Negative-Emissions Enabled Direct Air Capture with Coupled Electro-Production of Hydrogen at a 5 kg-per-hour Scale (DE-FE0032255)

Xin Gao, Jesse Thompson, and Kunlei Liu Institute for Decarbonization and Energy Advancement at PPL R&D Center University of Kentucky August 5th, 2024

Project Overview

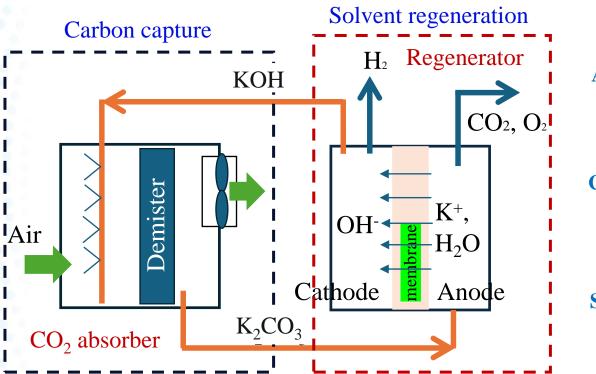
Project Title	Negative-Emissions Enabled Direct Air Capture with Coupled Electro-Production of Hydrogen at a 5 kg-per-hour Scale	
Award #	DE-FE0032255	
Project Goals	Develop an intensified and simplified DAC process at a TRL 5 scale that simultaneously produces H_2 to offset the process cost.	
Funding	DOE: \$2,999,681 Cost-Share: \$749,943	
Duration	08/1/2023 – 7/31/2026, 3 Budget Periods	
Project Participants	UKy, EPRI, PPL Corporation, and TotalEnergies	

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Solvent-Based Technology Applied to DAC

Process Sketch for DE-FE0032255



 $CO_2 \text{ capture}$ $CO_2 + 2OH^- \rightarrow CO_3^{2-} + H_2O$

Alkaline water electrolysis $2H_2O \rightarrow O_2 + 4H^+ + \text{electrons}$ $2H_2O + \text{electrons} \rightarrow H_2 + 2OH^-$

CO₂ release H⁺ + CO₃²⁻ → HCO₃⁻ H⁺ + HCO₃⁻ → CO₂ + H₂O

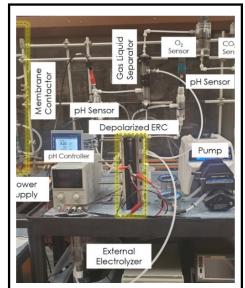
Solvent regeneration $K^+ + OH^- \rightarrow KOH$

Feature: producing H_2 for sale, offsetting DAC operating cost

History of DAC and H₂ Production Research

DAC 1.0, proof-of-concept

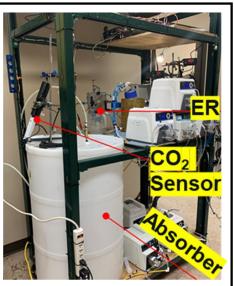
DAC 2.0, size up DAC 2.5, point-source integration



2020 - 2021

- 30 W regenerator
- 2 L min⁻¹ air contactor
- <1 kg yr⁻¹ CO₂ capture process
- <1 kg yr⁻¹ H₂ production
- · Standard operation and explored depolarized operation DE-FE0031962

Our publication



2021 - 2023

- 210 W regenerator
- 10 cfm air contactor
- 200 kg yr⁻¹ CO₂ capture
- 10 kg yr⁻¹ H₂
- · Zero-gap cell design, electrode material selection
- ~500 kJ mol⁻¹ regeneration

energy DE-FE0032125



2022 - 2023

- 600 W regenerator
- 14 cfm gas with 4,000 ppm CO₂ contactor
- Negative Emissions, Integrated with point source capture (3-5% CO₂) as polisher
- Carbon polisher, 1700 kg yr⁻¹ process
- H₂ production at 77 kg yr⁻¹

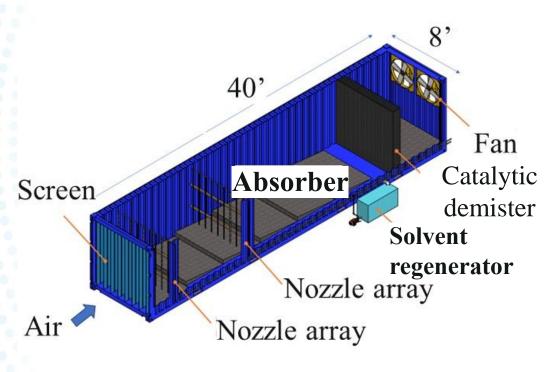
Journal of the Electrochemical Society 169 (4), 044527 ECS Advances 3 (2), 024501

International Journal of Applied Ceramic Technology 20 (5), 3014-3026 US 11857914B2

2023-2026: DAC 3.0 Packing assisted cross-flow absorber and stacking solvent regenerator

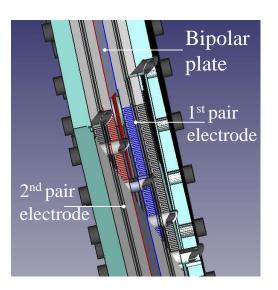
Equipment Sketch for DE-FE0032255

Capturing kiloton of CO₂ year⁻¹ from air



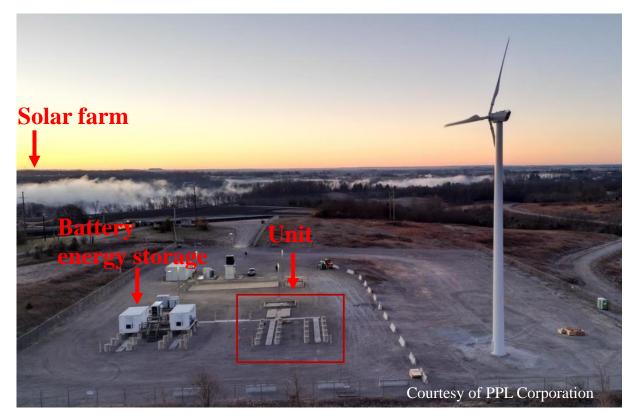
Solvent regenerator:

• Bipolar plate



*Packing structure is not shown.

Project Goal Renewable powered DAC and H₂ production at PPL testing site



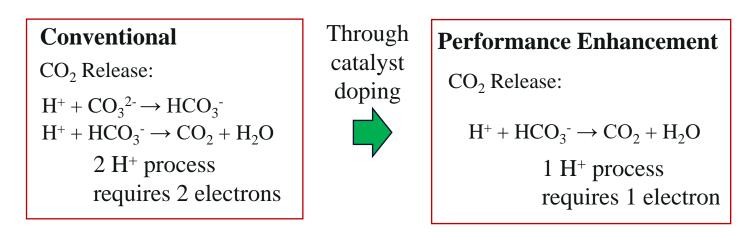
- The unit will be installed at the E.W. Brown Power Generation Plant affiliated with PPL Corporation.
- The unit will be powered by renewable energy coupled with battery energy storage, facilitating life cycle assessment.

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Motivation of Tasks 2 and 3 in BP 1 Reduce energy needed for solvent regeneration

Catalytic Demister for carbon capture (Task 2)



- Due to the small partial pressure of CO_2 in air, CO_3^{2-} is the major product.
- Using a catalyst to promote HCO₃⁻ formation, therefore reducing the number of electrons (electricity) for H⁺ production.

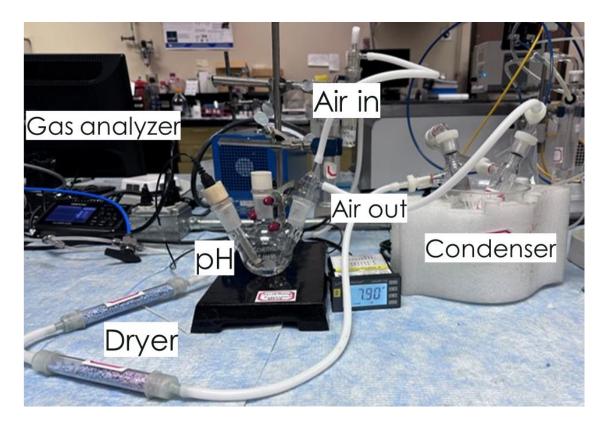
Catalytic electrode for solvent regeneration (Task 3)

• Using a catalytic material to minimize overpotential of water electrolysis or gas evolution reactions.

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Catalyst Development (Task 2) Experimental

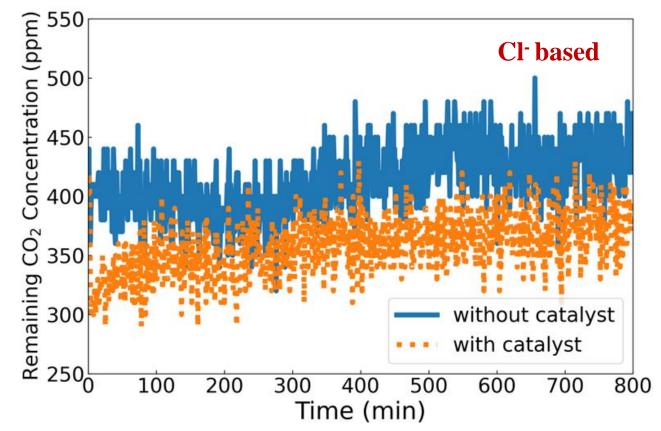


- Conditions: 0.5 L min⁻¹ of air, 5 mM catalyst in 1 M K_2CO_3 for air capture, Vaisala CO_2 gas analyzer
- Measured: remaining CO₂ concentration
- Goal: calculate carbon capture rate

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Catalyst Development CO₂ capture performance



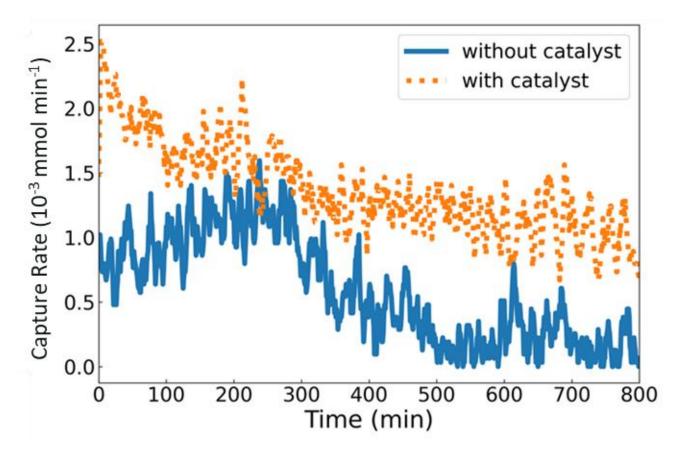
- BF_4^- based and Cl^- based catalysts have been synthesized.
- CA mimic shows the enhanced carbon capture performance at high pH, due to its enhanced surface charge, facilitating CO_2 reacting with CO_3^{2-} to produce HCO_3^{-} .

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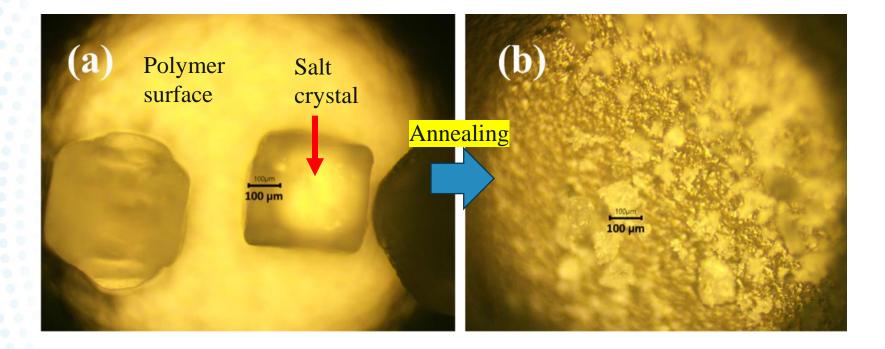


Catalyst Development Substantial increases in capture rate



• At 800 min, the rate without catalyst is almost diminished while the rate with catalyst is still measurable.

Catalyst Development Immobilization of non-soluble catalyst on demister



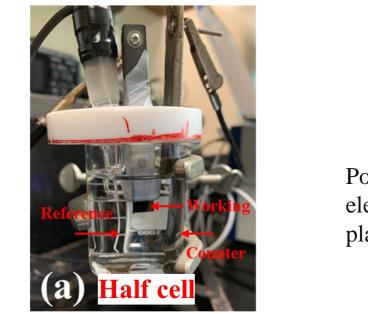
- Roughen surface of demister.
- Using water-soluble salt particles to induce surface pits on a demister through annealing, thereby establishing host sites for a catalyst.

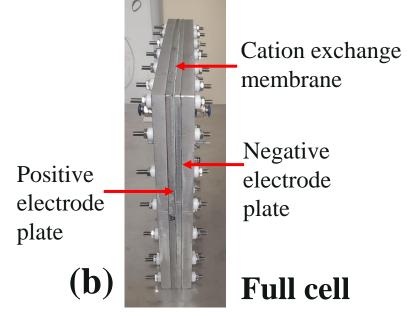
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Catalyst Electrode Selection (Task 3) Experimental





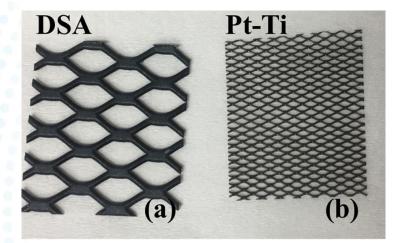
Half-cell: 3-electrode cell, cycling voltammetry, 100 mV s⁻¹, 1 - 1.5 M K₂CO₃ Full-cell: 400 cm² plate cell, constant current charging, varied charging currents, up to 2-6 M K⁺.

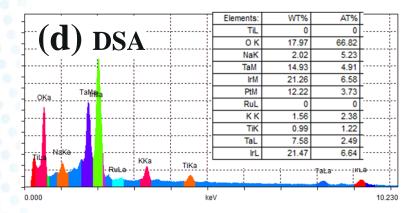
Measured: current vs voltage

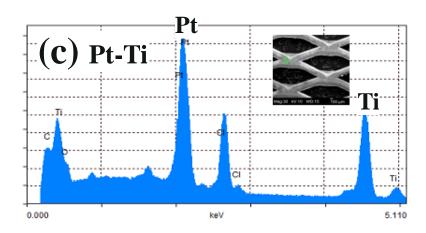
Goal: examine catalytic material stability under alkaline conditions



Catalyst Electrode Selection Catalytic electrode: DSA vs Pt-Ti





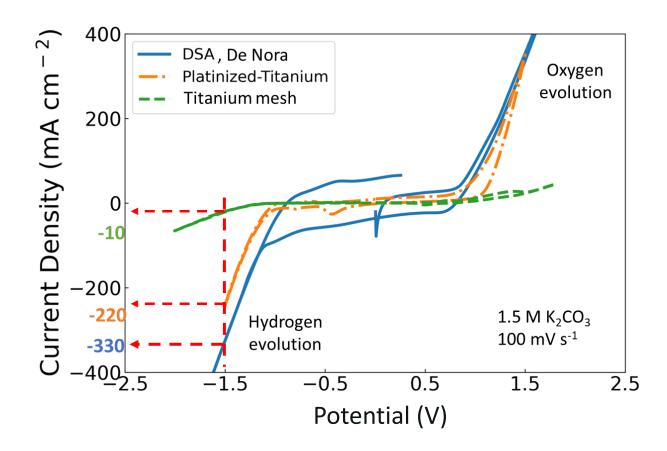


- Dimensional stable anode (DSA): a titanium mesh coated with Ir, Pt, etc
- Platinized titanium (Pt-Ti): a titanium mesh coated with Pt black.
- Both electrodes can catalyze gas evolution reactions.

https://www.denora.com/our-brands/DSA.html

https://www.denora.com/our-products/Anodes-for-Oxygen-Evolution/platinized-anodes.html

Catalyst Electrode Selection Catalytic effect in half-cell: DSA > Pt-Ti

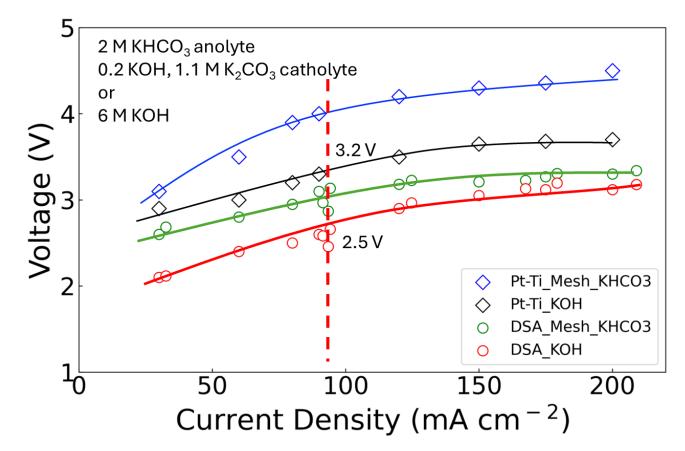


• DSA exhibits a more robust current response compared to Pt-Ti, indicating a potentially faster kinetic for gas evolution reactions.

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Catalyst Electrode Selection Operating voltage of a full cell: DSA < Pt-Ti

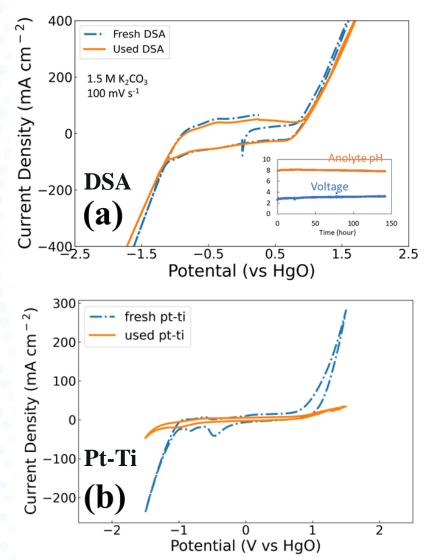


• DSA exhibits a lower voltage compared to Pt-Ti, consist with the results from the half-cell studies.

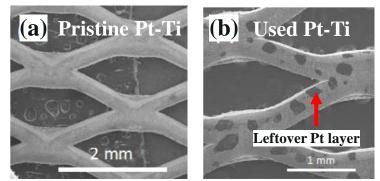
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Catalyst Electrode Selection Electrode stability: DAS > Pt-Ti



- Following a full-cell long-term test, half-cell tests for used anodes were repeated.
- DSA demonstrates greater electrochemical stability when it comes to gas evolution reactions.
- The decline in current behavior observed in Pt-Ti is attributed to the loss of the Pt catalytic layer.
- Select DSA as the catalytic electrode.



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Preliminary Techno-Economic Analysis (Task 4) Impact of catalyst on DAC cost

(\mathbf{a})	Cost of Capture, \$/tonne CO2					
Component	14X Scale (49,000 tpy)					
Component	Base Case	11% Enhanced	21% Enhanced	30% Enhanced		
Capital	212	203	199	194		
Fixed	80	80	80	80		
Variable	32	32	32	32		
Electricity	345	315	297	282		
Catalyst	0	14*	14*	14*		
Subtotal	669	644	622	602		
CO2 T&S	14	14	14	14		
H2 Sales Value (\$6/kg)	-402	-367	-347	-329		
Total	281	291	289	287		

*expected cost of the catalyst can range from \$0.30 to \$14 per tonne CO2

(b)		Catalyst Enhancement Scenario				
		Base Case	se Case 11% Enhanced 21%		30% Enhanced	
Solvent Molar Concer	trations					
КОН	mol/L	0.11	1.77E-03	7.96E-04	4.88E-04	
K2CO3	mol/L	1.44	1.41	1.32	1.23	
КНСОЗ	mol/L	4.24E-03	0.17	0.35	0.54	
CO2(aq)	mol/L	1.30E-09	2.17E-06	9.97E-06	2.48E-05	
Product Molar Flow R	ates					
CO2(g)	kg/hr	470	470	470	470	
H2(g)	kg/hr	31	29	27	26	
CO2 Purity into CO2 P	urificatio	n Unit				
CO2(g)	mol %	62	64	65	66	
O2 Balance, Dry Basis	kg/hr	214	195	184	175	
Performance Specific	ations					
ER Power Required	kW	1,717	1,567	1,481	1,404	
Power Reduction	%	-	8.74	13.77	18.27	
H2 Output Reduction	%	-	8.74	13.77	18.27	

- The base case show the cost of carbon capture is \$281 tonne CO_2 .
- Created 3 catalyst enhanced carbon capture scenarios at catalyst cost of \$14 tonne⁻¹.
- DAC cost with catalyst > base case.
 - High cost of making catalyst
 - Reduction in H₂ production
- The use of catalyst reduce the power consumption of solvent regeneration.

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Community Benefits in BP 1

- We have students and interns working on the tasks of (1) catalyst immobilization and (2) classroom teaching materials of decarbonization.
 - Students have learned decarbonation technologies, e.g., point source carbon capture, DAC, and green hydrogen production.
- The teaching materials will be disseminated to the students at UKy college of engineering in the Fall semester 2024.

Activity	Metrics and Data
Recruit student(s), BP1	• 1 student recruited to participate in project
Collaboratewithcommunitystakeholders todevelopeducationalcontent, BP2	• 2 topics to be in the course materials.
Provide access to developed content, including online posting, classroom instruction, and/or outreaches, BP3	 2 topics developed for instructional purposes will be shared on the UK-IDEA website At least 1 presentation from a recruited student

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Work Plan in BP 2 (August 2024 – July 2025)

Task 5 in BP 2

- Step 0: polish P&ID and 3-D CAD design
 - Finalizing mass chart and equipment selection.
- Step 1: procurement, balance of plant, fabrication
 - CO₂ absorber and solvent regenerator
- Step 2: process monitoring and control
 - Sensors (pH, conductivity, etc), datalogger, etc
 - HAZOP study
- Step 3: startup and commissioning
 - Testing unit at UK-IDEA
- Step 4: integration with solar power

Lessons Learned

Carbon Capture

• The duration of droplet suspension time is a critical factor in achieving efficient CO_2 capture.

Solvent Regeneration

• The membrane seal, which prevents mixing between the catholyte and anolyte, is vital in the solvent regeneration process as it enables CO_2 recovery through pH swings.

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Summary

- We have developed 2 catalytic materials, **catalytic 3-D demister** and **stable catalytic electrode**, to reduce the energy consumption for solvent regeneration.
- Preliminary TEA indicates that the expense of capturing 1 ton of CO₂ may fall **below \$300** when factoring in proceeds from H₂ sales (@ \$6/kg) and catalyst cost.

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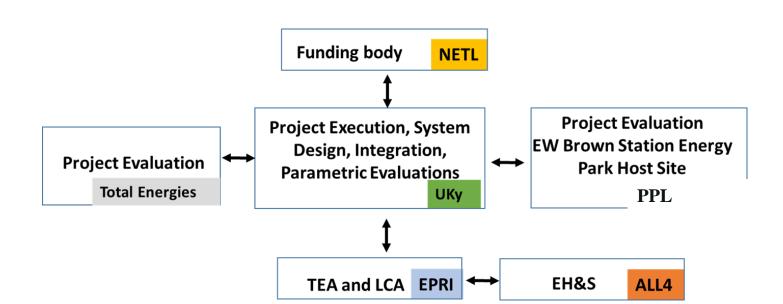
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Acknowledgements

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- UK-IDEA: Jinwen Wang, Pom Kharel, Su Shi, Steve Summers, Matt Button, Priyabrata Biswal, Siza Chaudhary, Lisa Richburg, Moushumi Sarma; **Student and Intern**: Emily Liu, Jenna Roseman, Maya Rao, Jesse Okorafor, Emmanuel Ohiomuba, Siza Chaudhary, Patrick Adoba

Project Team and Division of Responsibility



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	PLAN	PLAN	
TASK DESCRIPTION	START	END	
1 Project Management and Planning	8/1/2023	7/31/2026	
1.1 1A. Update Project Management Plan	8/1/2023	8/31/2023	
1.1 1B. Kickoff Meeting	8/1/2023	10/31/2023	
1.2 2A. Initial Technology Maturation Plan	8/1/2023	10/31/2023	
1.2 28. Final Technology Maturation Plan	1/1/2025	4/2/2026	
BP1 BP1: Design and Development	8/1/2023	7/31/2024	
2 DAC Hybrid Absorber Development			
	8/1/2023	3/31/2024	
2.1 CA Mimics Development	8/1/2023	10/31/2023	
2.2 Catalyst Immobilization	11/1/2023	3/31/2024	
2.3 Hybrid Absorber Design	1/1/2024	3/31/2024	
2.4 Fabrication and Testing of Absorber Components	3/1/2024	7/30/2024	
3 Electrochemical Regenerator R&D	8/1/2023	5/1/2024	
3.1 Commercial Electrode Selection	8/1/2023	12/31/2023	
3.2 Stability of ERC	12/1/2023	5/1/2024	
4 Recruitment, Initial Analysis and Design Package	8/1/2023	7/31/2024	
4.1 Student Recruiment and Mentoring	8/1/2023	7/31/2024	
4.2 Process Design Package	10/1/2023	3/29/2024	
4.2 Initial Technoeconomic Analysis	8/1/2023	11/29/2023	
4.3 Initial Life Cycle Analysis	8/1/2023	11/29/2023	
BP2 BP2 Scale up, System Integration and Modulation	8/1/2024	7/31/2025	
5.1 Procurement and Balance of Plant	8/1/2024	11/1/2024	
5.2 Process Control and Monitoring and P&ID	10/2/2024	2/2/2025	
5.3 Integration with Solar Energy Park	2/2/2025	5/2/2025	
5.4 Startup and Comissioning	3/3/2025	7/28/2025	
BP3 BP3: Parametric, Long-Term, and Technology Analyses	8/1/2025	7/31/2026	
6.1 Parametric Testing	8/1/2025	2/1/2026	
6.2 Long Term Testing and Analysis	12/1/2025	7/31/2026	
7.1 Final Technoeconomic Analysis	11/3/2025	5/2/2026	
8.1 Life Cycle Analysis	11/3/2025	5/2/2026	
9.1 EH&S Assessment	11/3/2025	5/2/2026	
10.1 Technology Gap Analysis	11/3/2025	5/2/2026	