

Energy-Efficient Direct Air Capture System for High-Purity CO₂ Separation

DE-FE0032128

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Project Overview

- 1) Funding: DOE share \$1,499,999 and cost share \$393,650
- 2) Overall Project Performance Dates: 10/1/2021 – 10/31/2024
- 3) Project Participants: University of Cincinnati (UC), BASF, Daeyoung, Trimeric
- 4) Overall Project Objectives: demonstrate the Recipient's DAC sorbent technology to capture CO₂ from ambient air and separate it at high purity.

Technology Background

- **Modified amine**-based sorbent technology with resistance to oxidative and thermal degradations
- Sorbents with high capacities, fast kinetics, small heat and mass-transfer resistances, and low desorption energy requirement
- Increased selectivity toward CO₂ over water vapor
- High throughput of air flow with minimum pressure drop through sorbent-washcoated monolith in air contactor
- Passive air contactor without energy requirement during adsorption

Technical Approach/Project Scope

- **Task 2: CFD and Adsorption Kinetics (UC)**
 - ✓ Air flow model through monolith in passive air contactor
 - ✓ Determine CO₂ adsorption kinetics
- **Task 3: Manufacture CO₂ sorbent (UC)**
 - ✓ Manufacture CO₂ sorbent
 - ✓ Evaluate long-term lab-scale performance
- **Task 4: Manufacture sorbent-washcoated monolith structure (UC, BASF, Daeyoung C&E)**
 - ✓ Develop sorbent-washcoated monolith
 - ✓ Determine cell size and length
- **Task 6: Evaluate performances of sorbent-washcoated monolith in air contactor system (UC)**
 - ✓ Measure temperature, humidity, velocity, and CO₂ concentration
 - ✓ Evaluate performance

Technical Approach/Project Scope

Major milestones

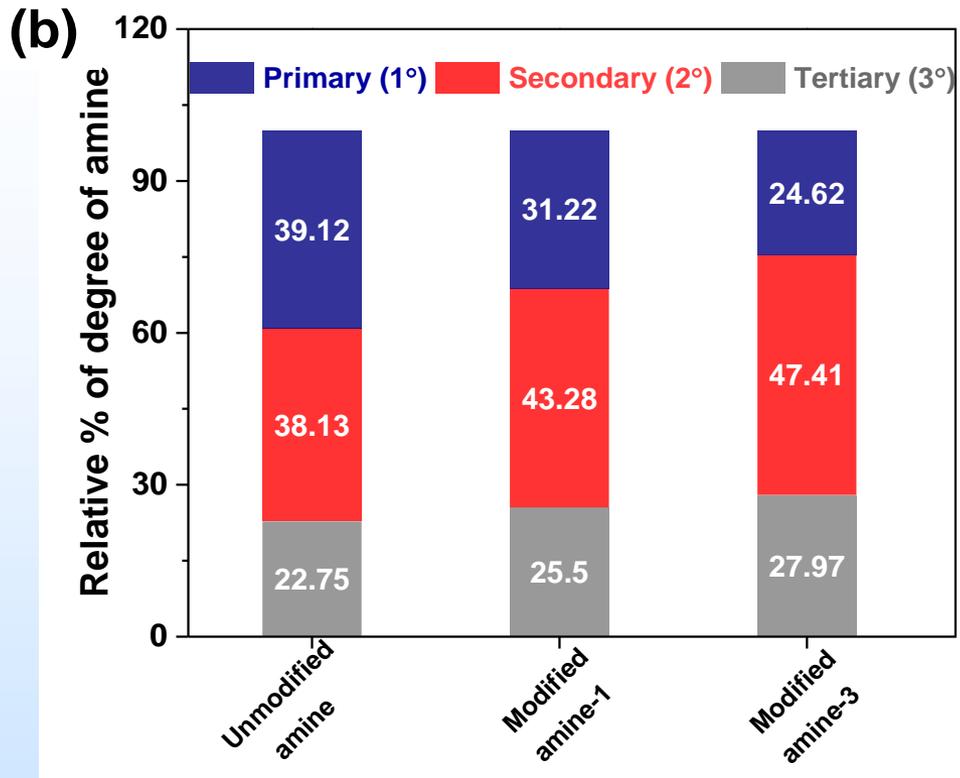
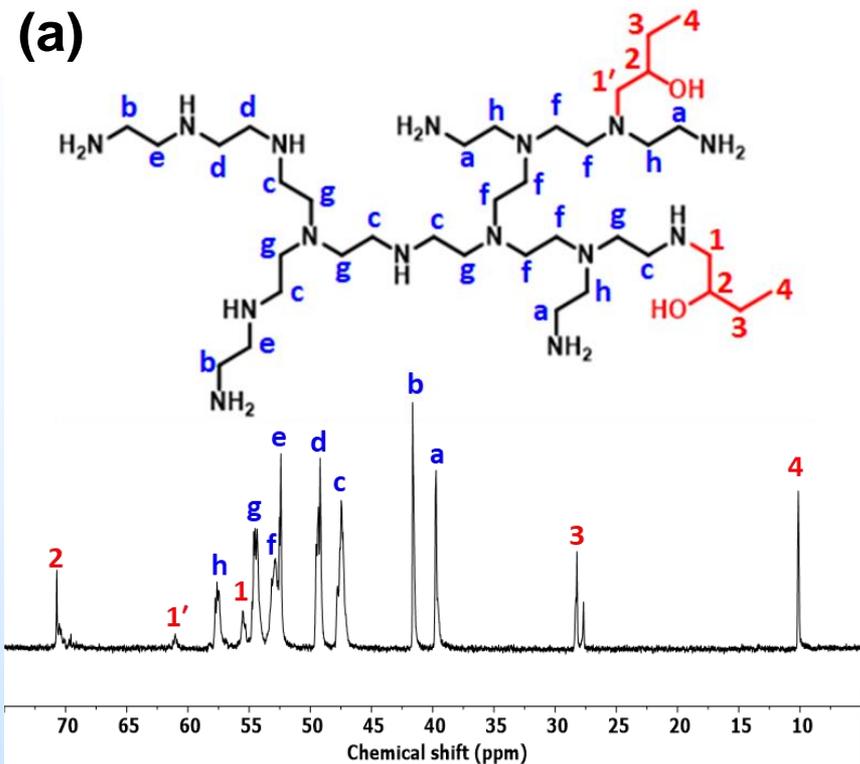
Task	Milestone Title & Description	Planned Completion Date
3	Manufacture of 10 kg of CO ₂ sorbent	PSD+23 months
4	Manufacture of two sorbent-washcoated monolith prototypes	PSD+24 months
6	CO ₂ capture efficiency, energy requirements, and overall volumetric CO ₂ productivity	PSD+39 months

Major Success criteria

- 70% average CO₂ capture efficiency in passive air contactor with monolith with pressure drop of <100 Pa
- Overall volumetric productivity of ~2 (gmol CO₂/(hr x V(l)))

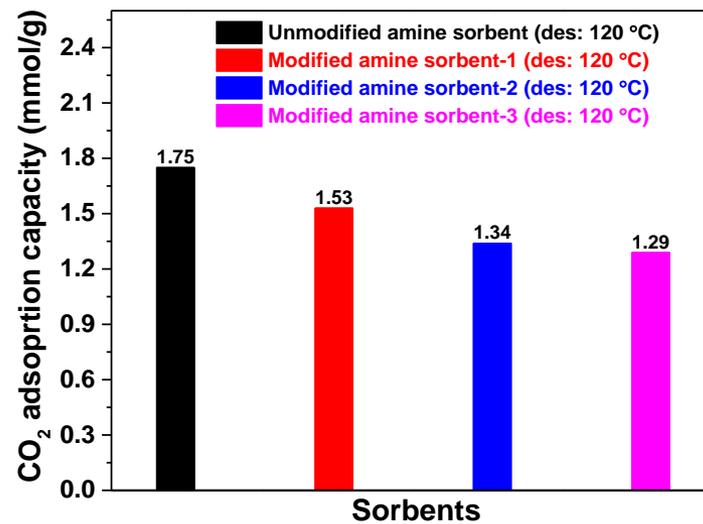
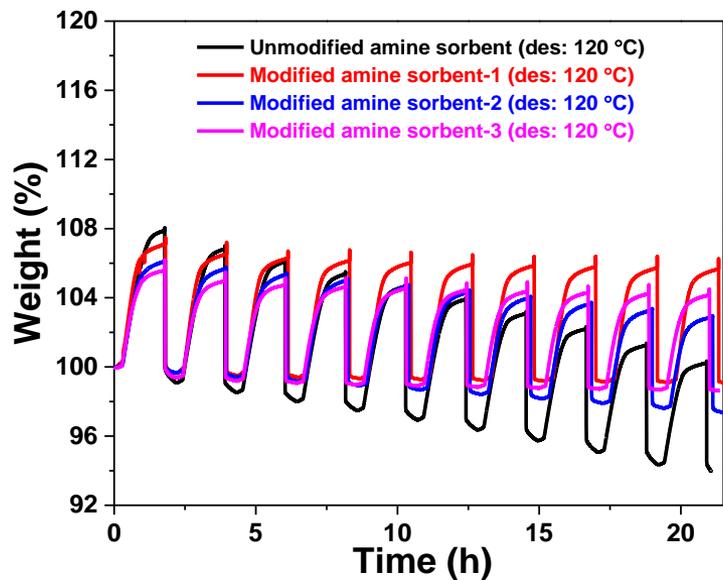
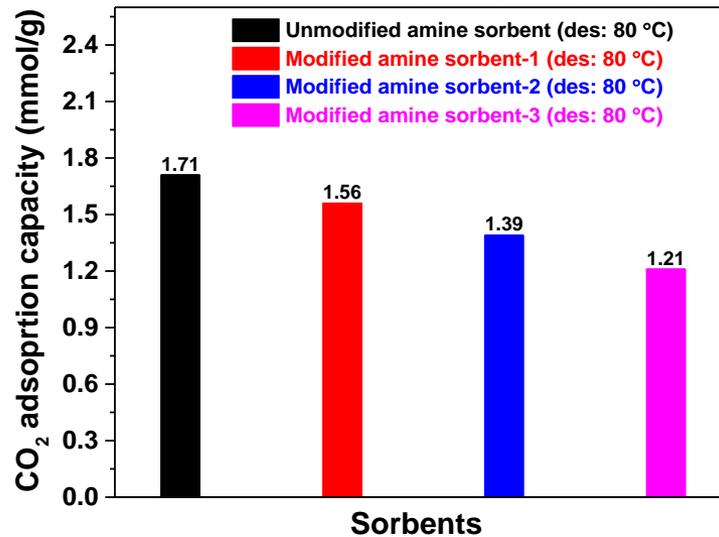
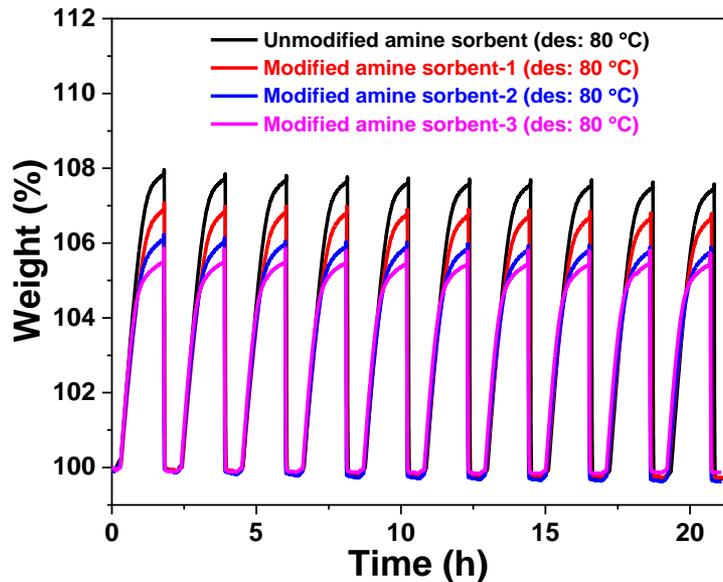
Project Risks and Mitigation Strategies

- Low performance of sorbent-washcoated monolith: BASF and Daeyoung will attempt many different coating formulations
- Low DAC system performance: parametric testing will be carried out to investigate the effects of parameters (i.e., operating conditions, materials, etc.)⁵

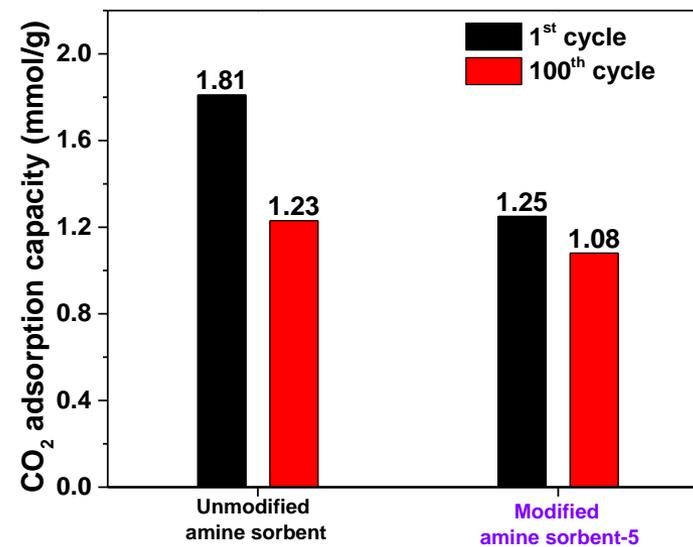
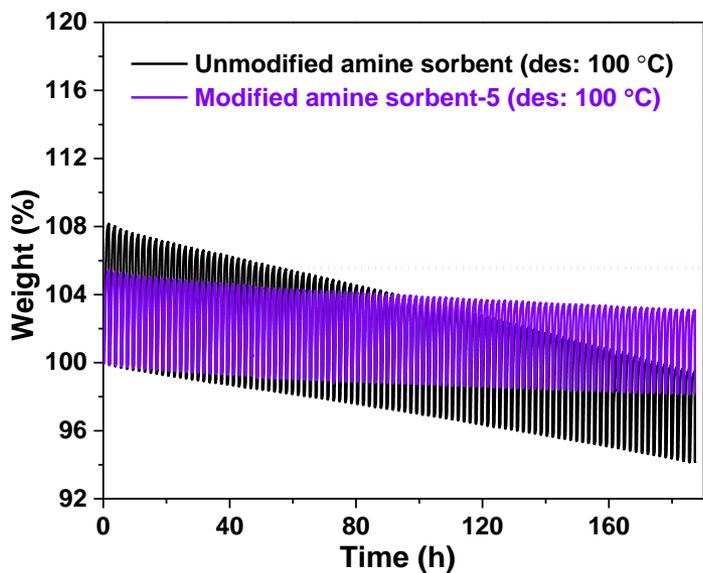
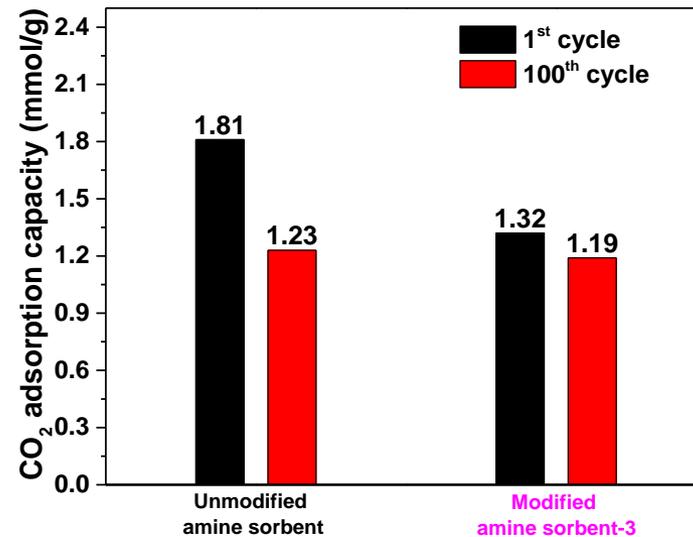
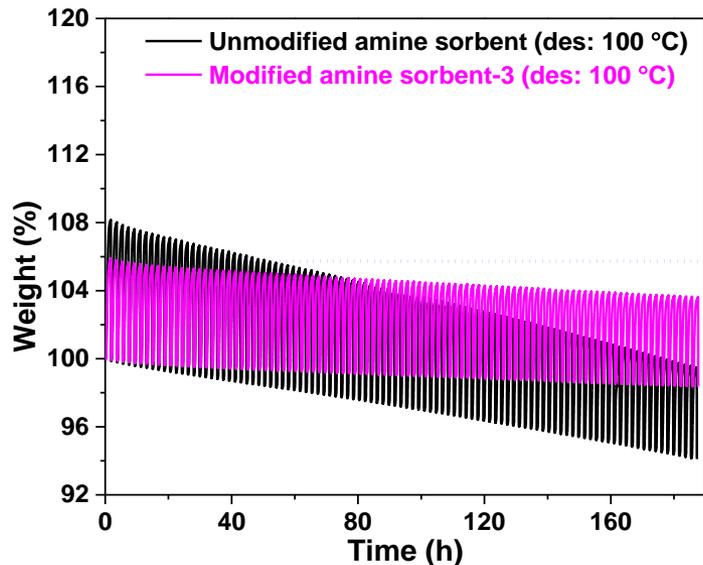


¹³C NMR spectrum for (a) modified amine and (b) distribution of amine states

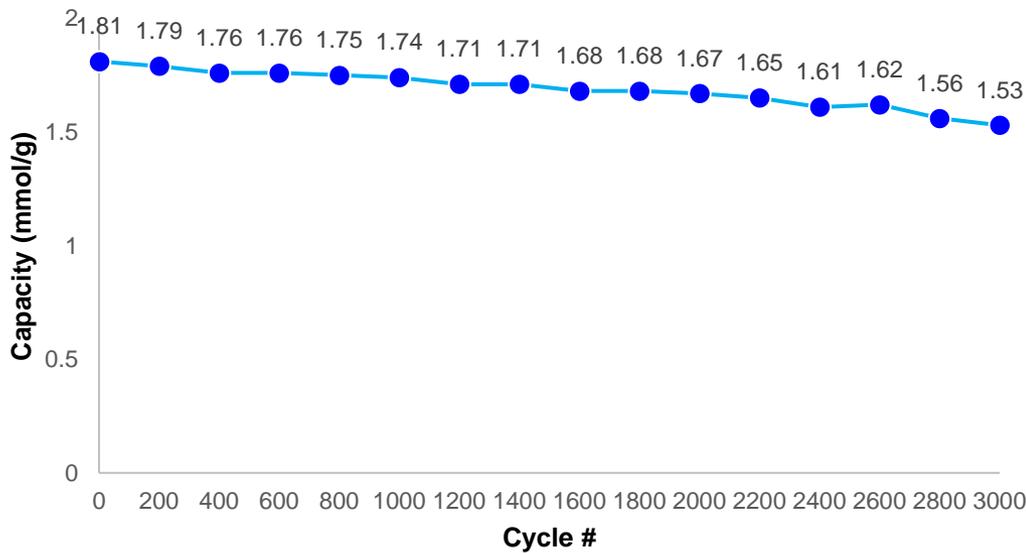
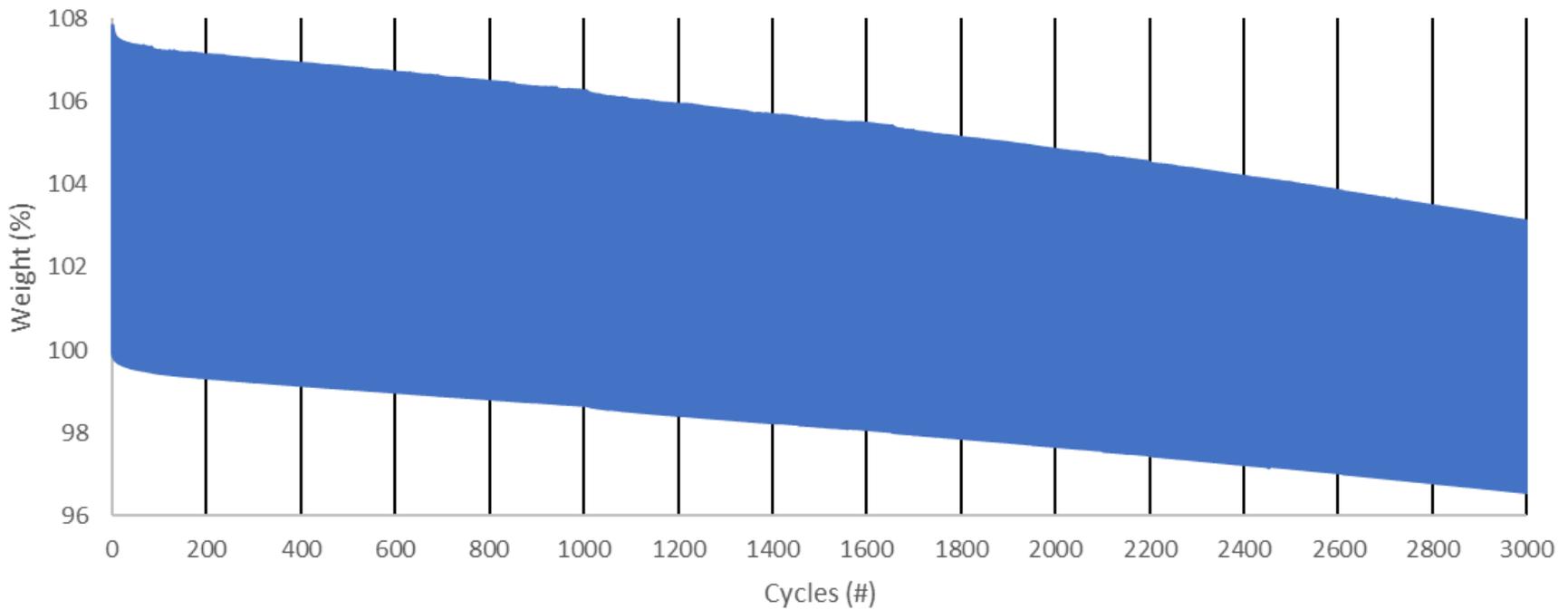
Increase the resistances to thermal and oxidative degradations by lowering the basicity and increasing steric hindrance.



Adsorption: 400 ppm CO₂ in dry air at 30 °C and Desorption: N₂ at 80 & 120 °C



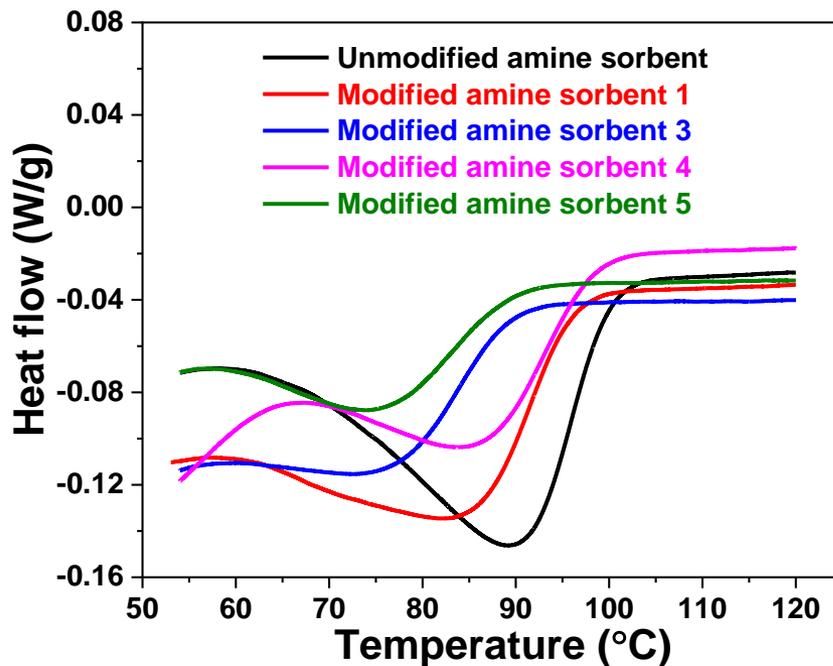
Adsorption: 400 ppm CO₂ in Dry Air at 30 °C and Desorption: N₂ at 100 °C



Adsorption under 400 ppm CO₂ in Dry Air at 30 °C and desorption under N₂ at 90 °C for desorption.

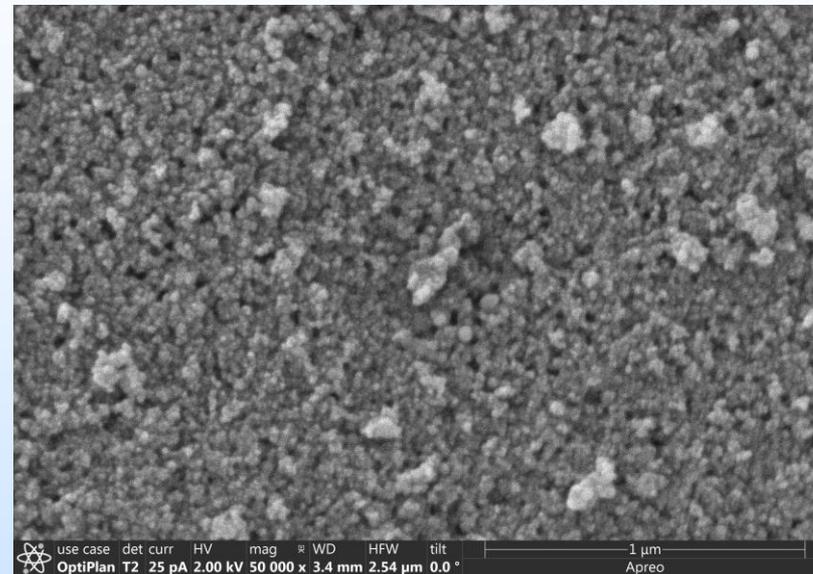
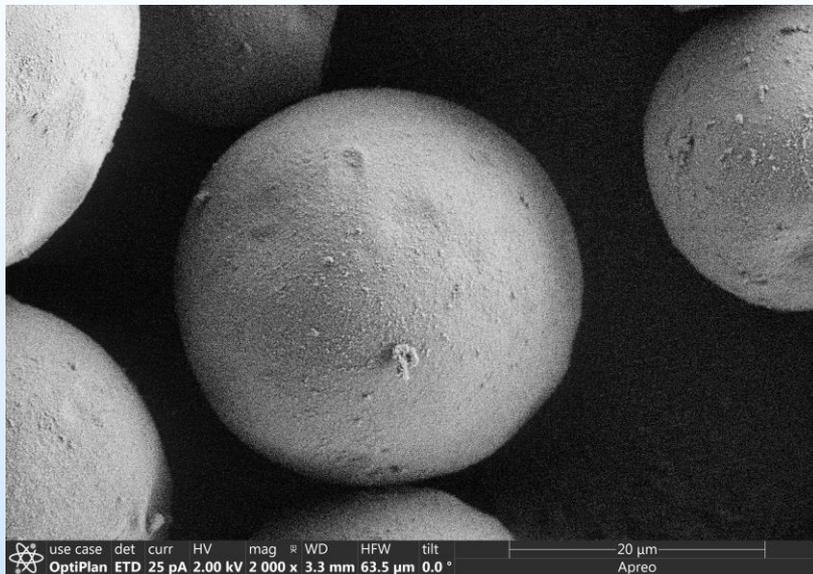
~20% loss in capacity over 3,000 cycles

Heat of Desorption for Sorbents

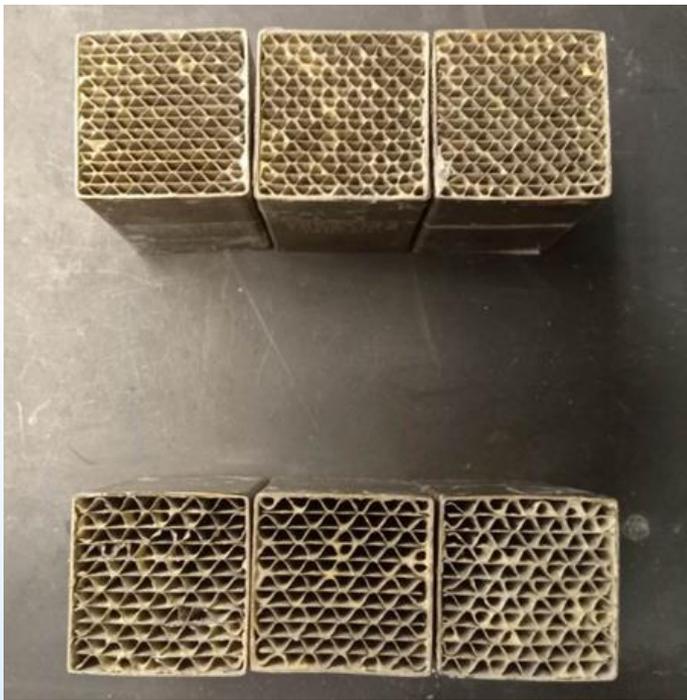


Sorbents	Heat of desorption (kJ/gmol CO ₂)	Energy savings relative to unmodified amine sorbent (%)*
Unmodified amine sorbent	73.74	0
Modified amine sorbent 1	56.87	-22.9
Modified amine sorbent 3	34.77	-52.8
Modified amine sorbent 4	35.83	-51.4
Modified amine sorbent 5	31.82	-56.8

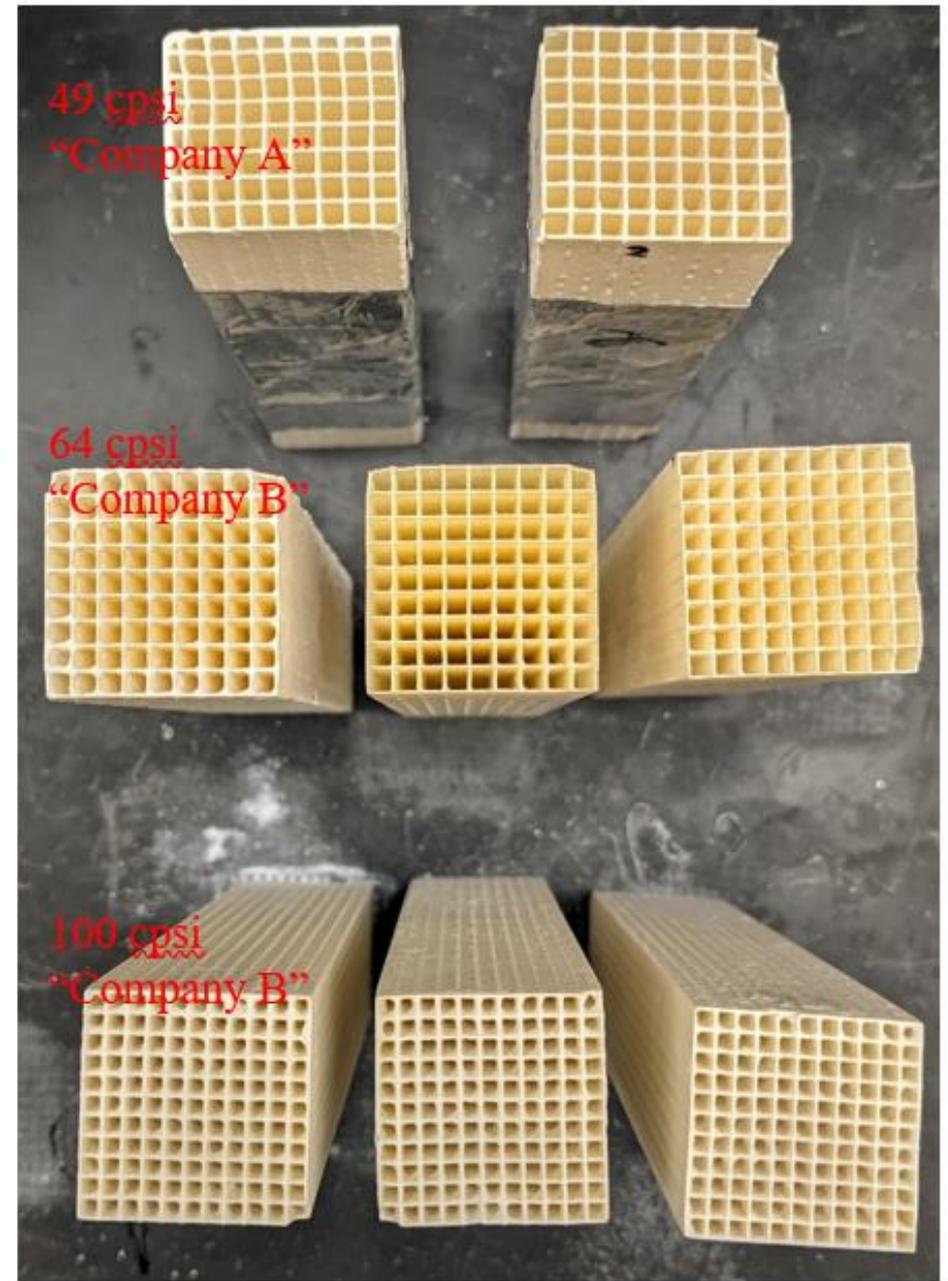
Technology Background



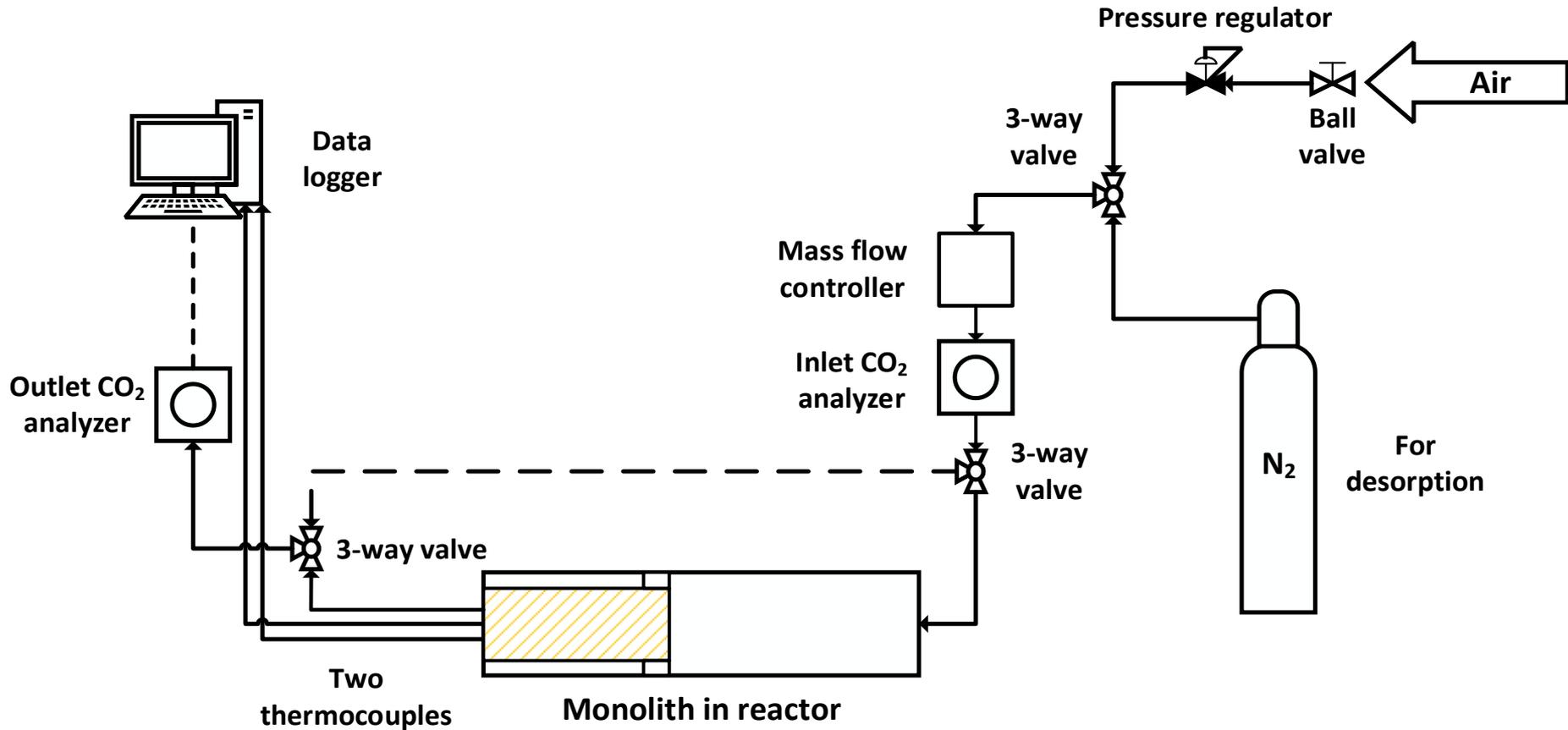
SEM images sorbent substrate: surface area ($\sim 350 \text{ m}^2/\text{g}$), pore volume ($\sim 1.5 \text{ cm}^3/\text{g}$), and average pore diameter ($\sim 20 \text{ nm}$)



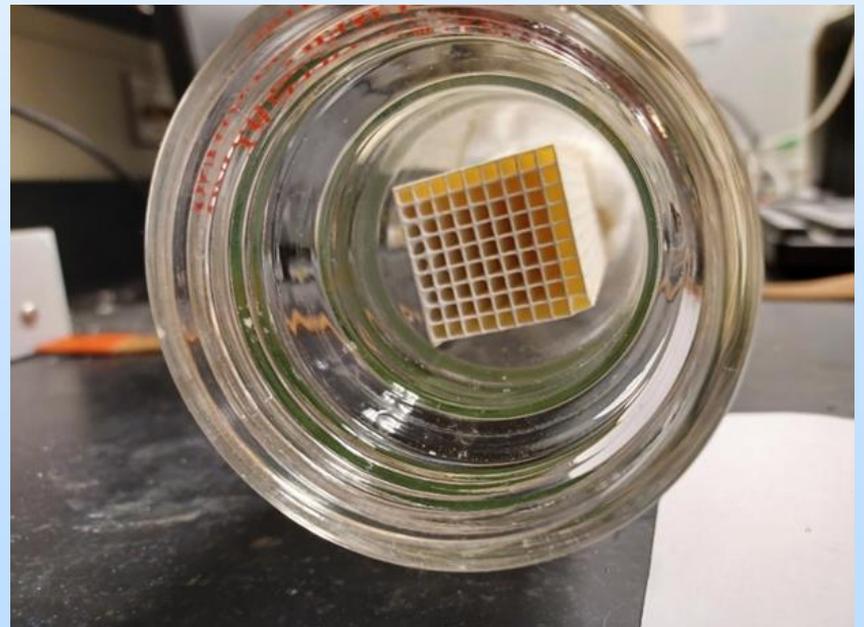
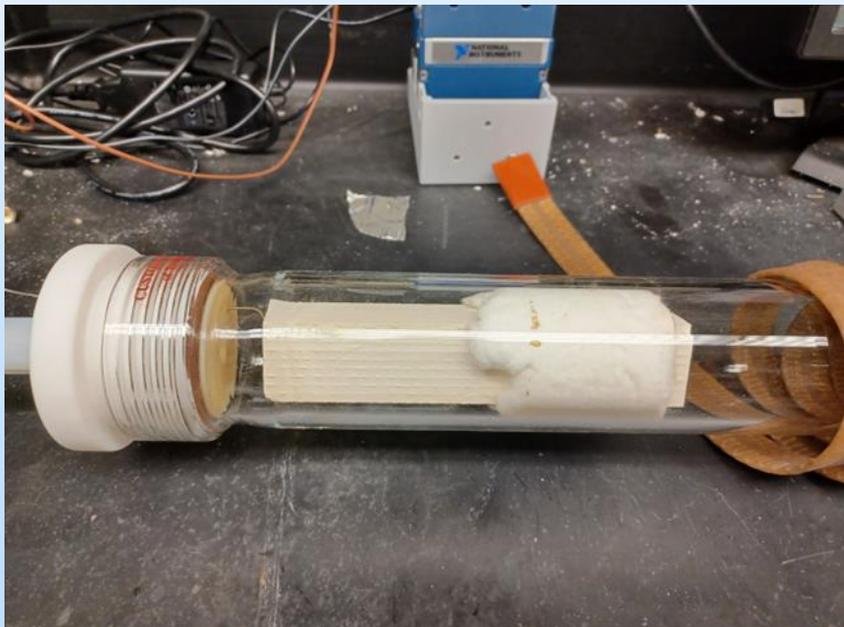
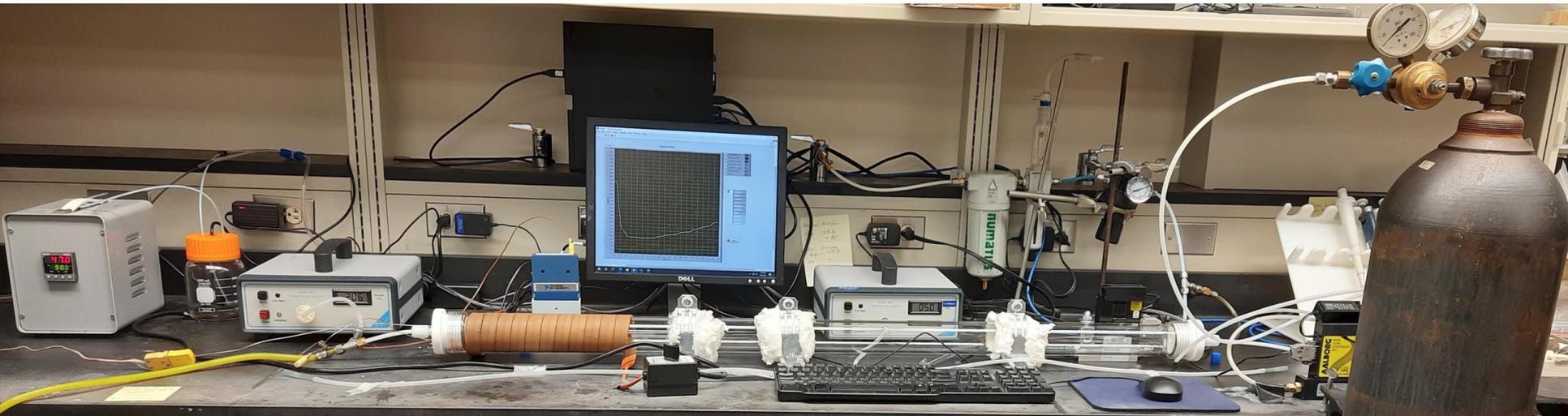
- Dimensions: 3 cm x 3 cm x 15 cm
- Company A's **metallic** monolith blocks with 100 and 150 cpsi
- Company A's **ceramic** monolith blocks with 49 cpsi
- Company B's **ceramic** monolith blocks with 64 and 100 cpsi



Reactor Set-up

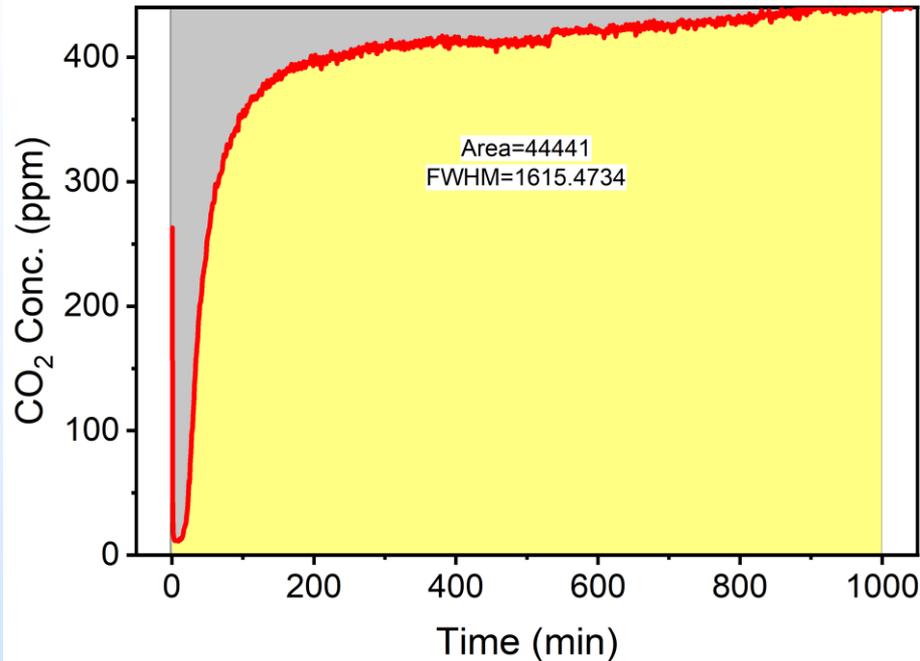


Reactor Set-up



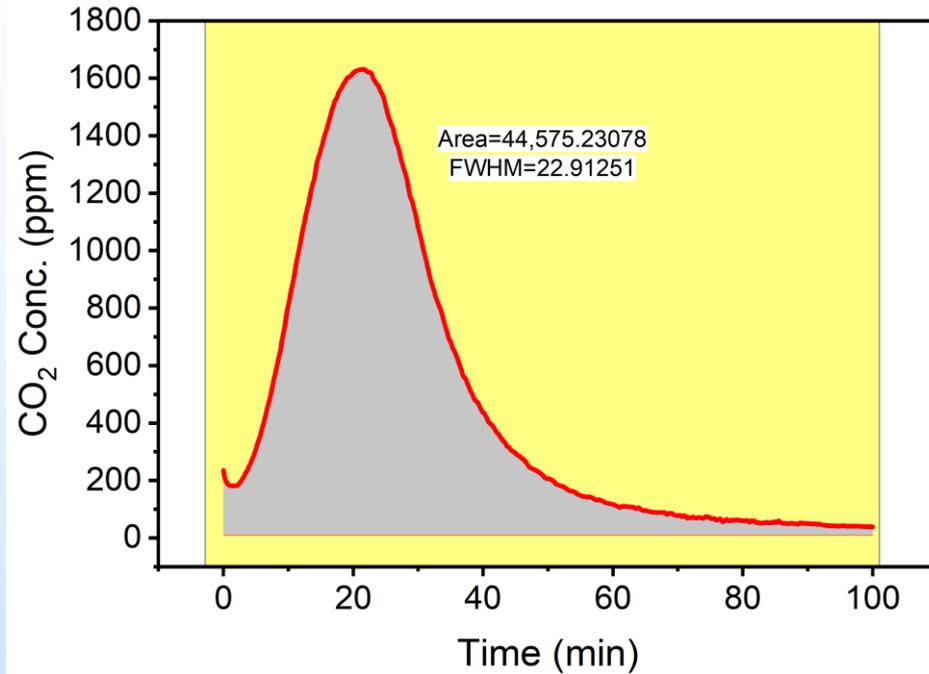
Adsorption and Desorption Breakthrough Curves

Adsorption



10 LPM of compressed indoor air

Desorption



8 LPM of industrial grade N₂

$$\text{CO}_2 \text{ adsorption capacity (mmol CO}_2\text{/g sorbent)} = \frac{\text{Air flowrate} \left(\frac{\text{L}}{\text{min}} \right) \times \frac{P(\text{kPa})}{R \left(\frac{\text{L} \cdot \text{kPa}}{\text{mol} \cdot \text{K}} \right) T(\text{K})} \times \int_{t_i}^{t_f} C_{\text{CO}_2} dt \text{ (ppm CO}_2 \cdot \text{min)} \times 10^{-6}}{\text{sorbent mass (g)}}$$

CO₂ Capacities for **Metallic** Monolith Blocks

Monolith	Ads. T (°C)	Adsorption capacity of powdered sorbent (mmol CO ₂ /g sorbent)	Avg. adsorption capacity of washcoated sorbent (mmol CO ₂ /g sorbent)	Avg. adsorption capacity of block (mmol CO ₂ /block)	Avg. desorption capacity of washcoated sorbent (mmol CO ₂ /g sorbent)
100 cpsi	24	1.78	0.64	5.06	0.72
100 cpsi	40	1.79	0.60	5.02	0.54
150 cpsi	24	1.55	0.70	5.03	0.58

Desorption T: 90 °C in N₂

CO₂ Capacities for 64 cpsi Monolith Blocks

Sorbent	Silica loading	Ads capacity of powdered sorbent (mmol CO ₂ /g sorbent)	Ads capacity of washcoated sorbent in monolith (mmol CO ₂ /g sorbent)	% Ads approach (coated sorbent / powdered sorbent) (%)	Ads capacity of monolith (mmol CO ₂ /monolith)
Unmod	Low	1.79	1.11 ± 0.15	62	25.80
Mod 1	Low	1.55	0.93 ± 0.10	60	19.46
Mod 4	Low	1.50	1.07 ± 0.25	71	18.72
Unmod	High	1.79	1.21 ± 0.15	68	28.41
Mod 1	High	1.55	1.05 ± 0.15	68	22.86
Mod 4	High	1.50	0.99 ± 0.20	66	24.99

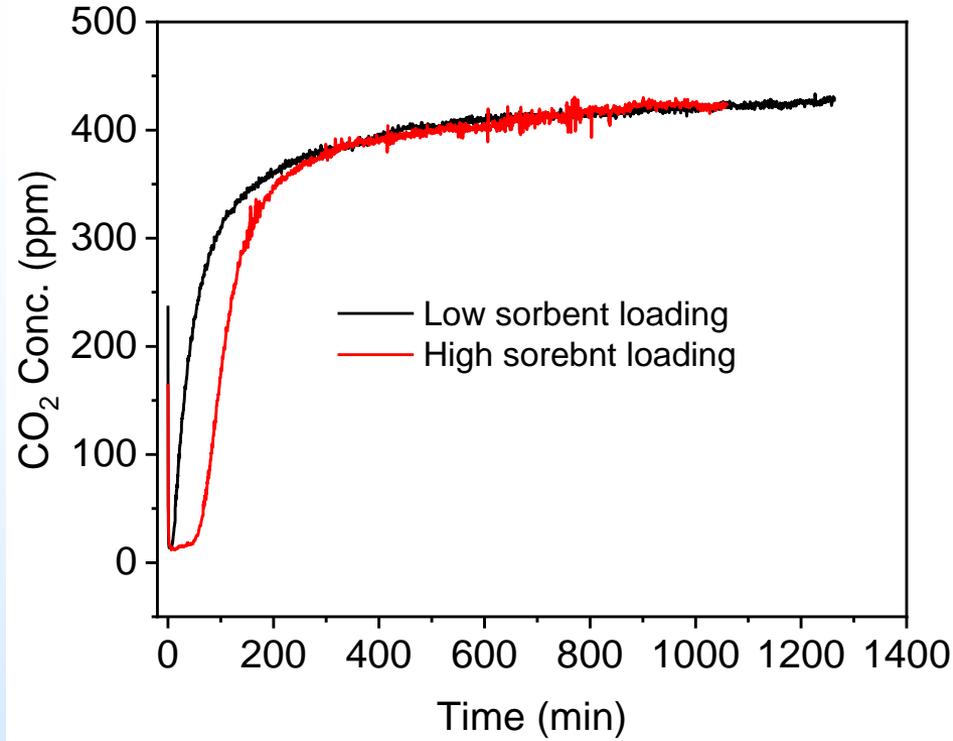
Adsorption T = 24 °C, Desorption T = 90 °C in N₂

CO₂ Capacities for **100 cpsi** Monolith Blocks

Sorbent	Silica loading	Ads capacity of powdered sorbent (mmol CO ₂ /g sorbent)	Ads capacity of washcoated sorbent in monolith (mmol CO ₂ /g sorbent)	% Ads approach (coated sorbent / powdered sorbent) (%)	Ads capacity of monolith (mmol CO ₂ / monolith)
Unmod	High	1.79	1.09 ± 0.11	61	27.88
Mod 1	High	1.55	0.91 ± 0.08	59	21.60
Mod 4	High	1.50	0.87 ± 0.05	58	21.75

Adsorption T = 24 °C, Desorption T = 90 °C in N₂

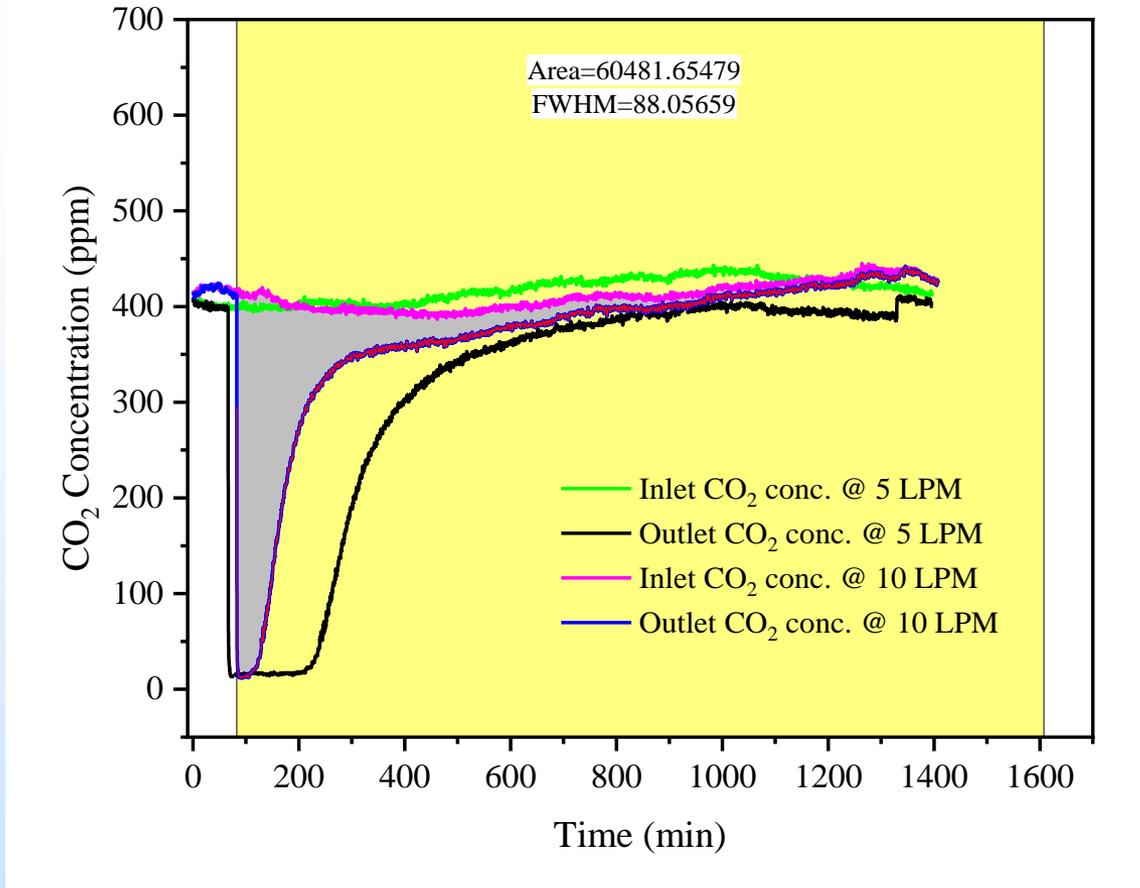
Monolith with High and Low Sorbent Loadings



Block	90% saturation @ ~380 ppm			100% saturation @ ~420 ppm		
	Time (min)	Capacity (mmol CO ₂ /g sorbent)	Capacity (mmol CO ₂ /monolith)	Time (min)	Capacity (mmol CO ₂ /g sorbent)	Capacity (mmol CO ₂ /monolith)
Low	451	0.84	17.51	~900	0.93	19.46
High	417	1.09	25.60	~900	1.21	28.44

Adsorption T = 24 °C, Air flowrate = 10 LPM

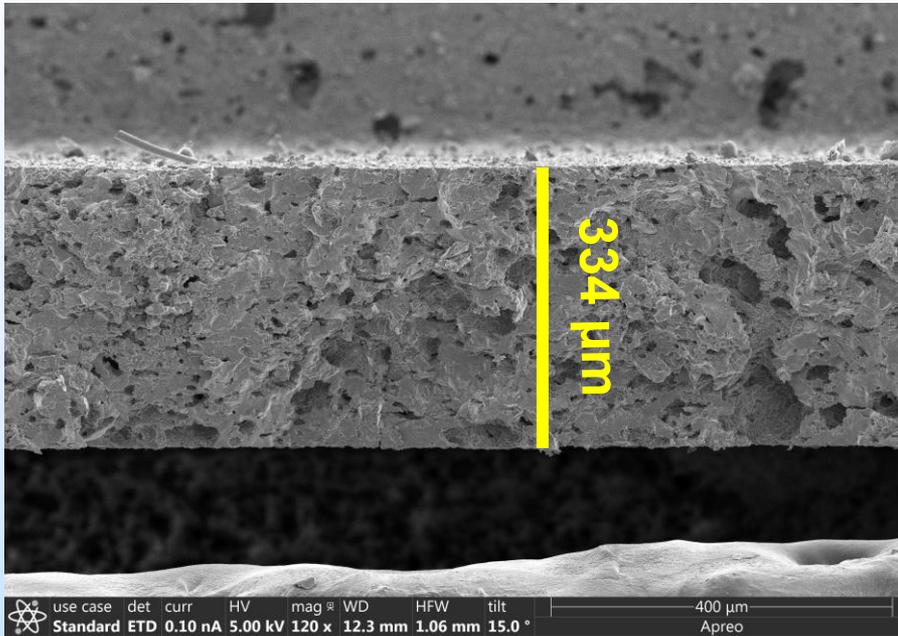
Breakthrough Curves under Different Flow Rates



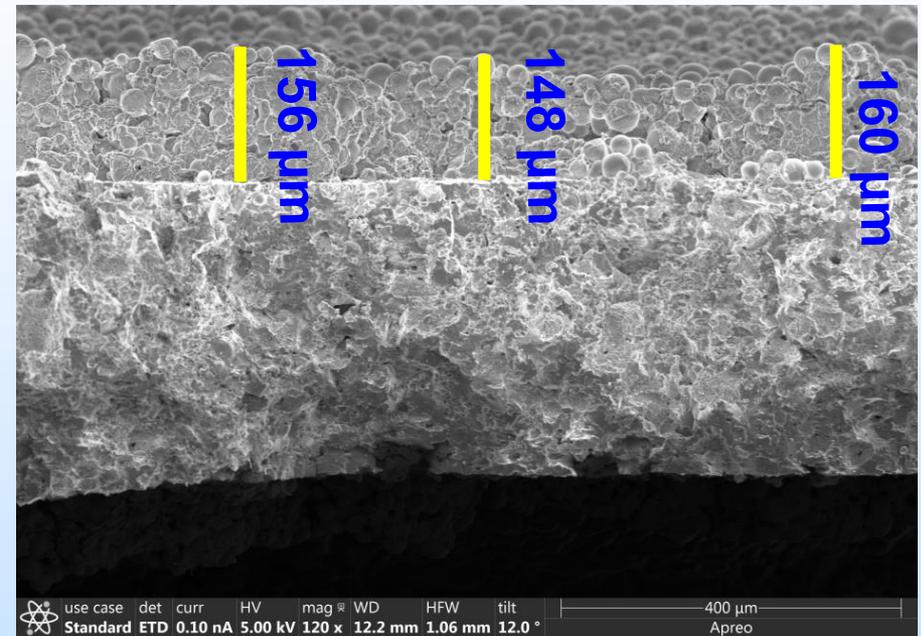
Flow rate (LPM)/ LV (cm/s)	Full capacity (mmol CO ₂ /g sorbent)	Time to reach specific saturation % of total capacity (hr)			
		70%	80%	90%	100%
5 (18)	1.2	5.6	8.8	14.0	21.0
10 (36)	1.1	3.5	6.1	10.5	20.9

Sorbent-washcoated Cell in Ceramic Monolith Blocks

Bare monolith

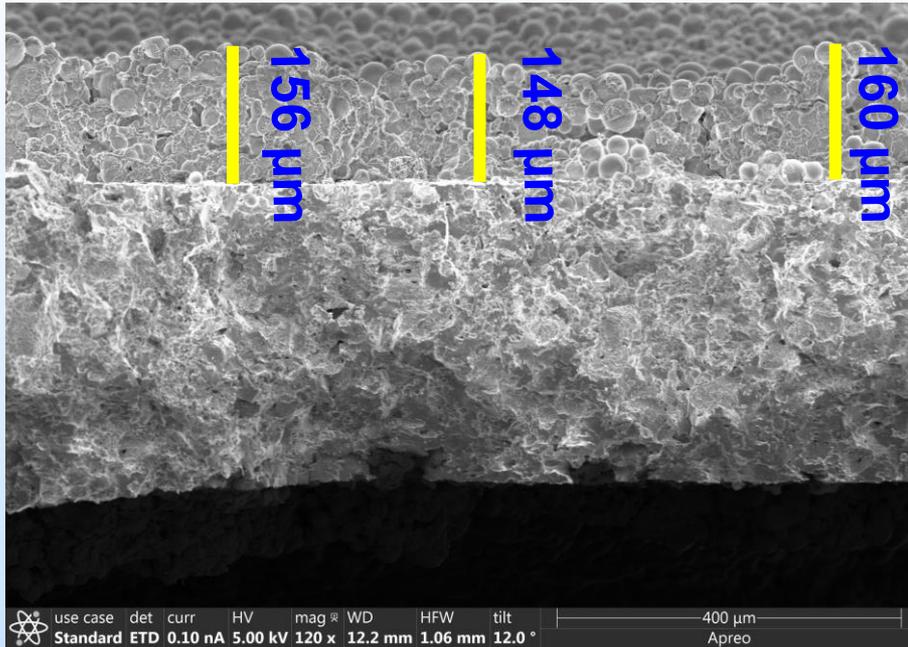


Substrate-coated monolith

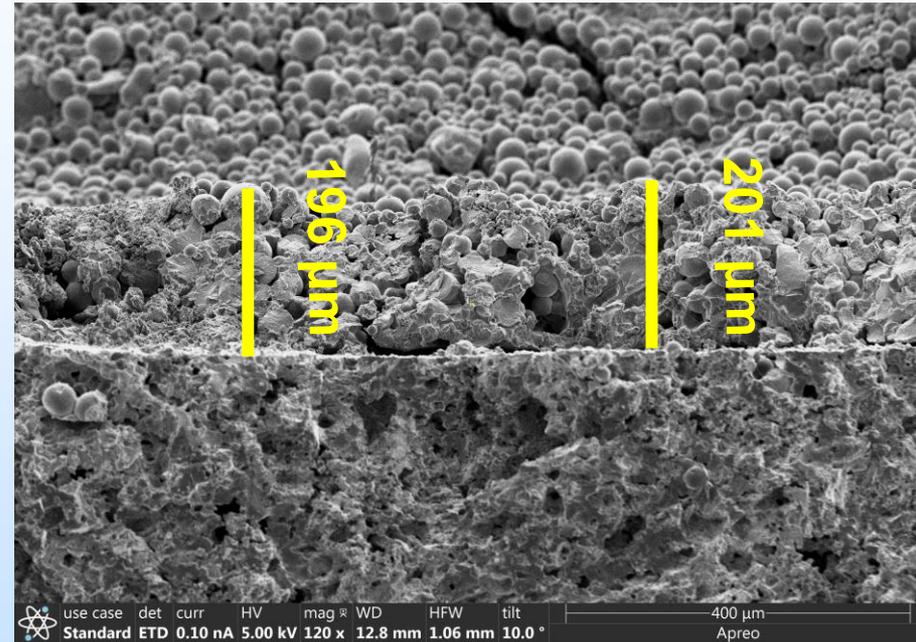


Sorbent-washcoated Cell in Ceramic Monolith Blocks

Substrate-coated monolith

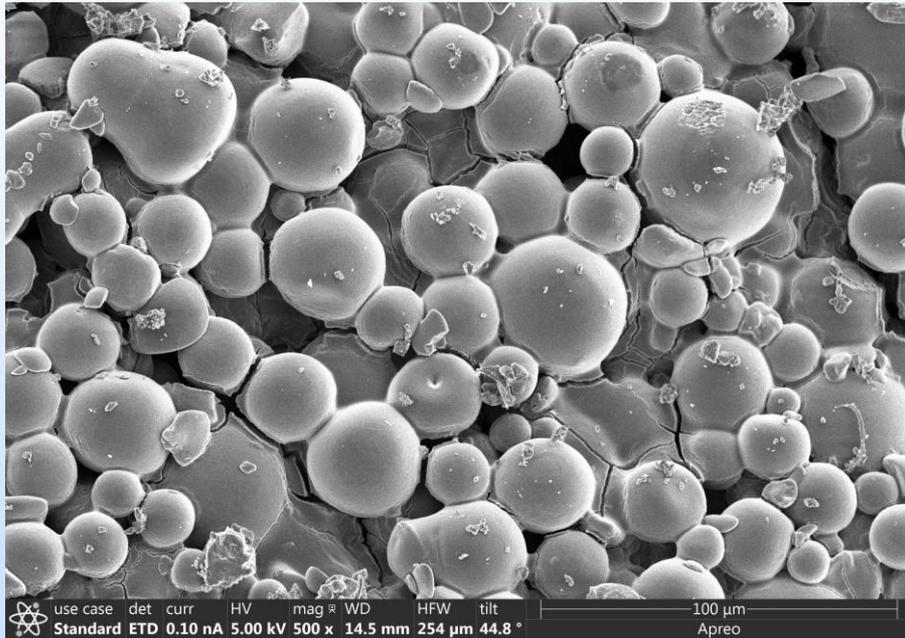


Amine-doped sorbent-washcoated monolith



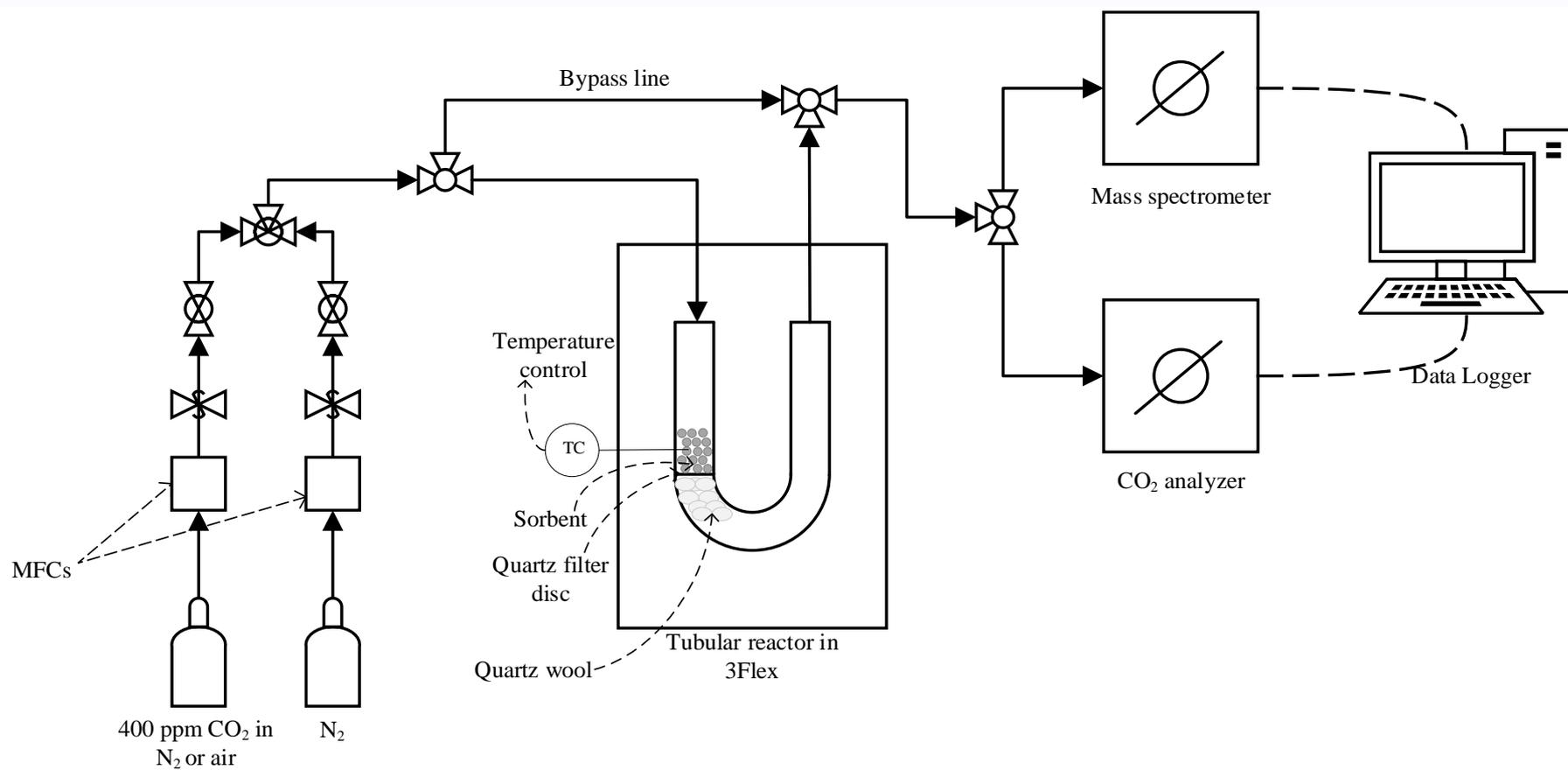
Sorbent-washcoated Cell in Ceramic Monolith Blocks

Amine-doped sorbent-washcoated monolith



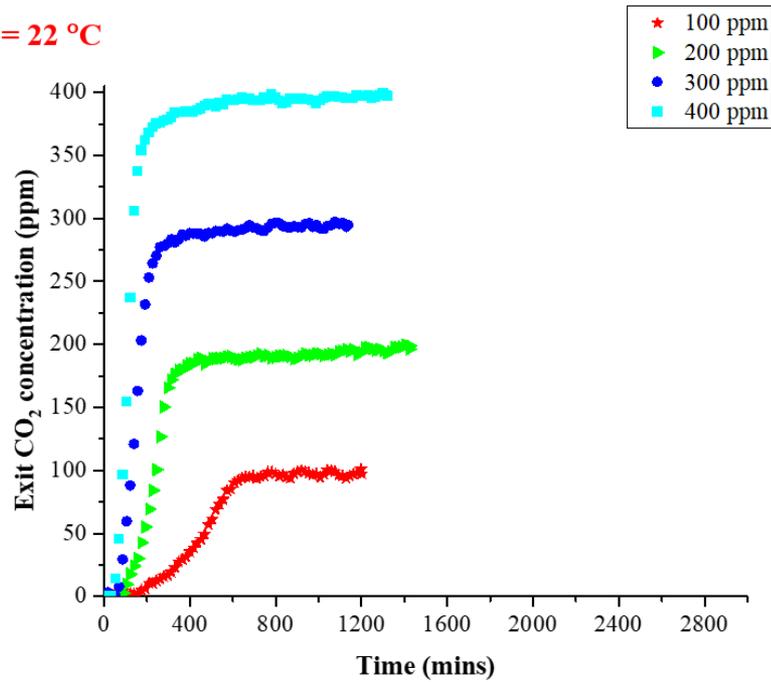
Poor amine doping around the edge of the monolith block

CO₂ Adsorption Kinetics

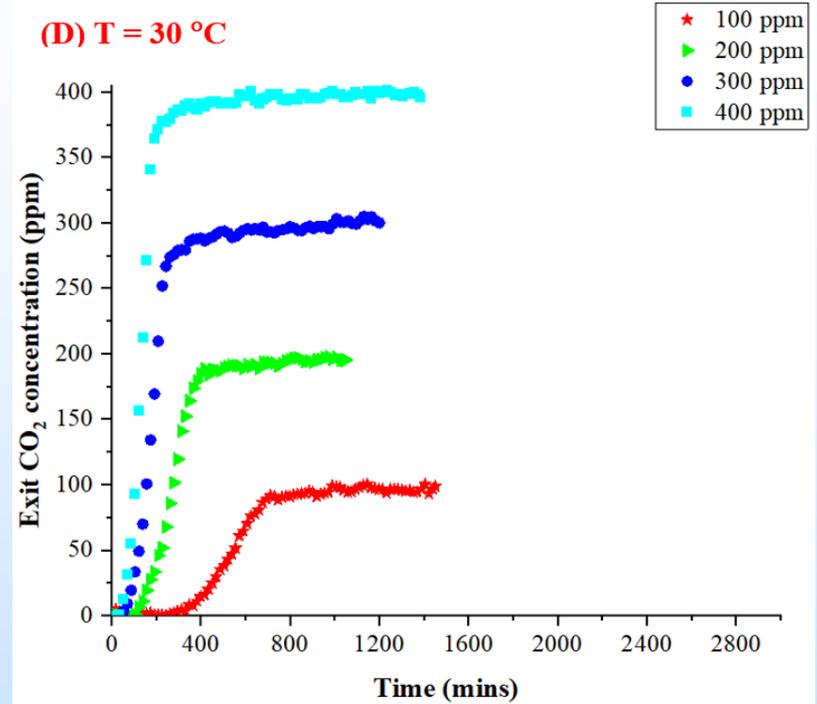


CO₂ Adsorption Kinetics for Modified Amine Sorbent 1

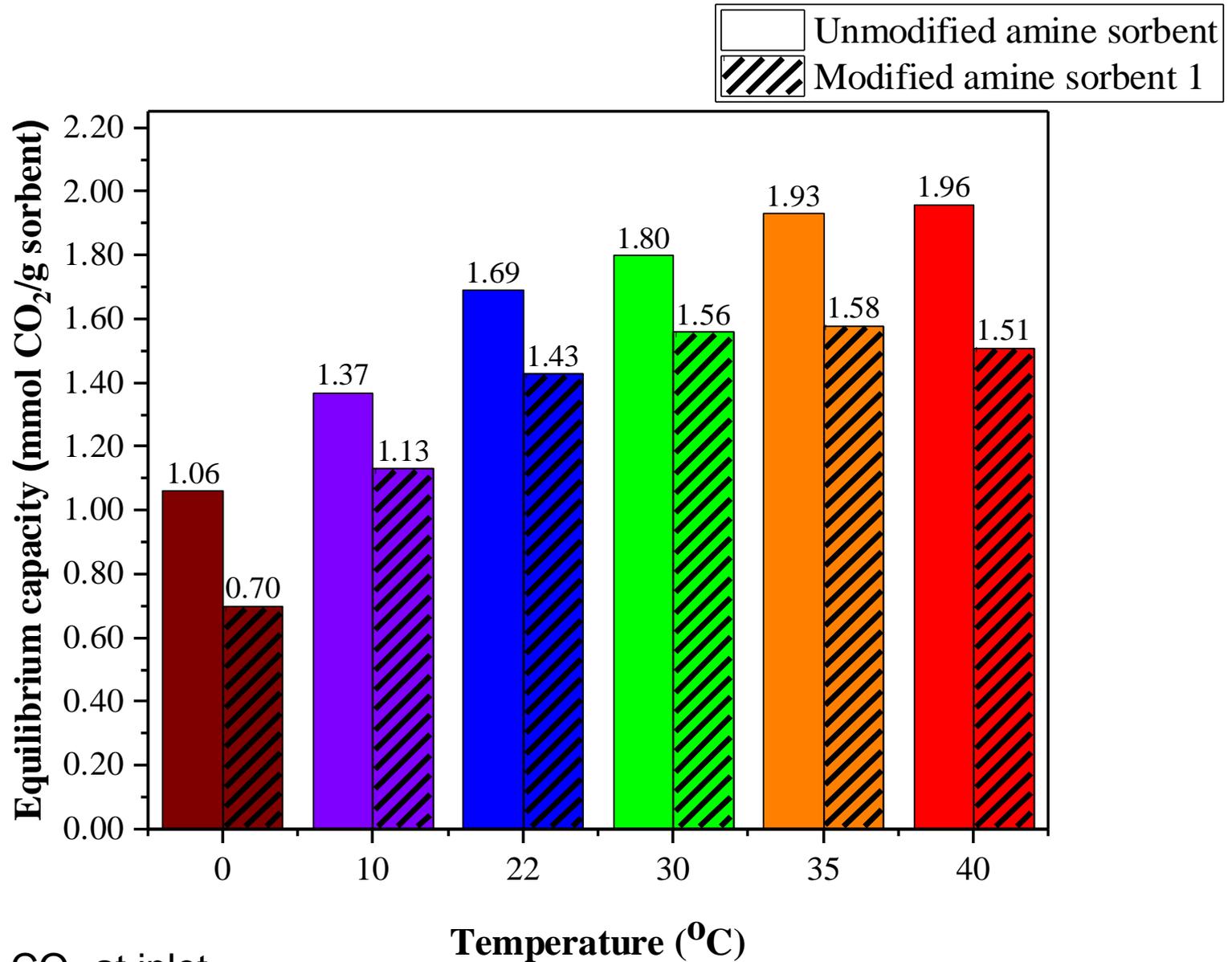
(C) T = 22 °C



(D) T = 30 °C

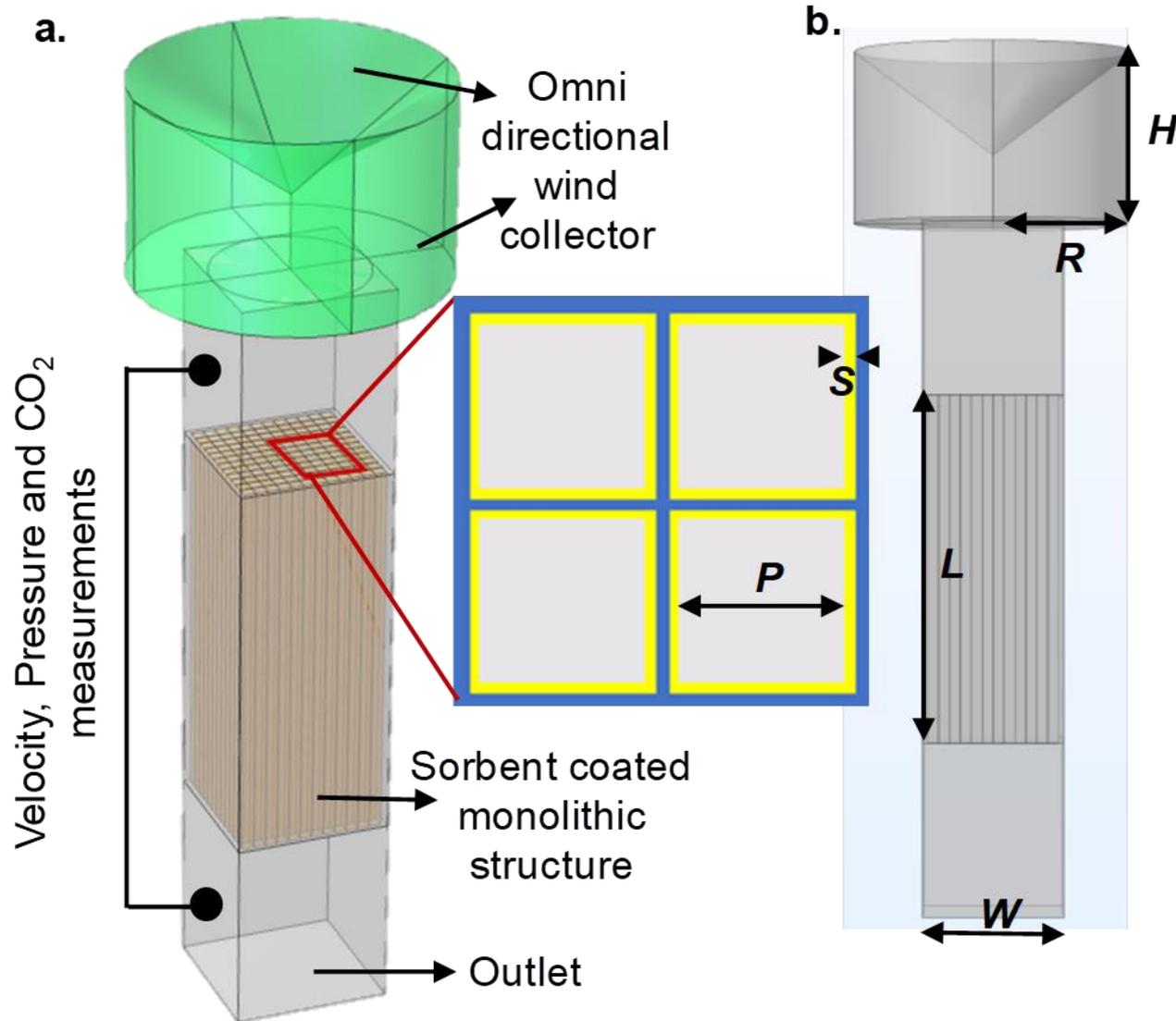


Equilibrium CO₂ Adsorption Capacities

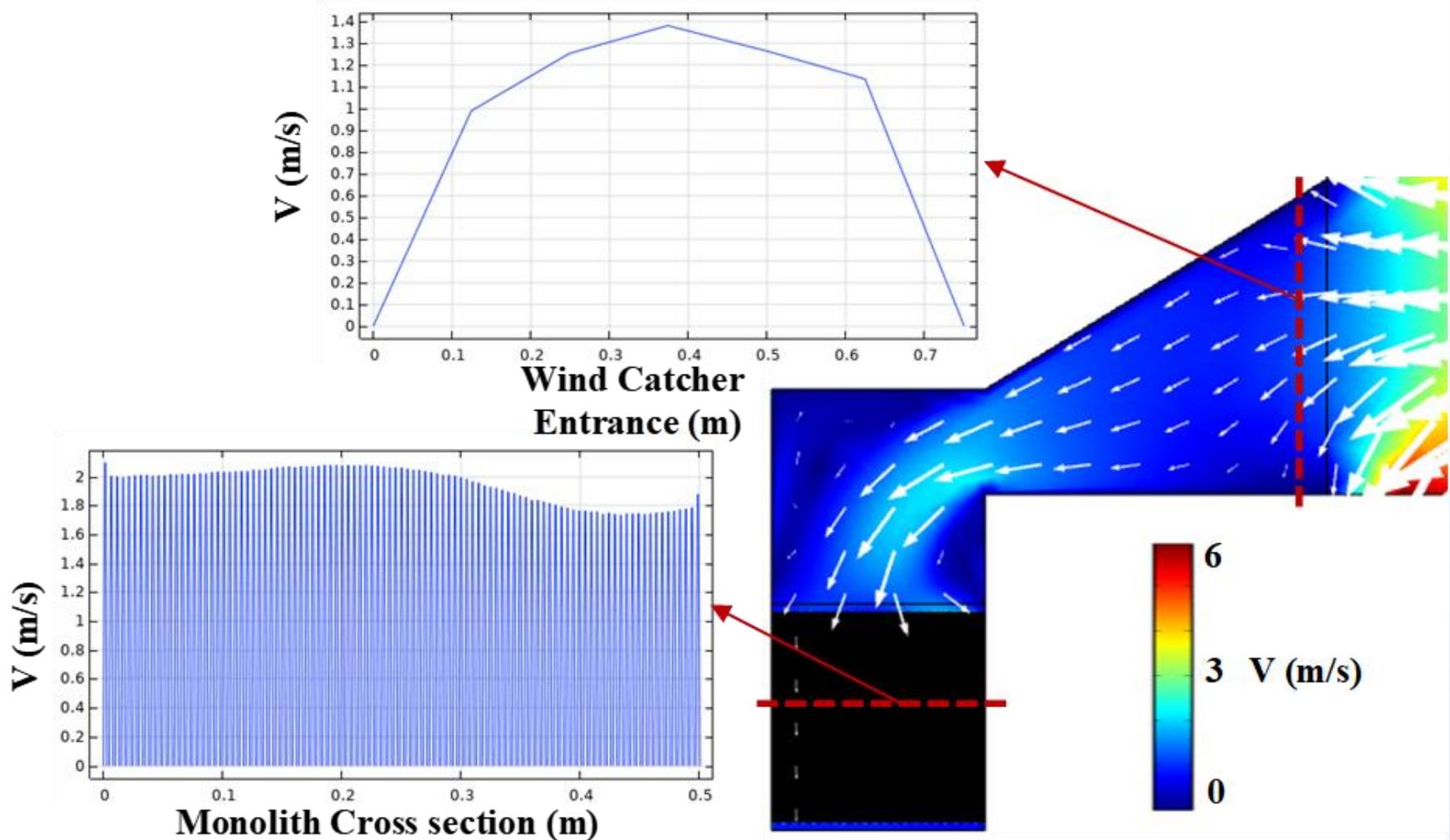


400 ppm CO₂ at inlet

Passive Air Contactor

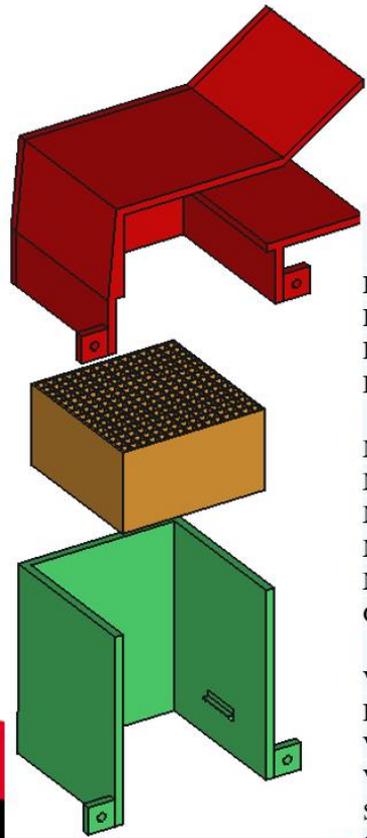


CFD for Passive Air Contactor



Wind speed: 5 m/s; pitch: 2 mm; linear velocity: ~ 2 m/s at middle height; Re : ~ 270

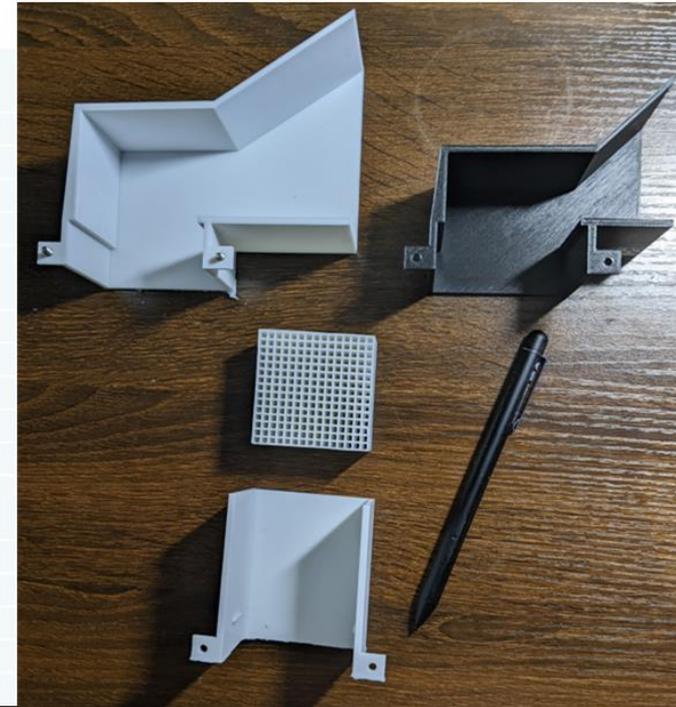
Experimental Validation of CFD Model



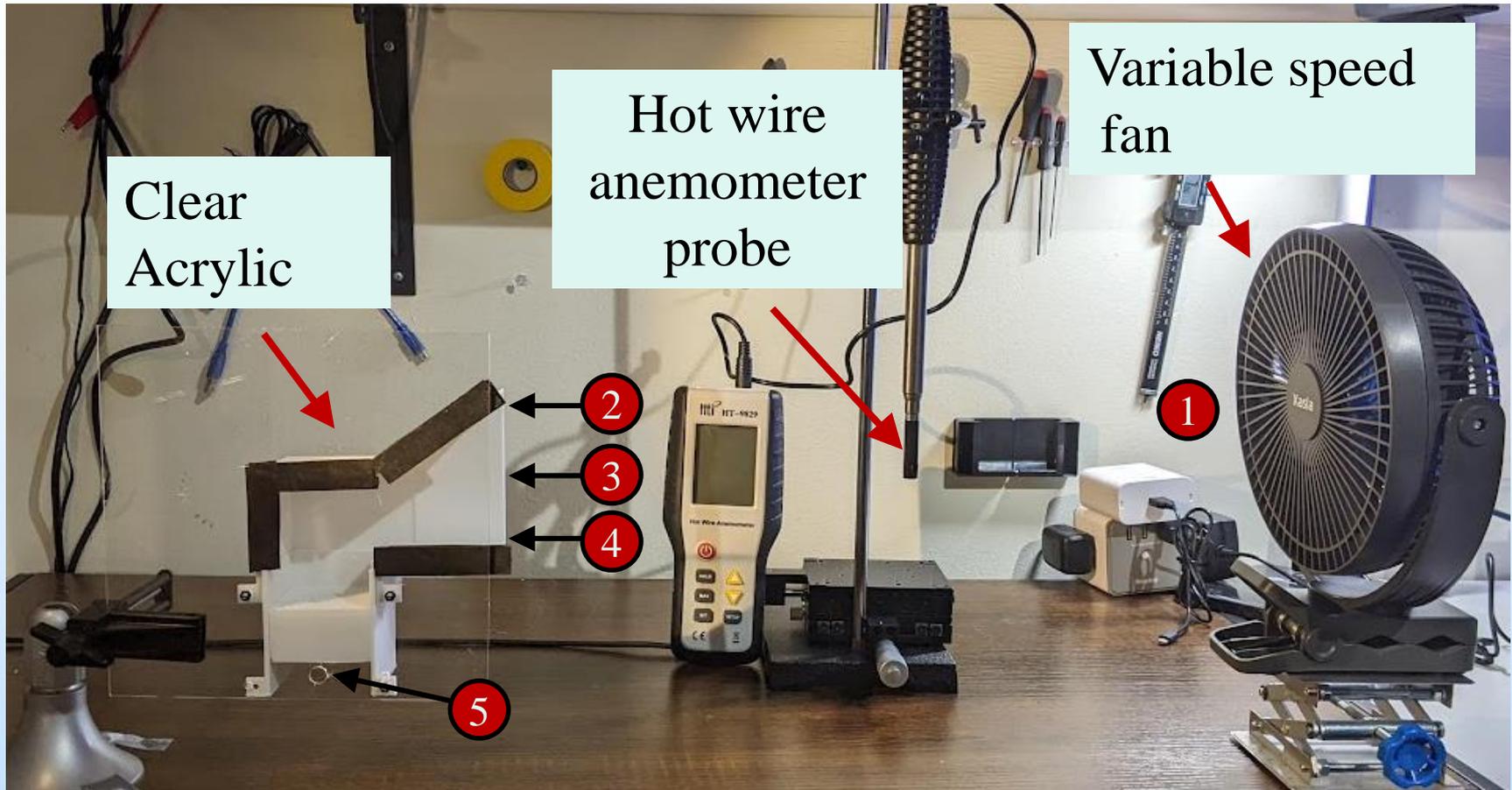
Fused Deposition 3D Printing

Parameterized Variables	Value	Units	Description
React_h	70 mm		Height of the DAC Reactor
React_w	60 mm		Width of the DAC Reactor
React_d	60 mm		Depth of the DAC Reactor
React_th	3 mm		Wall thickness of the reactor
			Position of the Monolith from the reactor bottom
MonoL_holder_pos	15 mm		
MonoL_holder_th	2 mm		Thickness of monolith holder
MonoL_cell_d	3 mm		Pitch of each monolith cell
MonoL_gap	0.5 mm		Gap between consecutive monolith cells
MonoL_h	30 mm		Height of the monolith
Clearance_fit	0.5 mm		Clearance factor for 3D printer
			Height above the monolith to windcatcher section
Windc_h	20 mm		
React_in_h	30 mm		Height of the reactor inlet
Windc_w	30 mm		Width of windcatcher section
Windc_in_h	50 mm		Height of windcatcher inlet
Screw_hole	3.2 mm		Screw hole dia for M3 Screws
Screw_mount	10 mm		Screw mount size

Modular system with interchangeable windcatcher and monolith sections



Experimental Validation of CFD Model

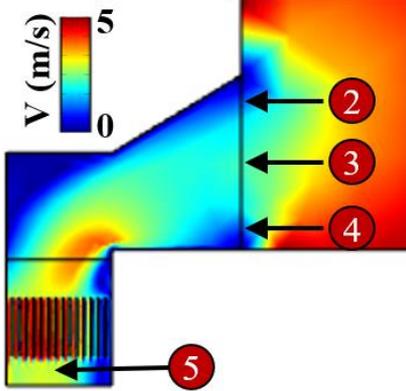


Experimental Validation of CFD Model

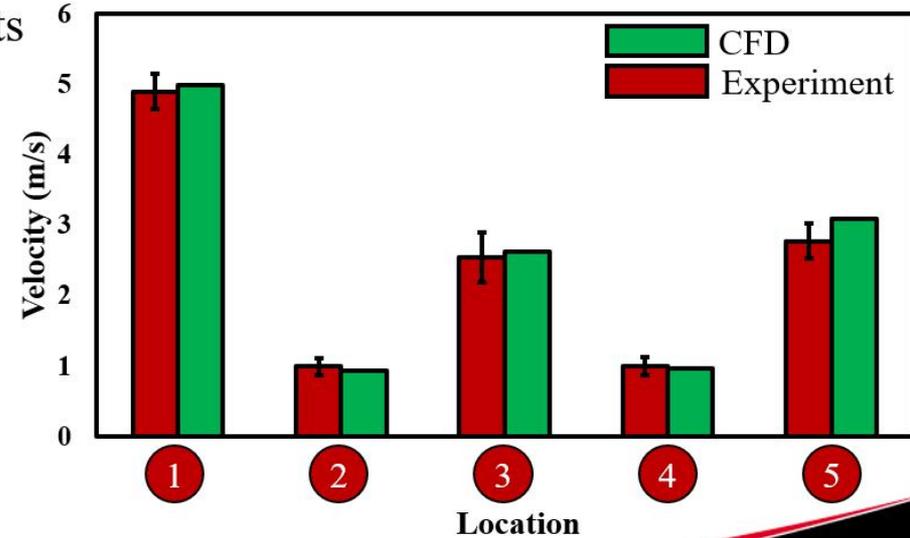
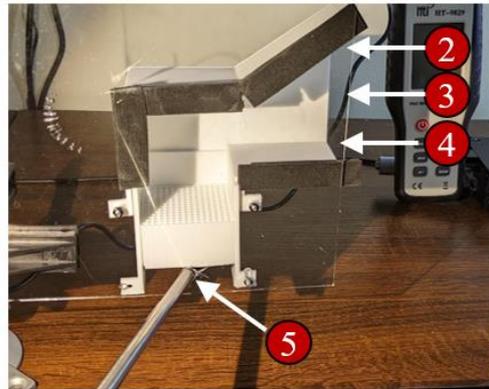
$$\text{Error} = \frac{|CFD \text{ value} - \text{Exp. value}|}{\text{Exp. value}}$$

Error 2-11%

CFD probing points



Experimental probing points



Plans for future testing/development

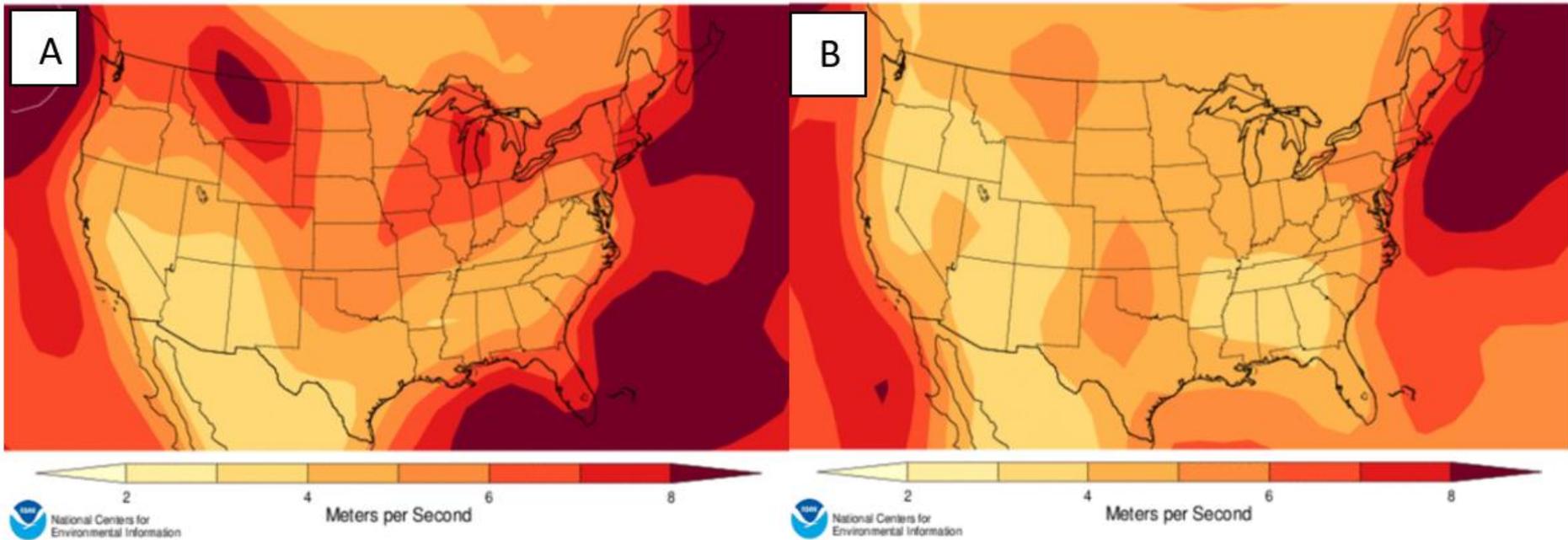
- **Task 2:** CFD combined with adsorption kinetics for DAC
- **Task 4:** Sorbent-washcoated monolith structure
 - ✓ Determine final coating formulations and cell size
 - ✓ Scale up monolith: 15 cm x 15 cm x 30 cm
- **Task 5:** Design, construction and start-up of DAC system in environmental chamber
- **Task 6:** Performance evaluation of sorbent-washcoated monolith in DAC system
 - ✓ Performance evaluation wrt T, RH, wind speeds and directions
 - ✓ Evaluate desorption options
- **Future Plan:** Outdoor demonstration and Commercialization

Summary Slide

- Robust and energy-efficient sorbent technology
- Systematic and rational PAC design using CFD confirmed with experimental data
- Successful development of sorbent-washcoated monolith for scalable PAC system
- Performance evaluations of scaled monolith in DAC system
- Open to partnerships for demonstration and commercialization

Appendix

Average Wind Speeds in Continental U.S.



Monthly average wind speed data for the month of (A) November 2020 and (B) May 2020 across the U.S. Accessed from the U.S. Wind Climatology database on National Centers for Environmental Information (NOAA) retried on June 29, 2021.