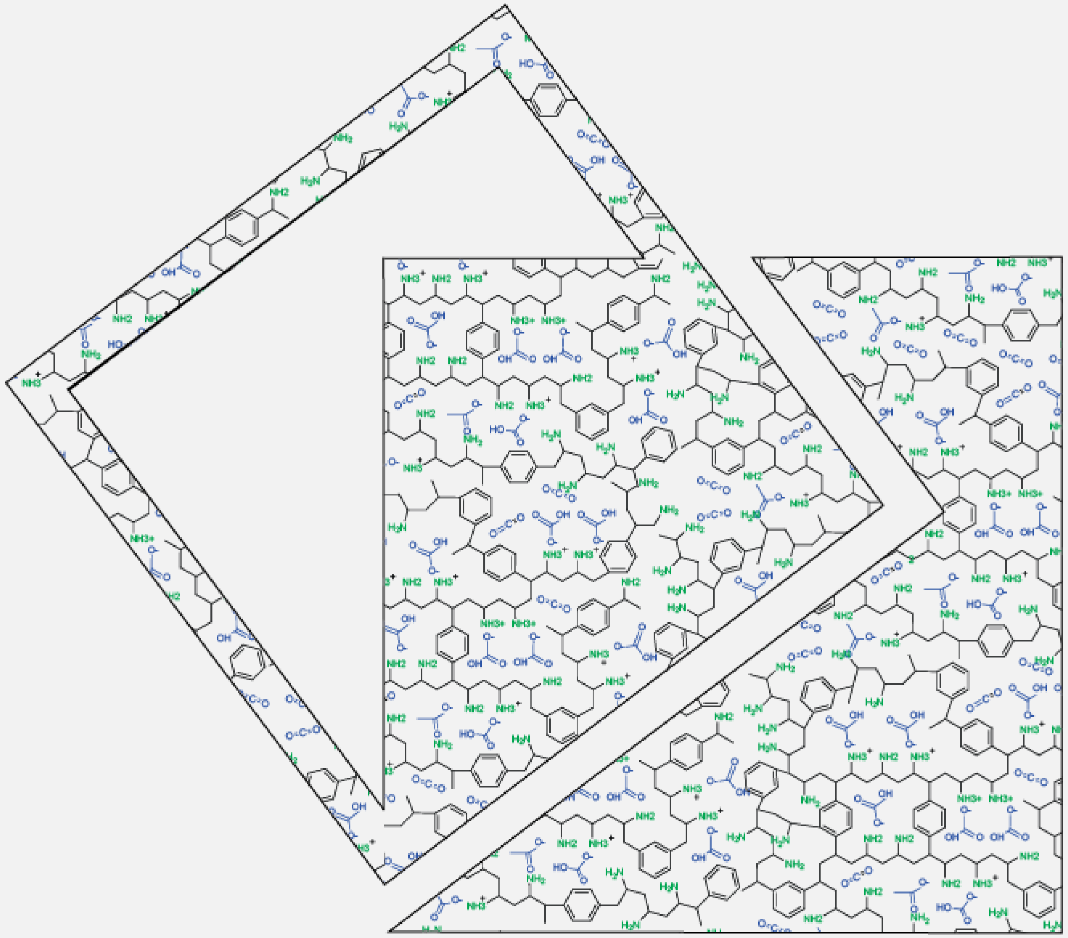
Aerogel Adsorbent Polymers for Direct Air Capture of CO_2



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Project Overview

Award Number: DE-FE0032251

Principal Investigator: Jonathan Bachman, Ph.D.

Project Period: 10/1/2023–9/30/2026

Funding: $2,999,642 Federal, $749,907 Cost Share

Key Participants: SRI International

Project Objectives:

- Optimize the structured adsorbent, contactor, and DAC system operation for improved volumetric productivity, pressure drop, and capacity fade towards the general target DAC cost of < $100/ton CO_2e.
- Identify a low-cost, scalable manufacturing method for structured adsorbent production.
- Develop a laboratory-scale DAC system with a continuous production rate of > 1 kg CO_2/day at a purity of > 90% CO_2, demonstrating < 0.005% / cycle capacity fade over 1,000 h of operation.

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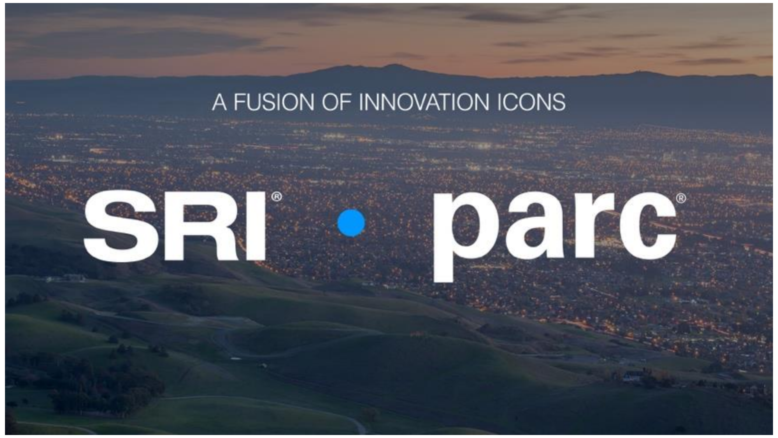
Project History

Project Location: Palo Alto, CA at the PARC campus of SRI International.

Project History: follows-up on previous work accomplished in DE-FE0031951 (Tunable, Rapid-Uptake Aminopolymers for Direct Air Capture of CO_2) and builds on a history of research on polymer resins at PARC, dating back to development of printer inks with Xerox.

Impact on DOE goals: Sorbent performance effects every aspect of the technoeconomics of direct air capture and next-generation materials are needed to achieve DOEs' $100/ton CO_2e goal.



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Project Scope

High Level Execution Plan:

- Conduct structured adsorbent testing, contactor fabrication, and system design.
- Commission bench-scale DAC system and conduct preliminary cycle testing.
- Optimize and conduct long-term cycling on bench-scale DAC system.

Key Milestones/Success Criteria:

- Develop a structured adsorbent with > 1.35 mmol CO_2/g equilibrium capacity and > 0.087 mmol $CO_2/g_{sorbent}$/min adsorption rate.
- Construct a 1 kg CO_2/day bench-scale DAC system that continuously produces CO_2 from air with > 90% purity.
- Demonstrate > 1,000 h of continuous cyclic operation with < 0.005%/cycle capacity fade.

High Probability Risk & Mitigations:

- Risk: Poor liquid water stability causes pore collapse, reducing sorbent performance.
- Mitigation: Instead of using direct steam for regeneration, use a 2-fluid contactor design with indirect heating.

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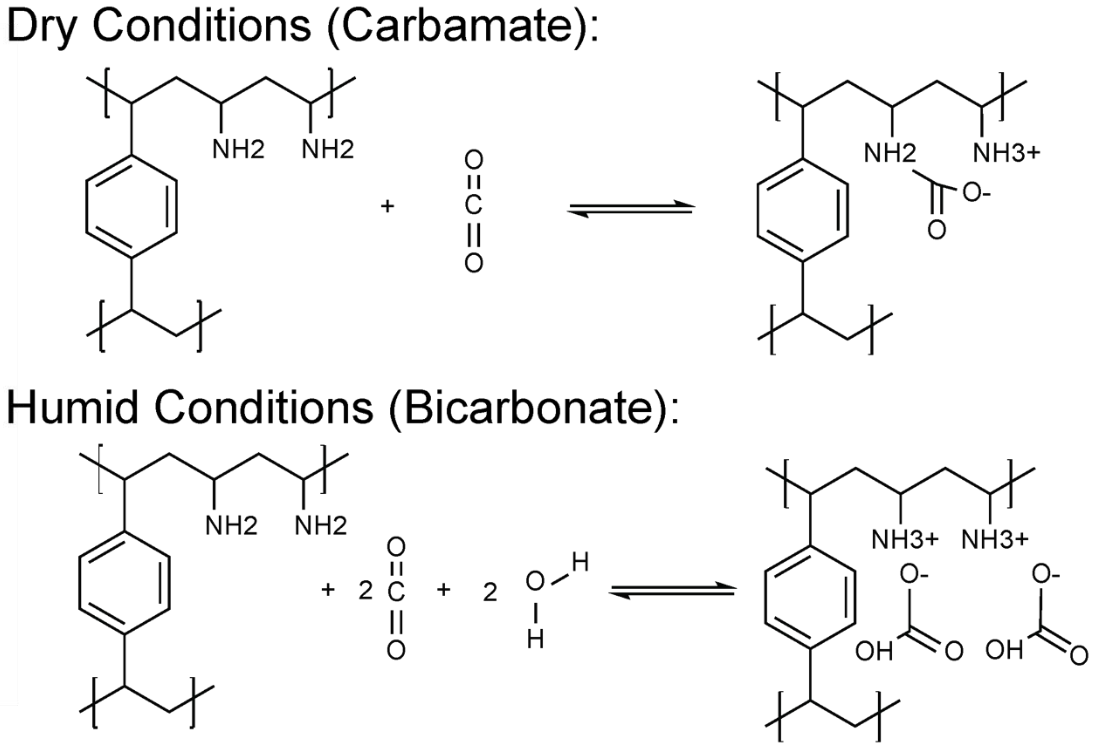
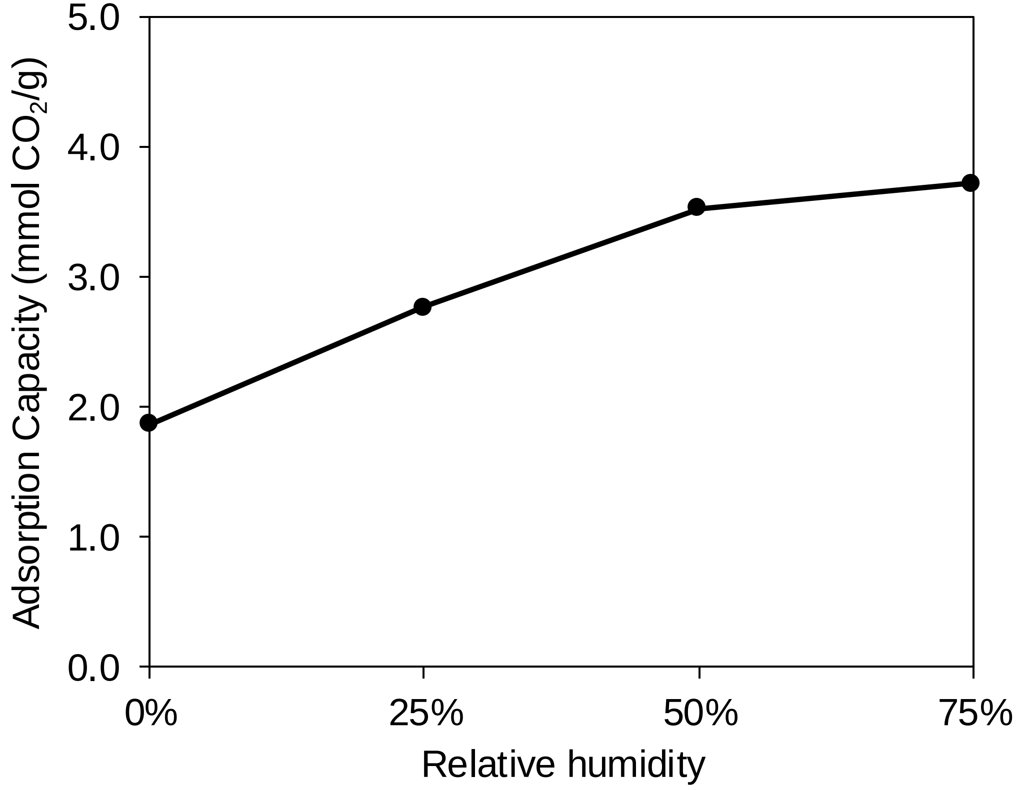
Background: Amine Polymer Resin Adsorbent

Adsorption Mechanism



CO_2 Adsorption Capacity



- Low MW (43.07 g/mol) vinylamine segments provide a high density of amine sites and DVB provides mesoporosity in the polymer resin.
- Amine efficiency increases from 1:2 to 1:1 CO_2:amine in the presence of water.

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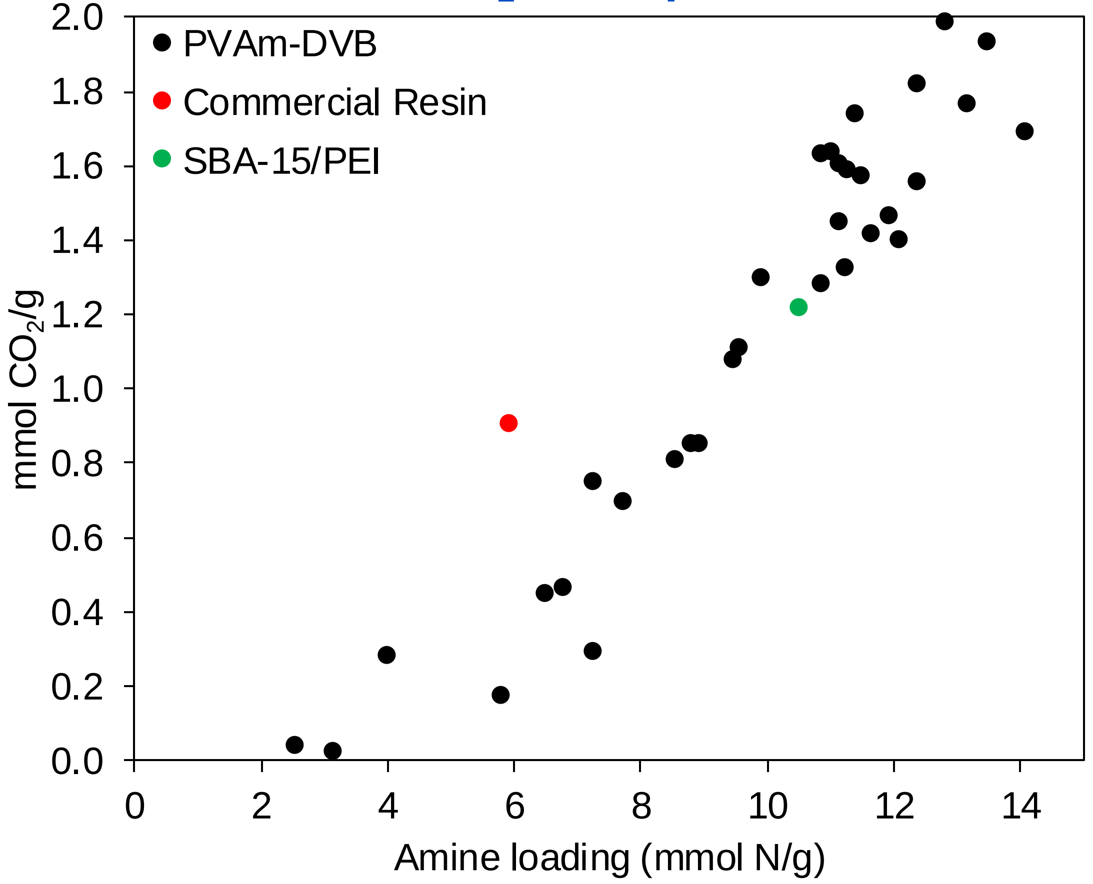
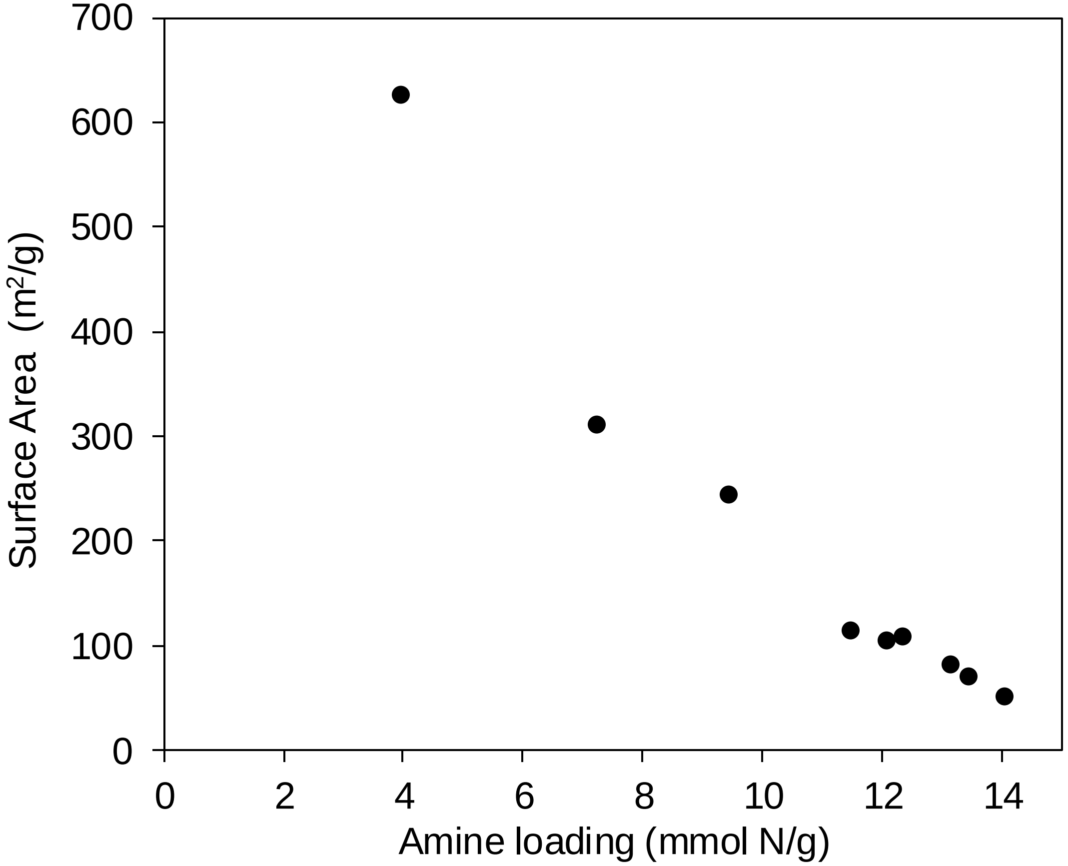
Background: Structure-Property Relationships

CO_2 Adsorption:



Surface Area:



- Increasing amine content increases CO_2 adsorption and amine efficiency
- Inverse correlation between CO_2 adsorption and surface area (but nonporous samples have no CO_2 adsorption)

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Project Milestones for Budget Period 1

Task/ Subtask	Milestone Title & Description	Status
2	**M2**: Outreach opportunity pursued.	Complete
3	**D3**: Submit initial technoeconomic analysis.	Complete
4	**D4**: Submit initial life cycle analysis.	Complete
5.1	**M5.1.1**: Structured adsorbent thickness control demonstrated.	Complete
5.1	**M5.1.2**: Accelerated oxidative aging testing completed.	Complete
5.1	**M5.1.3**: Liquid water stability determined.	Complete
5.2	**M5.2.1**: Target equilibrium capacity achieved for the structured adsorbent.	Complete
5.2	**M5.2.2**: Target adsorption rate achieved for the structured adsorbent.	Complete
5.2	**M5.2.3**: Baseline pressure drop determined.	Complete
5.2	**M5.2.4**: Baseline volumetric productivity determined.	Complete
5.3	**M5.3**: Initial design of DAC system completed.	Complete

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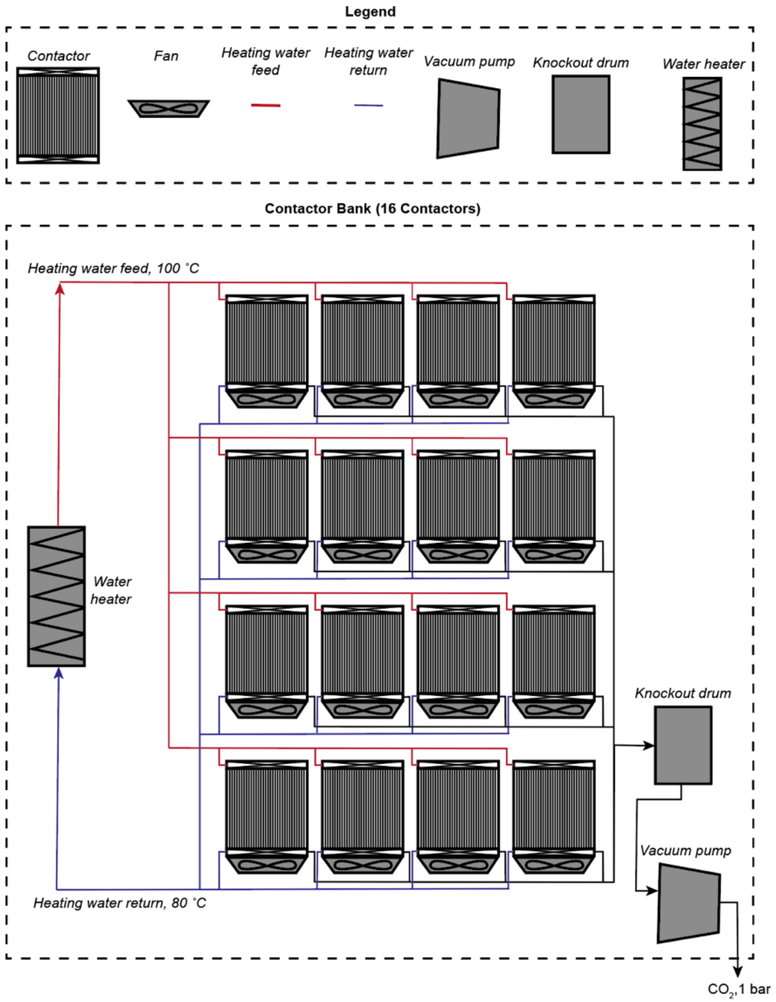
Initial Technoeconomic Analysis

D3: Submit initial technoeconomic analysis.



- The initial TEA resulted in an estimated total cost of capture of **\$162/t CO_2e**, with an annual operating cost of \$145,490,000 and a fixed capital investment requirement of \$403,200,000.

Summary of Cost Breakout

Cost category	Contribution to capture cost	Percentage of capture cost
Capital expenditure	\$45/t CO_2e	28%
Direct sorbent cost	\$7/t CO_2e	4%
Other OPEX	\$45/t CO_2e	28%
Utilities cost	\$65/t CO_2e	40%

Summary of Energy Breakout

Energy category	Energy requirement	Percentage of energy
Blower fan	0.49 GJ/t CO_2e	6%
Vacuum pump	0.63 GJ/t CO_2e	8%
Heating	7.04 GJ/t CO_2e	86%

DAC Facility Lifetime Performance

Performance category	Performance value
Nominal plant lifetime capture	20,000,000 ton CO_2
Energy-based emissions generated	2,080,800 ton CO_2
Net CO_2 captured	17,919,000 ton CO_2e

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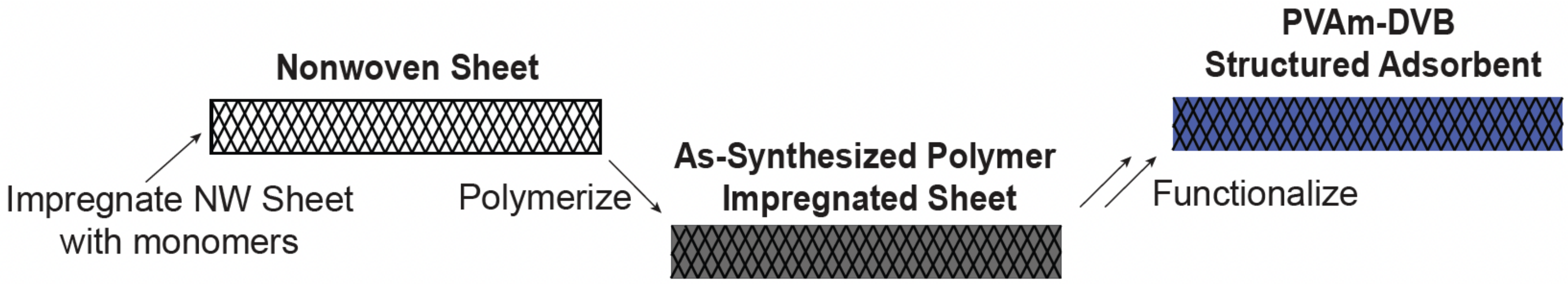
Adsorbent Structuring Approaches

M5.1.1: Structured adsorbent thickness control demonstrated.
Description: Structured adsorbents of ≥ 3 varying thickness (100 micrometers – 600 micrometers) fabricated.

In-situ polymerization for free-standing structured adsorbents:



- Manufacturing techniques from ion exchange membrane production are applied due to similarities in polymer chemistry.
- Free-standing structured sheets are produced in the first step of manufacturing.
- Thickness of the structured adsorbent can be controlled by changing the thickness and areal density of the nonwoven substrate.
- Substrates with weights of 20, 25, 30, and 40 g/m^2 were used to produce structured adsorbents with thicknesses of 165(7), 235(10), 286(26), and 447(43) µm, respectively.

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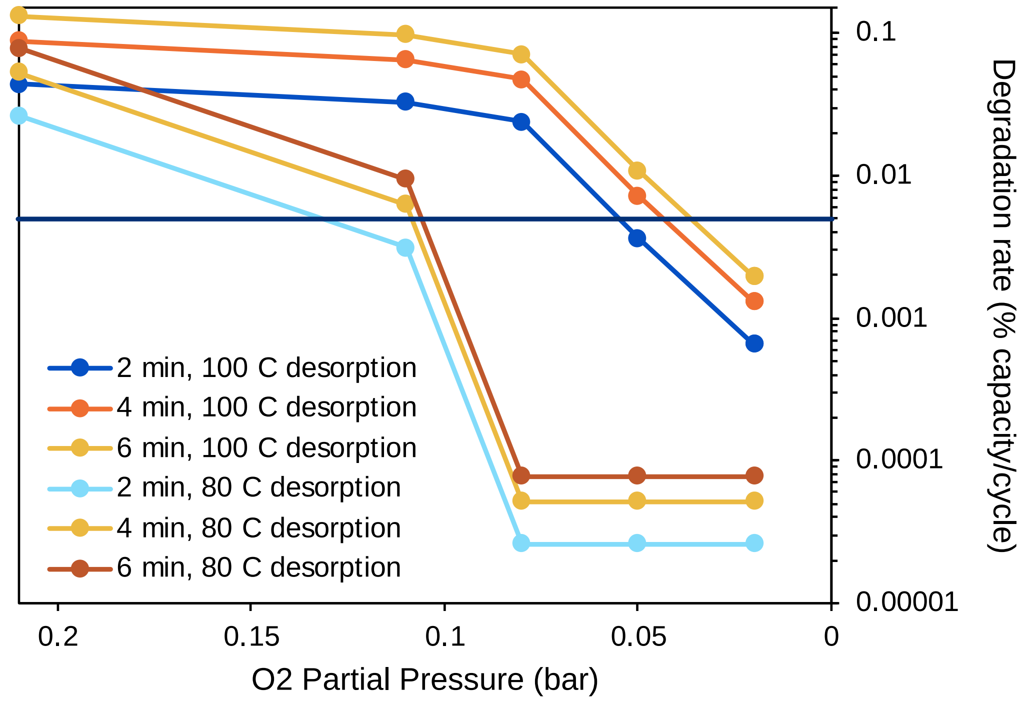
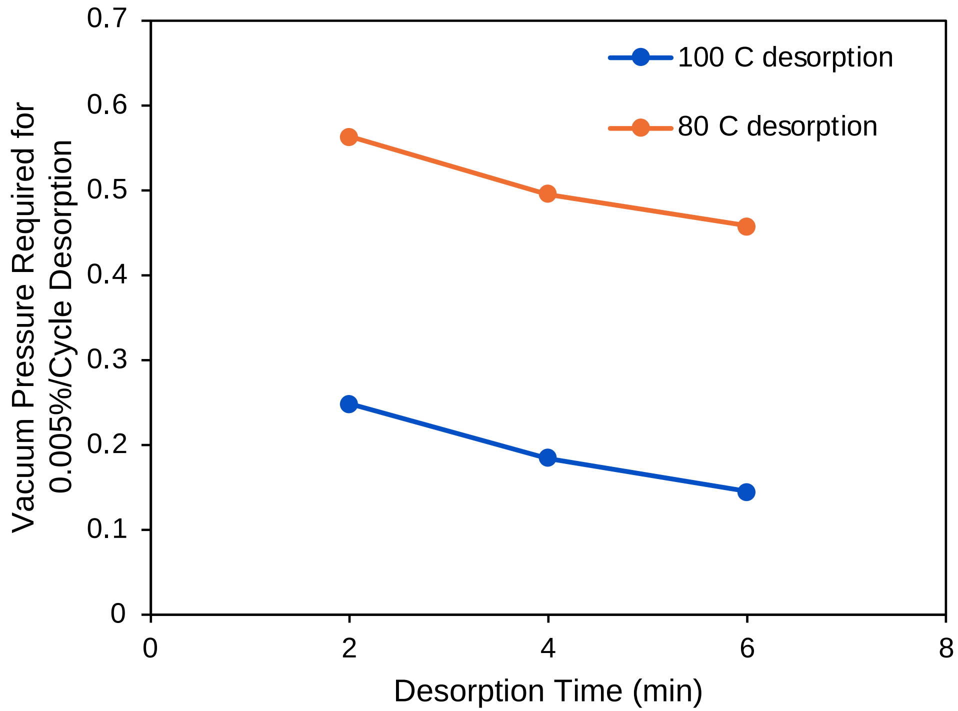
Oxidative Degradation

M5.1.2: Accelerated oxidative aging testing completed.
Description: Oxidative stability evaluated by thermogravimetric analysis (TGA). Degradation rate (% capacity/min) measured vs. oxygen concentration (0% – 21% O_2) and oxidation temperature (80 – 100 ˚C). Identify a vacuum pressure and temperature that would result in an oxidative degradation rate of < 0.005% / cycle.





- At 100 ˚C regeneration, depending on desorption time, a total vacuum pressure of 0.15-0.25 bar would result in a degradation rate of < 0.005 %/min.

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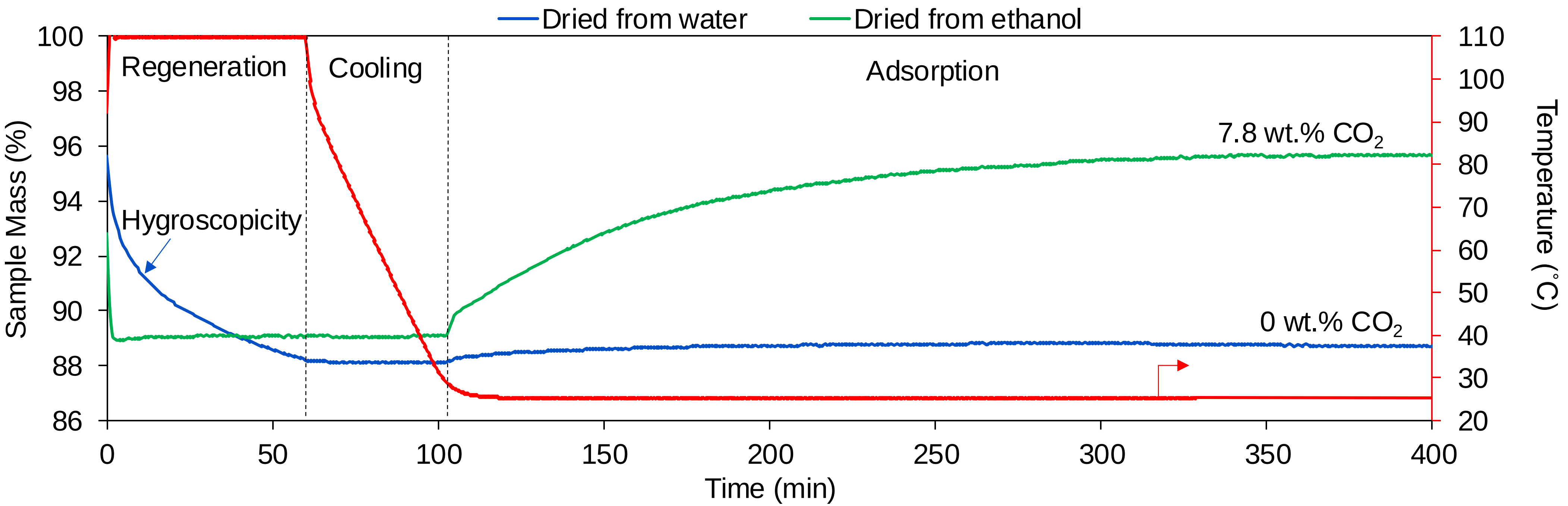
Liquid Water Stability

M5.1.3: Liquid water stability determined.
Description: Equilibrium CO_2 adsorption capacity measured before and after water exposure. ≥ 3 water-to-sorbent ratios and ≥ 3 exposure times tested. Based on the results, an S-TVSD or VTSA DAC process chosen.



- Drying from liquid water causes pore collapse, creating domains within the polymer that trap liquid water; bulk density dramatically increases.
- Indirect heating (i.e., a VTSA) process is required to maintain sorbent functionality.

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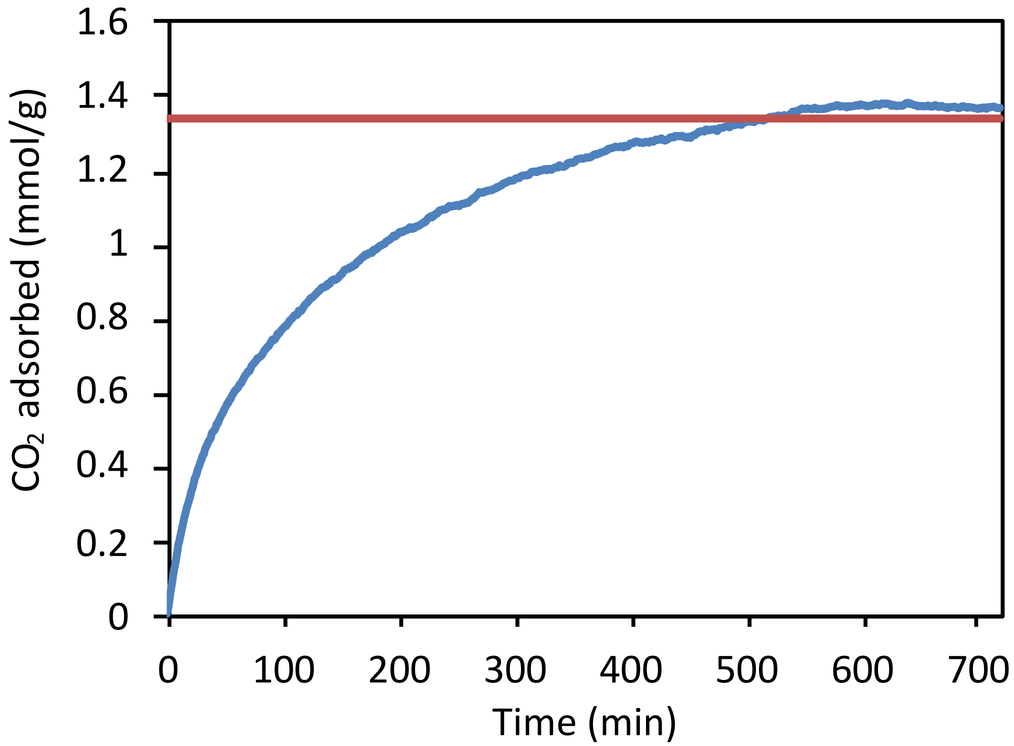
Optimizing Structured Adsorbent Synthesis

M5.2.1: Target equilibrium capacity achieved for the structured adsorbent.
Description: Equilibrium adsorption capacity of 1.35-2.7 mmol CO_2/g achieved under 0-75% RH under ambient air conditions measured on the structured adsorbent.

- Equilibrium capacity of 1.36 mmol $CO_2/g_{sorbent}$ under 0% relative humidity, and 25 ˚C, and 420 ppm CO_2 was achieved.

- Increasing both functional monomer content and solvent content during polymerization results in structured adsorbents with high equilibrium capacity.

- The structured adsorbent comprised 80 wt.% of active material – the normalized equilibrium capacity is 1.7 mmol $CO_2/g_{sorbent}$.



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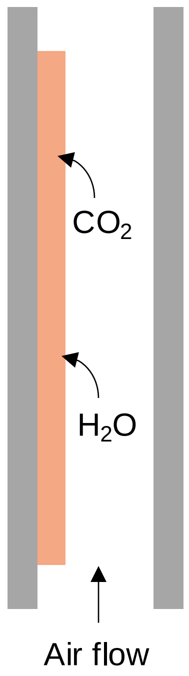
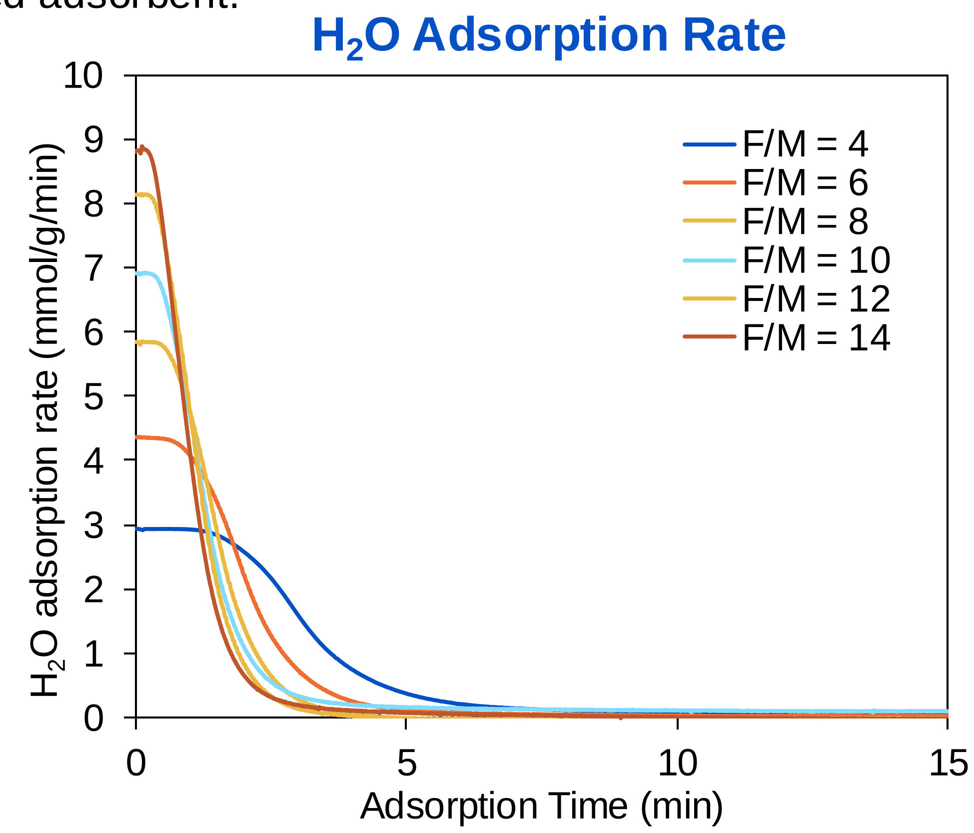
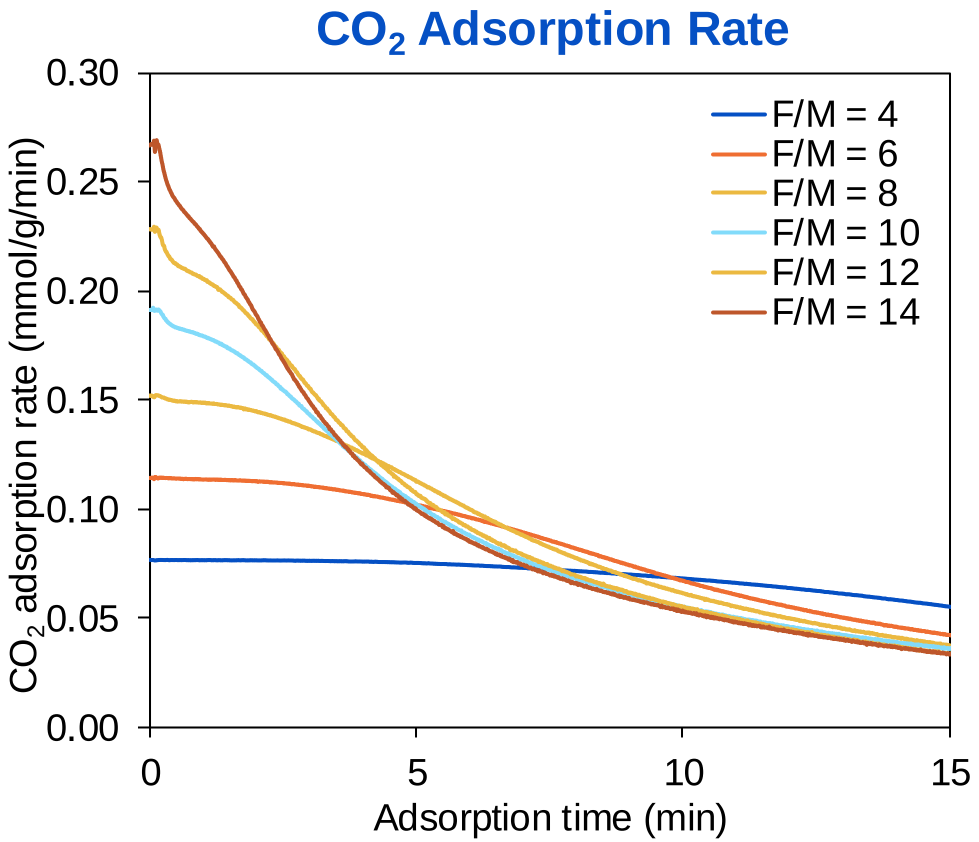
Adsorption Kinetics

M5.2.2: Target adsorption rate achieved for the structured adsorbent.

Description: Adsorption rate of > 0.087 mmol CO_2/g/min under 0% RH and ambient air conditions measured via breakthrough testing on the structured adsorbent.







- Adsorption is studied at variable air flow rates; flow-limited transport indicates that internal diffusion is not limiting.
- Initial CO_2 and H_2O adsorption rates as high as 0.26 and 9.0 mmol/g/min, correspond to the species feed rates.

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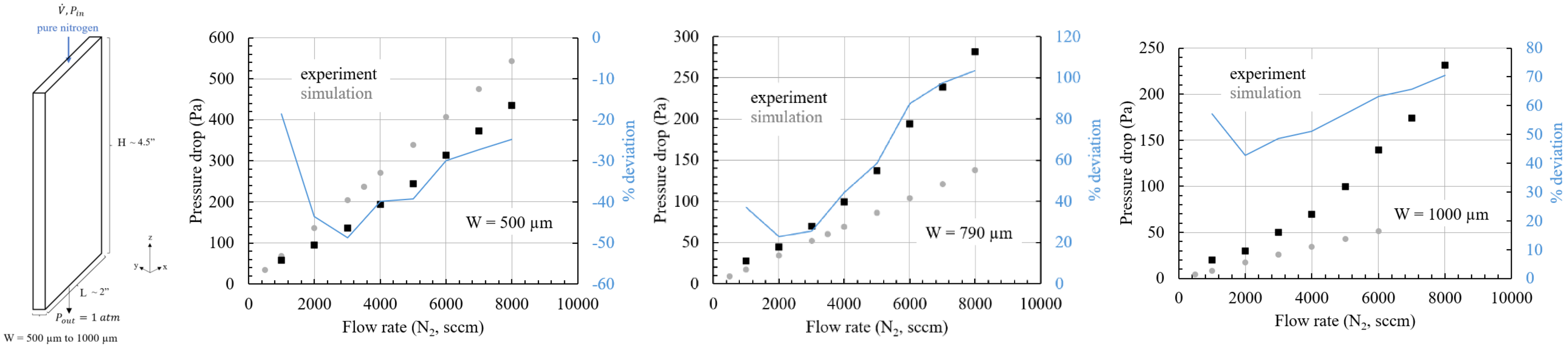
Pressure Drop

M5.2.3: Baseline pressure drop determined.

Description: Pressure drop as a function of air flow channel dimension and air flow rate determined by computational fluid dynamics. Pressure drop measured and compared with simulated values for ≥ 1 air flow channel dimension and ≥ 3 flow rates. Baseline air flow channel dimension and air flow rate established.

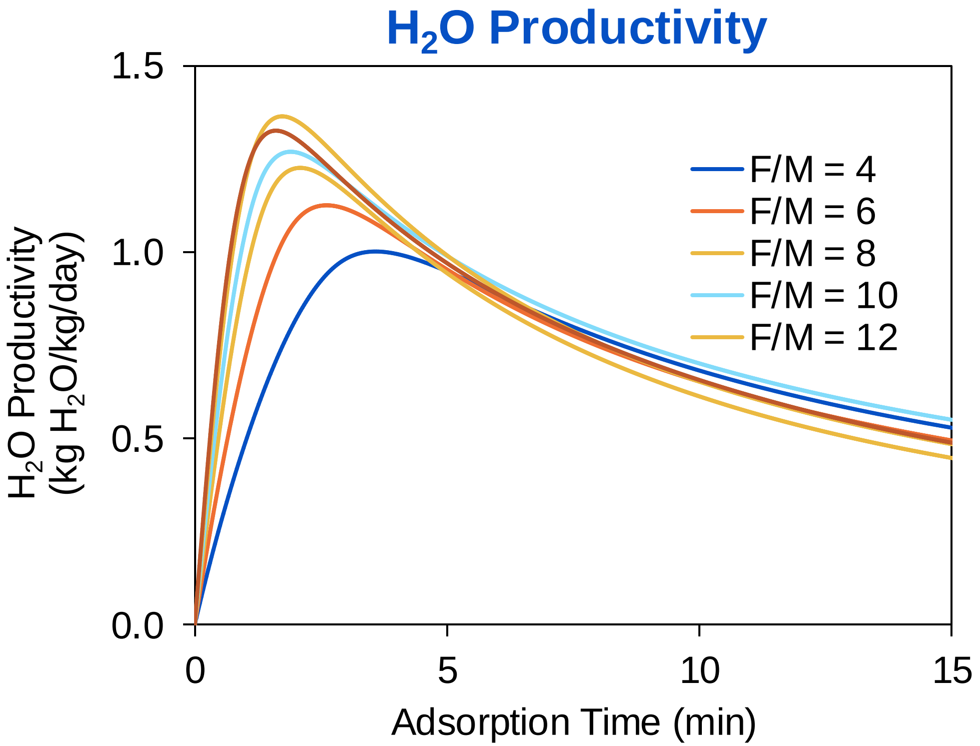


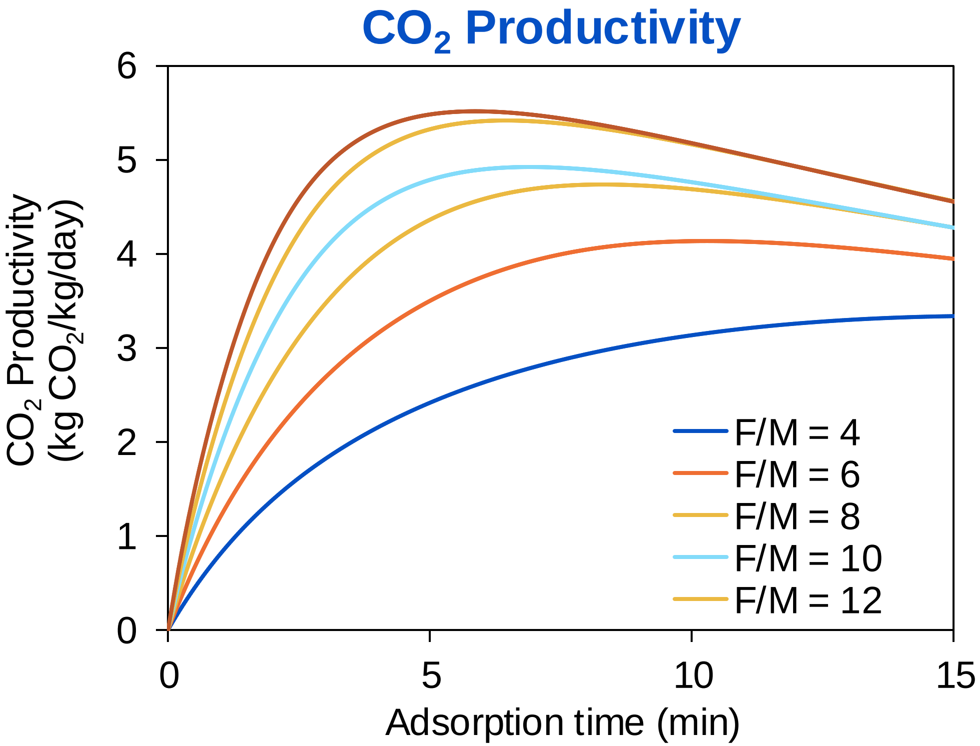
- Pressure drop measurements were conducted for 3 flow channel dimensions (0.5, 0.79, and 1.0 mm) at a range of flow rates between 500 and 8,000 sccm.
- Results indicate that a baseline pressure drop of < 400 Pa is achieved.

Volumetric Productivity

M5.2.4: Baseline volumetric productivity determined.

Description: The measured adsorption rate from M5.1.2, baseline air flow channel dimension from M5.2.3, and measured structured adsorbent density used to determine a baseline volumetric productivity. Cycle time determined based on optimized adsorption time and predicted desorption time.





- A baseline volumetric productivity of 0.71 ton CO_2/m^3/day was established, based on contactor geometry and sorbent properties.

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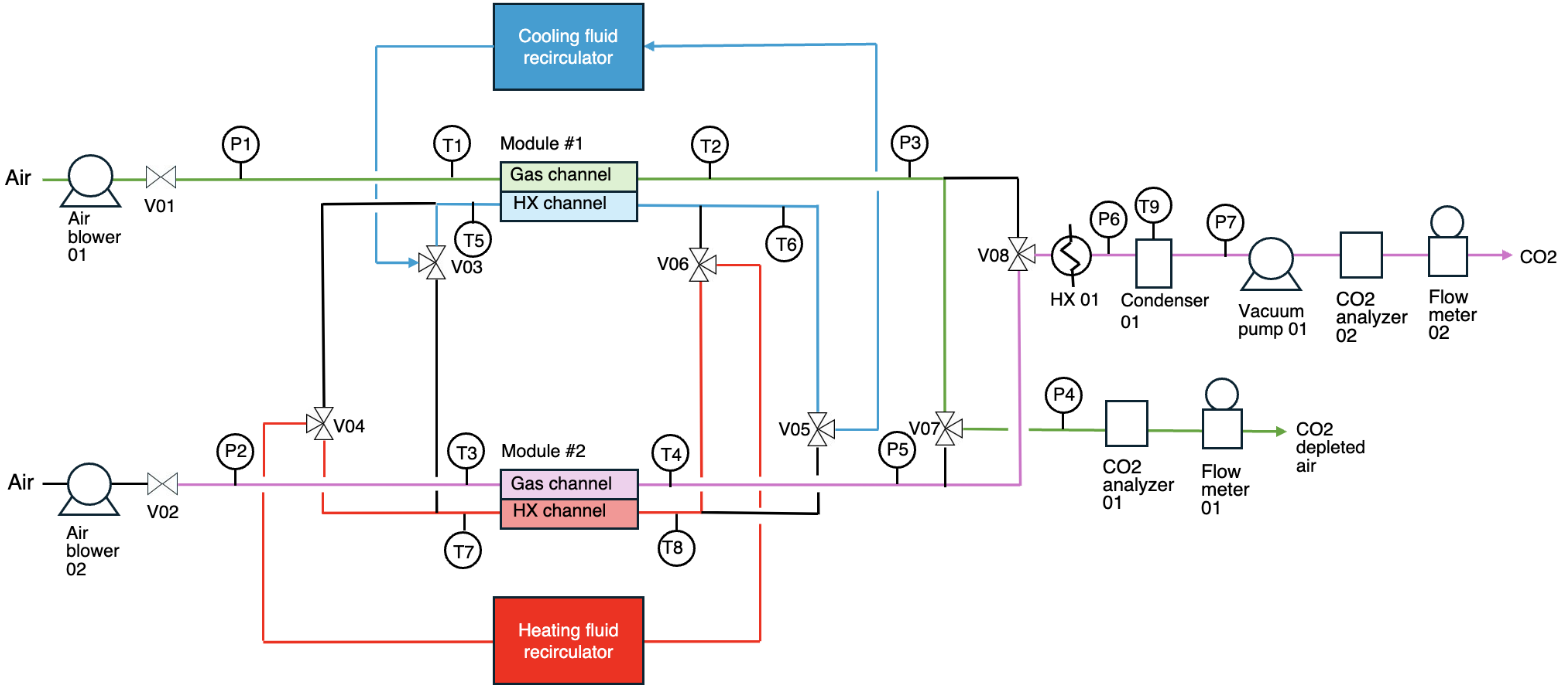
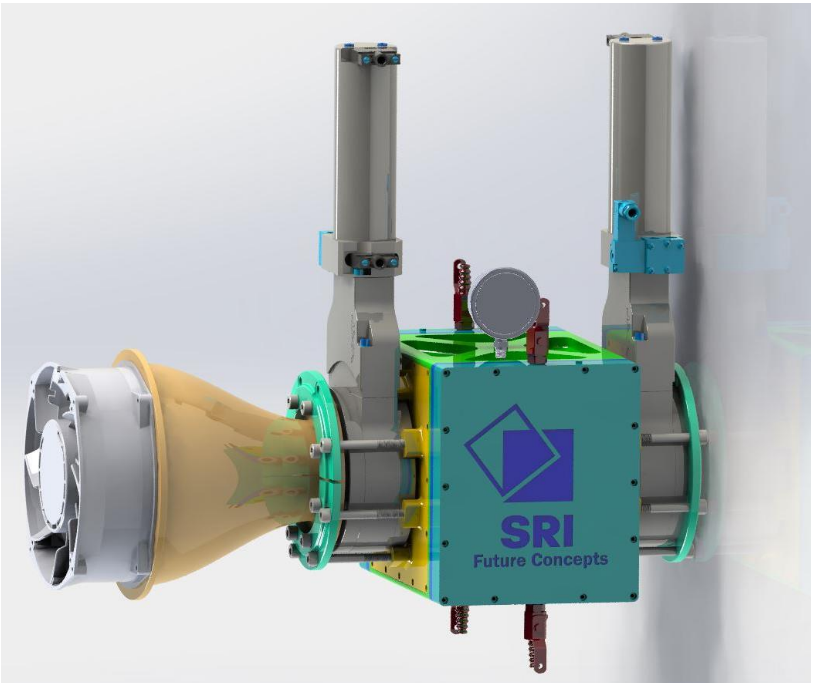
Bench-scale DAC System Design

M5.3: Initial design of DAC system completed.
Description: Initial design of the DAC system to produce > 1 kg CO_2/day at > 90% purity established. Process flow diagram and initial unit operation specifications established. Initial P&ID established along with overview of process controls to be implemented.

Initial P&ID of Bench-Scale System



Bench-Scale Air Contactor



- Vacuum-temperature swing adsorption (VTSA) system using indirect heating via cycling hot and cold water.

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Community Benefits Plan

M2: Outreach opportunity pursued.
Description: At least one outreach opportunities pursued (e.g., giving a seminar at a local community college, attending/hosting recruitment events at a minority serving institution, etc.).

- Outreach opportunities will be pursued (e.g., giving a seminar at a local community college, attending/hosting recruitment events at a minority serving institution, etc.) at least once per year.
- In May, the Student Chapter of the American Institute of Chemical Engineers at San Jose State University invited me to give a seminar.
- The focus of the event was on opportunities for ChemE's in clean energy careers, with a focus on carbon dioxide removal.
- Feedback was positive with students being surprisingly engaged in the research aspects – many were conducting undergraduate research on related fields.
- In the 2024-2025 school year, I hope to further engage with undergraduates at SJSU about opportunities in clean energy and CDR.

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Learnings & Next Steps

- Structured adsorbent synthesis for contactor assembly
- Single contactor optimization
- Large-scale structured adsorbent manufacturing design
- Bench-scale DAC system integration
- Initial cycle testing on bench-scale DAC system

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