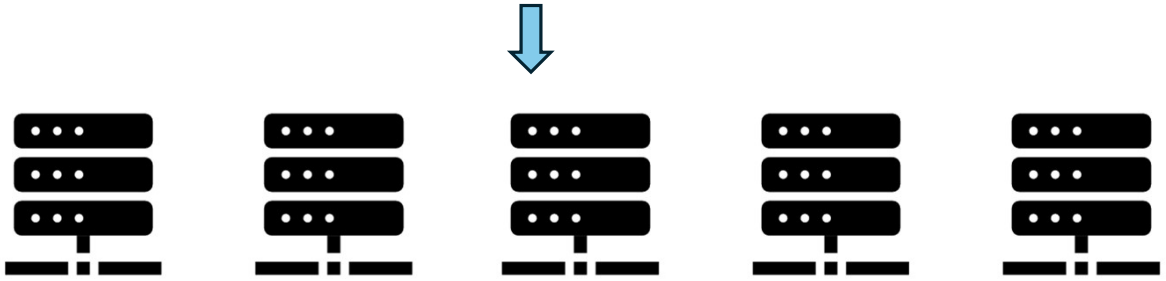
Detailed DACCU System Description – Milestone 4

"Groves" of 8 DAC Units
Capturing 100 MT/Y CO_2 per unit
Capturing 1,600 MT/Y CO_2 total



CO_2 RR eMethanol Cell Stacks
190kW Capacity Each
1,140kW Capacity Total
Generating 1,000 MT MeOH/Y

Electricity Input:
27.3MWH/D for electrolysis



Storage & Utilization
Generating 1,000 MT MeOH/Y for use on-site in facility or transportation to point of use.

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Community Benefits/Societal Considerations

Milestone 2: CBP Initial Assistance & Validation – We've met with the DOE team to review our CBP plan and solicit feedback on how we can optimize our approach. We are planning a virtual townhall meeting to invite local community stakeholders to share the innovations being made in their local community and welcome questions about the work.

Milestone 3: DEIA in Hiring – Workforce Diversity – Aircapture has successfully run its annual internship program again this year, increasing the size of the program by 50% and using equitable hiring processes.

Milestone 5: Complete Justice40 Research Plan - We have assembled our Justice40 Research Plan which will guide our assessment of how building and operating a scaled-up electrochemical methanol plant could impact the economic, environmental, and societal welfare of the surrounding communities.

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Lessons Learned

- Commercial electrochemical cells can be applied for CO2RR process development
- Bubble flowmeters are great to check flowrates
- COMSOL struggles to keep a balanced mass flow due to Finite Element math
- We have established a coordinated process of novel CO2RR development and scale-up between computational modelling and experimental methods

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Future Plans

In this project, we will continue testing and verification – building a more sophisticated software model and confirming the generation of methanol to meet the <$800/metric tonne target.

Upcoming Milestones:

Milestone 8: Demonstrating Quality Jobs

Milestone 9: Model Validation from Experimental Work

We've begun to investigate local areas that could be suitable for one of these sites with attention paid to their economic and environmental status/outlook and local employment prospects.

After the successful completion of this project, we intend to scale the capacity of this process to using emerging, commercially available fuel cells that are new to the market.

We look forward to working with DOE and commercial stakeholders to continue development.

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Summary

Electrogenerating MeOH at smaller potentials than water electrolysis will lead to a lower energy and economic production cost than traditional reactions with hydrogen produced by water electrolysis.

We have initiated and are coordinating experiments and computational studies that suggest CO2RR occurs with larger current densities and at potentials lower than water electrolysis.

We are focused to engineer and scale-up increased current densities for the low voltage electrogeneration of MeOH, from 1 to 100's mA/cm2 leading to a more capital efficient MeOH process with exceptional LCA.

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Acknowledgement

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Thank you to AirCapture, Corning, Hyundai Motor Corporation

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