Amine Infused ePTFE/SiO_2 Laminate Structured Sorbents as an Advanced Direct Air Capture System

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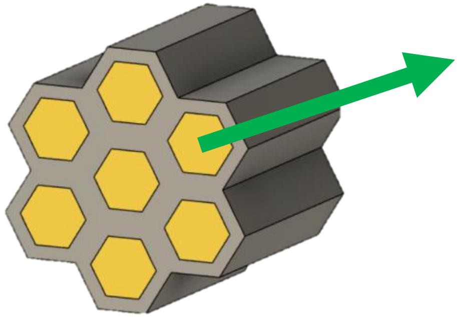
August 5 – 9, 2024
Lab/Bench-Scale DAC Research, 2:55 – 3:10 Monday August 5th

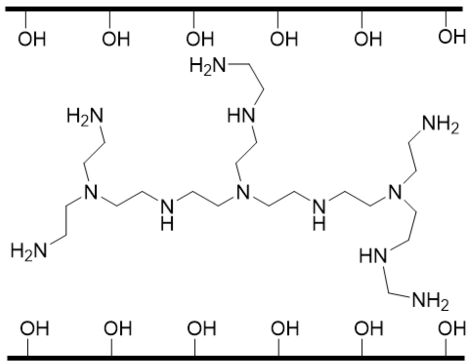
Project Overview

- Funding
  - Federal share (DOE): $745,006
  - Cost Share: $186,567
- Overall Project Performance Dates
  - 09/01/2023 – 08/31/2025
- Project Participants
  - Georgia Institute of Technology (Christopher Jones, Matthew Realff)
  - W.L.Gore & Associates Inc. (Gina Dell, Uwe Beuscher)

DAC by Solid-supported Amine Sorbents

Solid-supported amine sorbents

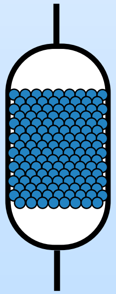




Immobilized amine-bearing polymers

- CO_2 adsorption by amine-bearing polymers immobilized on inorganic porous supports
- Requirements for practical DAC applications:
  - High CO_2 capacity
  - Rapid CO_2 adsorption/desorption kinetics
  - High recyclability under DAC conditions

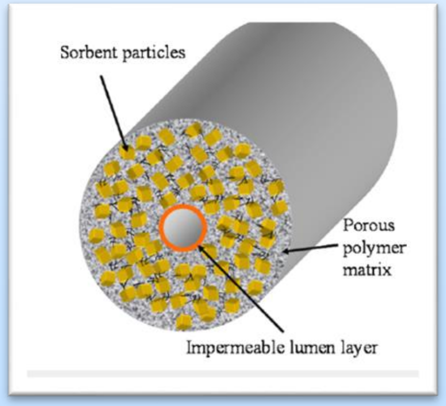
< Lab scale >



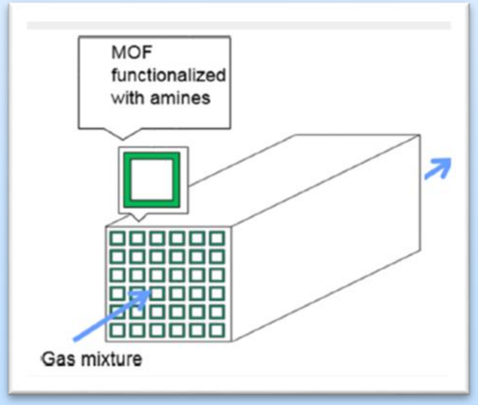
Fixed bed

Large pressure drop

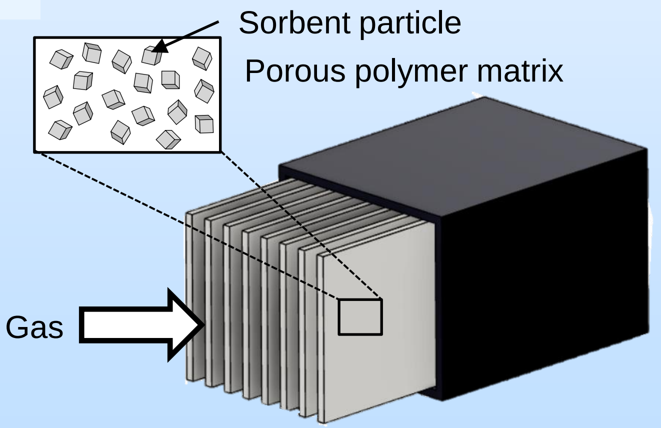
< Bench scale >



Fiber



Monolith



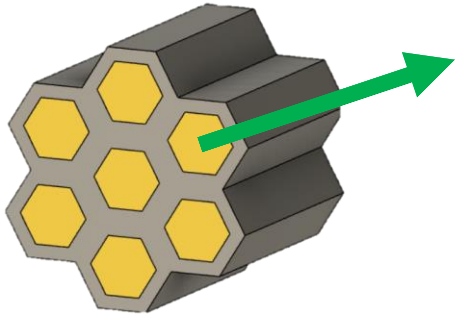
Laminate

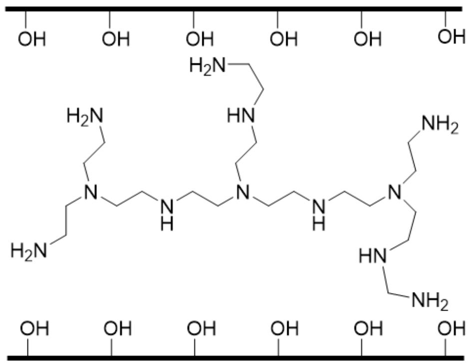
Darunte *et al.*, *ACS Appl. Mater. Interfaces* **2017**, 9 (20), 17042-17050

Lively *et al.*, *Chem. Eng. J.* **2011**, 171 (3), 801-810

DAC by Solid-supported Amine Sorbents

Solid-supported amine sorbents





Immobilized amine-bearing polymers

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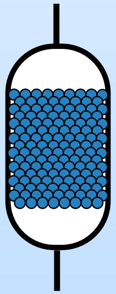
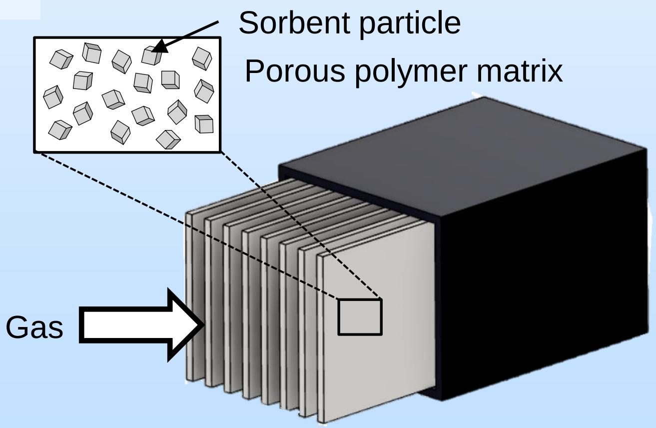


Fixed bed

Large pressure drop

< Bench scale >

This project →



Laminate

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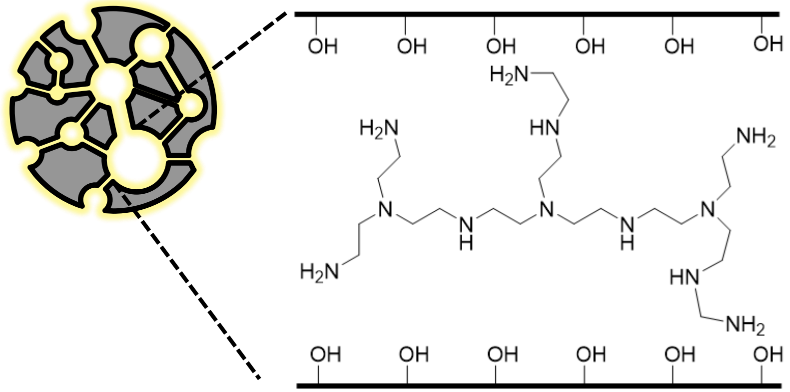
Free Standing Solid-supported Amine Sorbents

Advantages of polymeric inorganic/organic hybrid sorbents

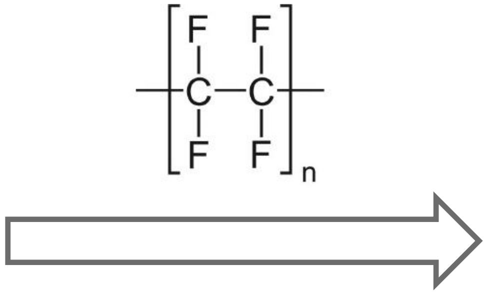
- High volume-loading of solid adsorbents (silica particles)
- Macroporous polymer – bicontinuous pore network for rapid CO_2 mass transport
- Tunable material properties: thermally stable, tunable porosity & **hydrophobic**

< PEI-ePTFE/silica hybrid sorbent for DAC >

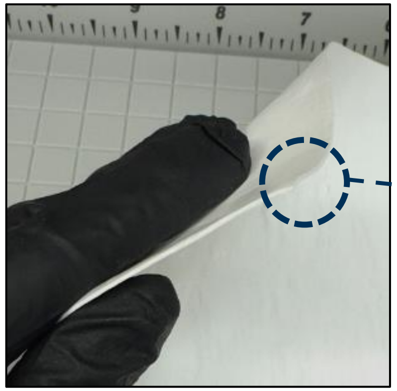


Immobilized Poly(ethyleneimine) (PEI) on silica pore surfaces

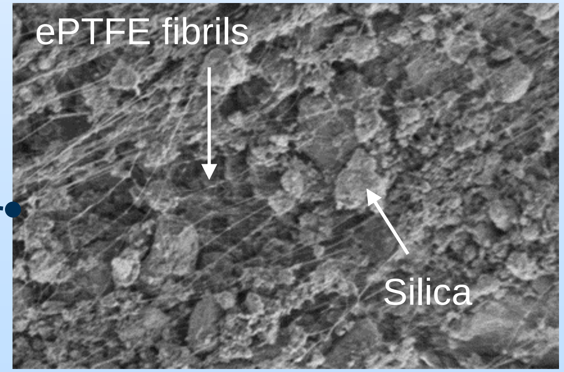
Hydrophobicity



Expanded poly(tetra fluoroethylene) (ePTFE)

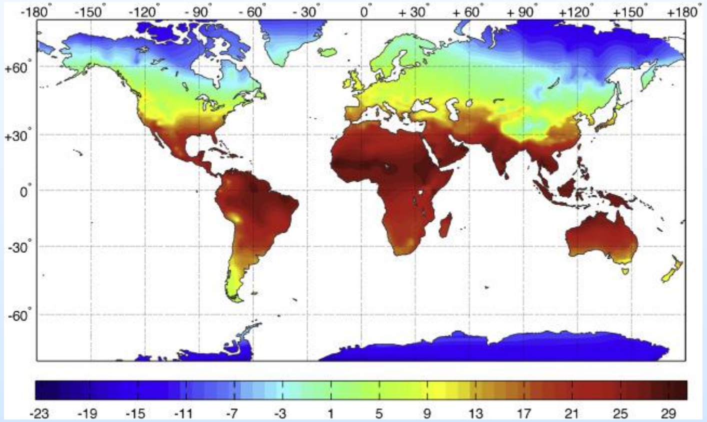


Cross-sectional image



DAC system with S-TVSA

- Wide range conditions for DAC system



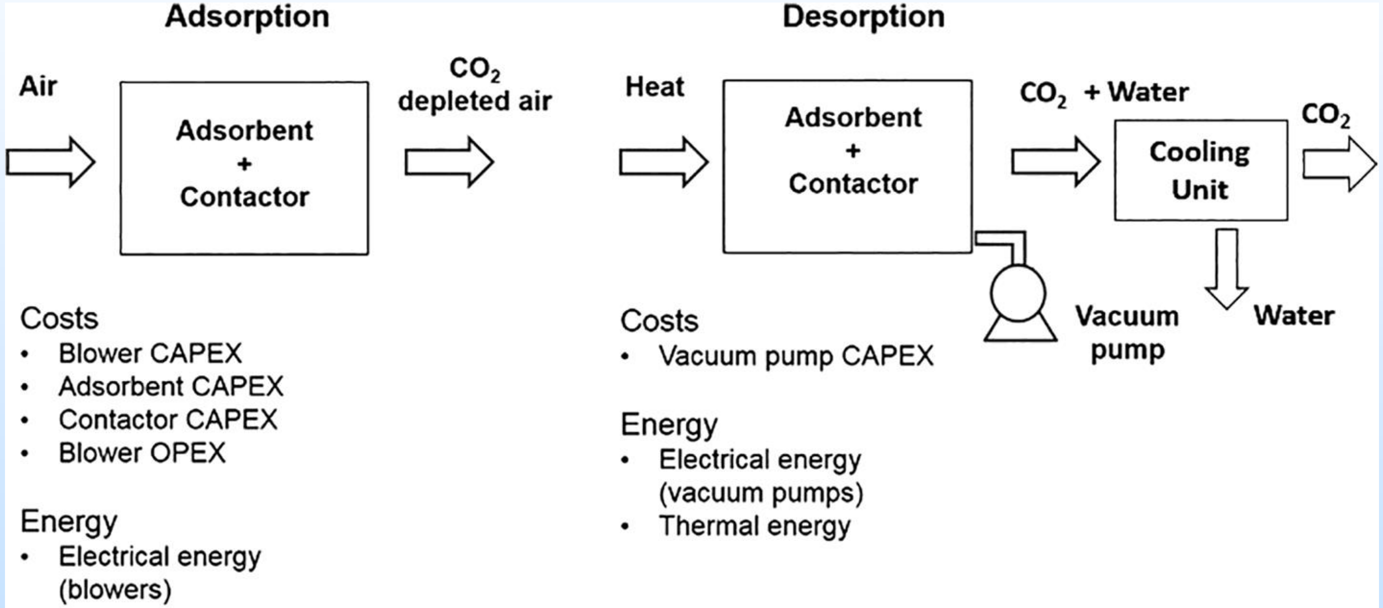
World average temperature (°C)

Mourshed *et al., Renewable Energy* **2016**, *94*, 55– 71

Aim to investigate the PEI-ePTFE/silica laminate DAC system performance in wide range of temperature and humidity conditions:

-20 to 35 °C and 0-80% RH

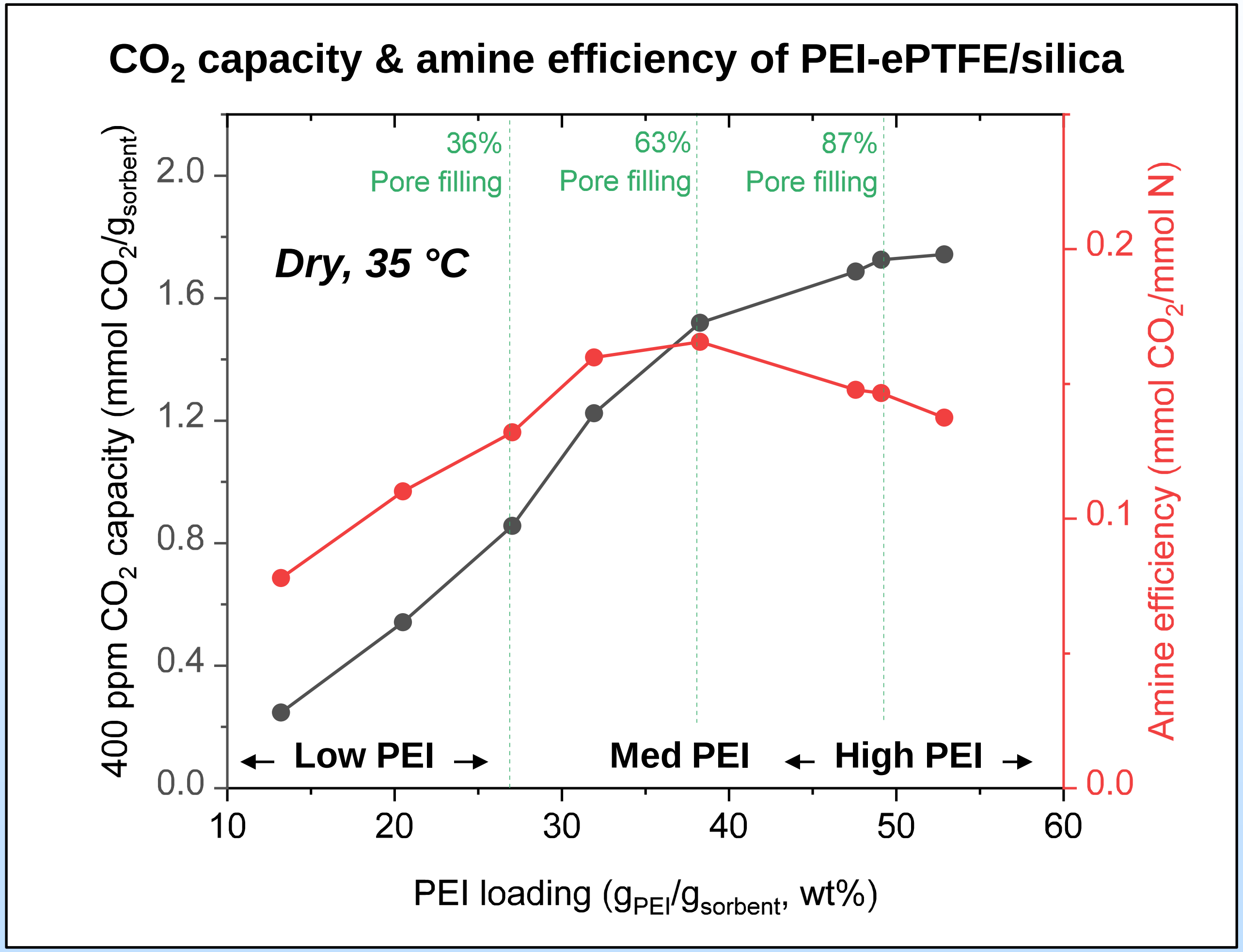
- **Steam-assisted temperature vacuum swing adsorption (S-TVSA)**



Sinha et al. *AIChE J*. **2019**, 65, e16607

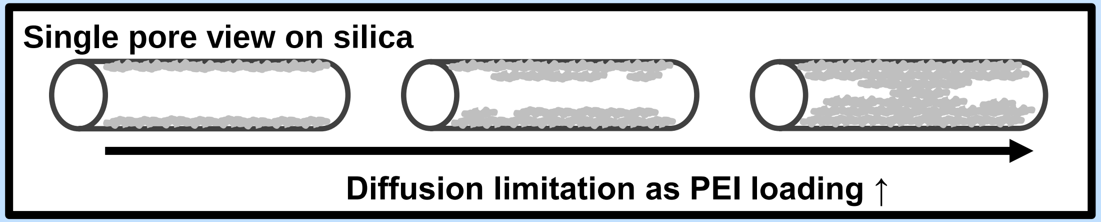
- Structured gas-solid contactor with **hydrophobic domain (ePTFE)**
  : Enhanced mass transfer rate & reduction in energy consumption.
- Steam-assisted temperature vacuum swing adsorption (**S-TVSA**)
  : Rapid heat transfer for sorbent regeneration.

Effect of Amine Loading



❑ **Changes in CO_2 capacity and amine efficiency**

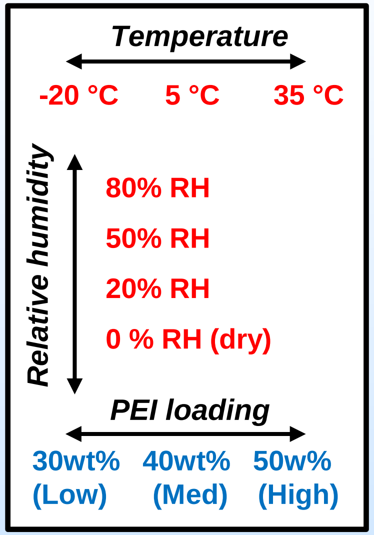
- **PEI loading ∝ Total number of amine sites ∝ CO_2 capacity of PEI-ePTFE/silica.**
- **Low** PEI loading
  : Interaction of amine sites ($-NH_2$) with the silica wall (- OH).
- **High** PEI loading
  : Amine sites with high diffusion limitation.

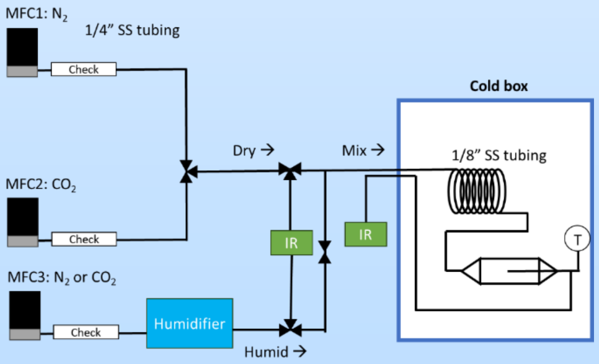


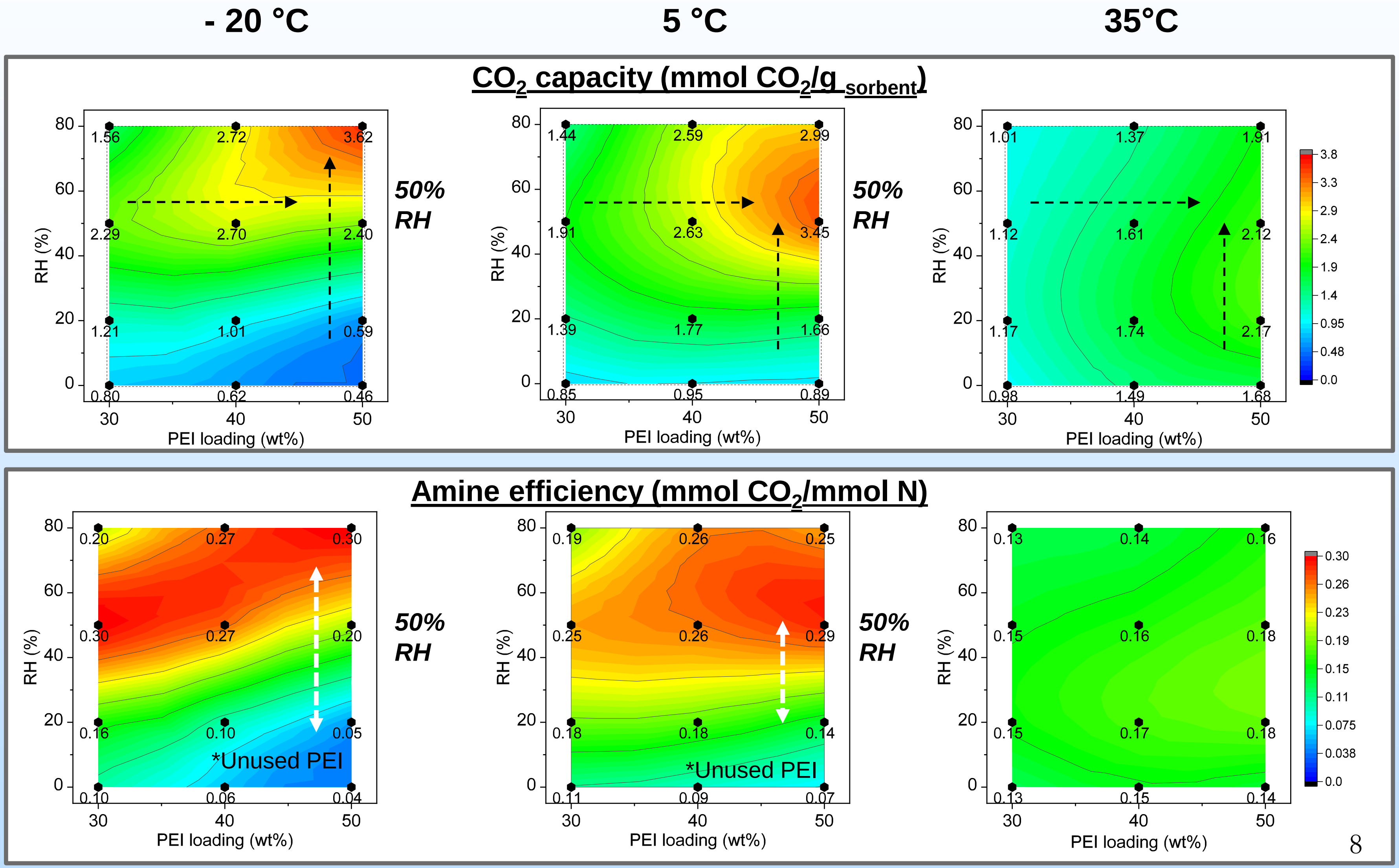
$$Amine\ Efficiency\left(\frac{mmol\ CO_2}{mmol\ N}\right) = \frac{moles\ of\ captured\ CO_2}{moles\ of\ amine\ sites\ on\ sorbent}$$

Changes in CO_2 capacity and amine efficiency

Simulate various atmospheric conditions



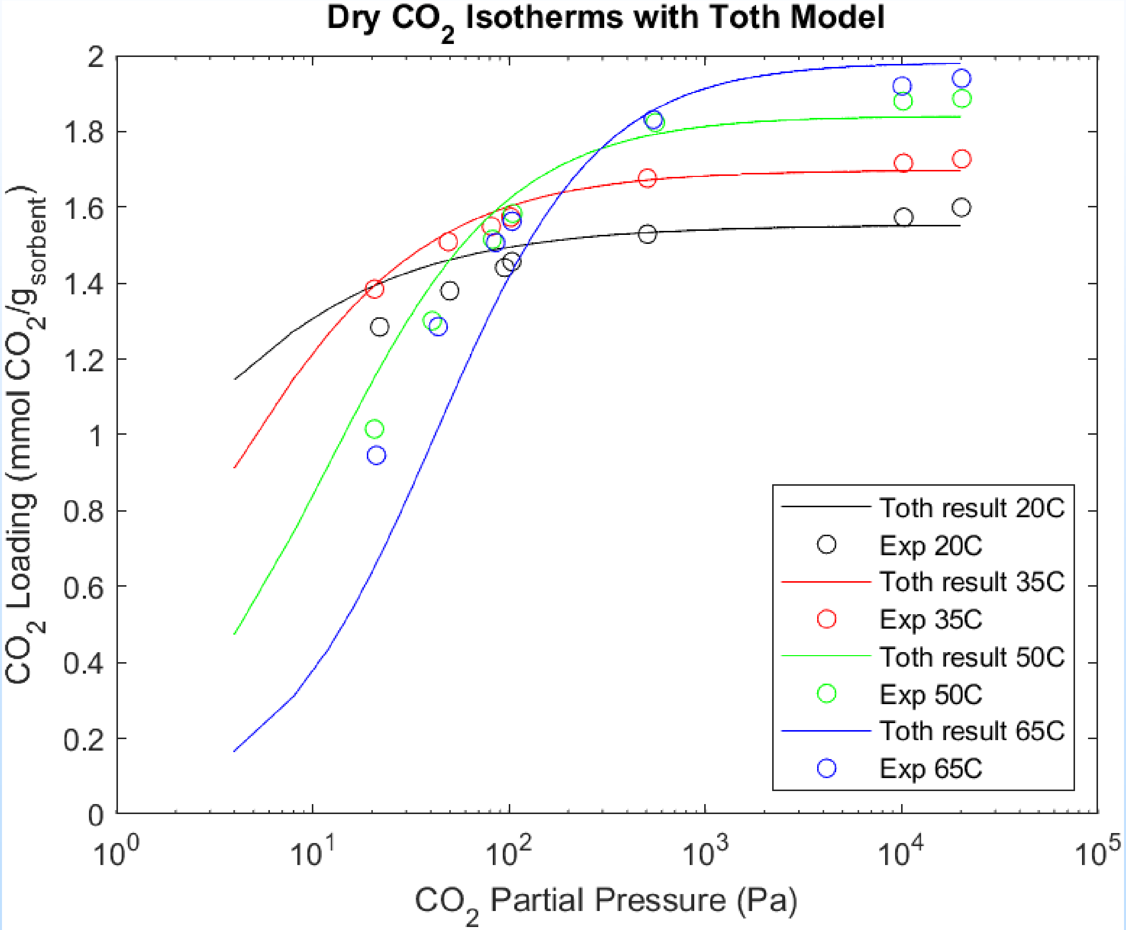




*Pre-saturation using humid N_2 stream

*Measured in a custom-built fixed bed configuration

Equilibrium Parameters



40 wt% PEI sample

Toth isotherm model for CO_2 adsorption

$$q_{eq,CO_2} = \frac{q_{max,CO_2} b P_{CO_2}}{\left(1 + \left(bP_{CO_2}\right)^n\right)^{1/n}}$$

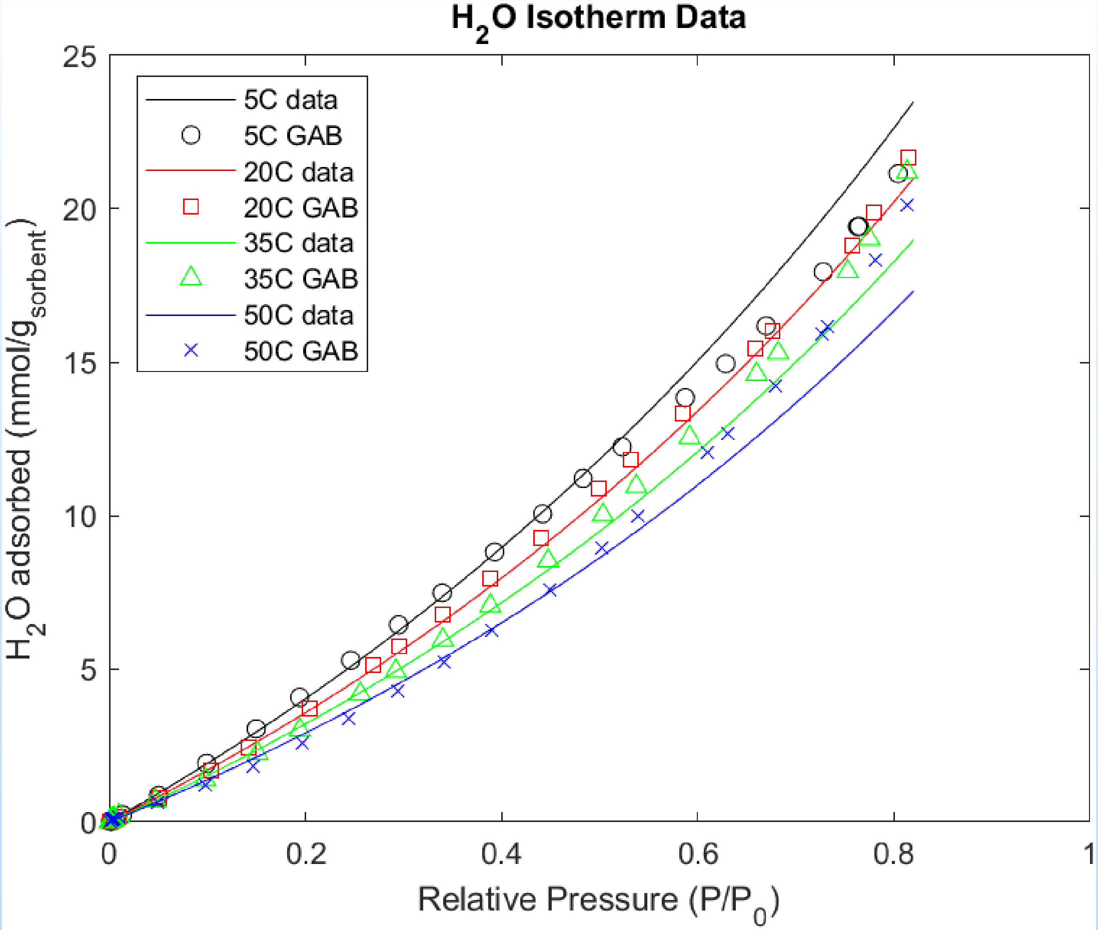
$$q_{max,CO_2} = q_{max,0} \exp(\chi(1 - \frac{T_0}{T}))$$

$$b = b_0 \exp(\frac{\Delta H}{RT_0}\left(\frac{T_0}{T} - 1\right))$$

$$n = A + B(1 - \frac{T_0}{T})$$

Toth isotherm parameters	
$q_{max,0}$ (mol CO_2/kg sorbent)	1.55
χ	1.83
b_0 (Pa^{-1})	2.30
ΔH (kJ/mol CO_2)	84.5
A	0.67
B	2.85

Equilibrium Parameters



40 wt% PEI sample

GAB isotherm model for H_2O adsorption

$$q_{eq,H_2O}(p, T) = \frac{q_{m,H_2O} K C p}{(1 - Kp)\big(1 - Kp(1 - C)\big)}$$

$$C = C_0 \exp\left(\frac{\Delta H_c}{RT}\right)$$

$$K = K_0 \exp\left(\frac{\Delta H_K}{RT}\right)$$

GAB isotherm parameters	
q_{m,H_2O} (mol H_2O/kg sorbent)	15.9
C_0	0.2
ΔH_c (kJ/mol H_2O)	6.5
K_0	0.4
ΔH_k (kJ/mol H_2O)	-1.0

Kinetic Parameters

Linear driving force approximation for CO_2 adsorption

CO_2 adsorption on surface & bulk amine sites

$$\frac{\partial q_1}{\partial t} = \boldsymbol{K}_{\mathbf{ov},\boldsymbol{k}}\left(q_{eq,CO_2}\psi - q_1\right)$$

$$\frac{\partial q_2}{\partial t} = \boldsymbol{K}_{\mathbf{ov},\boldsymbol{p}}\left(q_{eq,CO_2}(1-\psi) - q_2\right)$$

$$\boldsymbol{q}_{\mathbf{tot},\boldsymbol{CO_2}} = \boldsymbol{q_1} + \boldsymbol{q_2}$$

ψ: ratio between the surface amine sites to the total amine sites

Mass transfer resistance in series

$$\frac{\mathbf{1}}{\boldsymbol{K}_{\mathbf{ov},\boldsymbol{k}}} = \frac{1}{K_g} + \frac{1}{K_c} + \frac{1}{K_{s,k}}$$

$$\frac{\mathbf{1}}{\boldsymbol{K}_{\mathbf{ov},\boldsymbol{p}}} = \frac{1}{K_g} + \frac{1}{K_c} + \frac{1}{K_{s,k}} + \frac{1}{K_{s,p}}$$

$\frac{1}{K_g}$: External mass transfer resistance

$$K_g = \frac{2k_g}{d_0\rho_c\frac{\partial q_{eq,CO_2}}{\partial C_g}}$$

$$K_{s,k} = \frac{15D_K}{r_s^2\rho_s\frac{\partial q_{eq,CO_2}}{\partial C_g}(1-\varepsilon_{module})\psi}$$

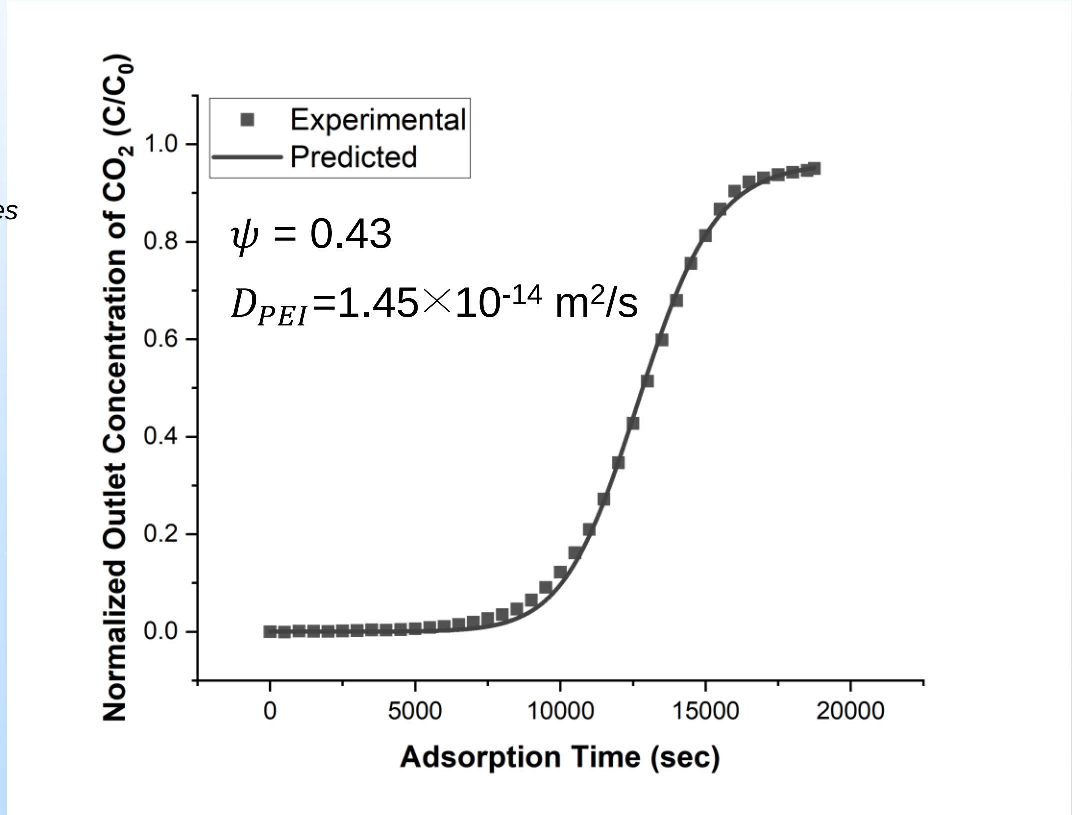
$\frac{1}{K_c}$: interparticle mass transfer resistance

$$K_c = \frac{12\varepsilon_c D_m}{{d_0}^2\rho_c\frac{\partial q_{eq,CO_2}}{\partial C_g}(1-\varepsilon_{module})}$$

$\frac{1}{K_{s,k}}, \frac{1}{K_{s,p}}$: intraparticle mass transfer resistance

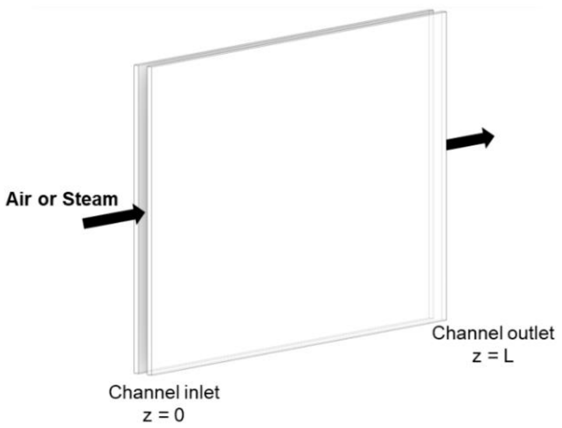
$$K_{s,p} = \frac{15D_{PEI}}{r_s^2\rho_c\frac{\partial q_{eq,CO_2}}{\partial C_g}(1-\varepsilon_{module})(1-\psi)}$$

Fitted curve of the kinetic model and experimental data at 35 °C, dry CO_2 adsorption

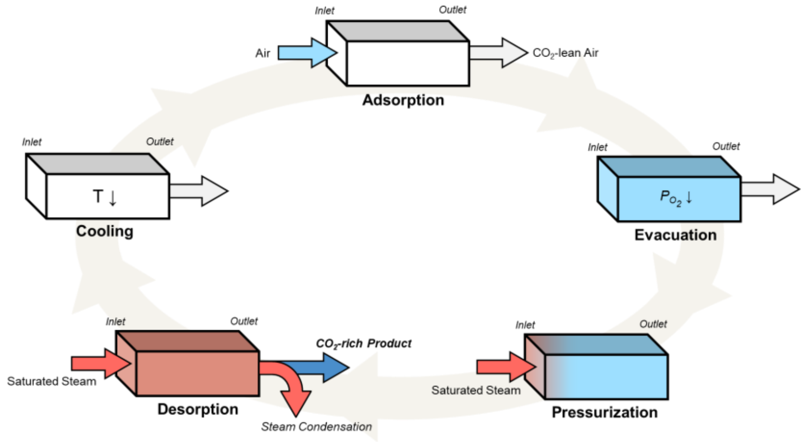


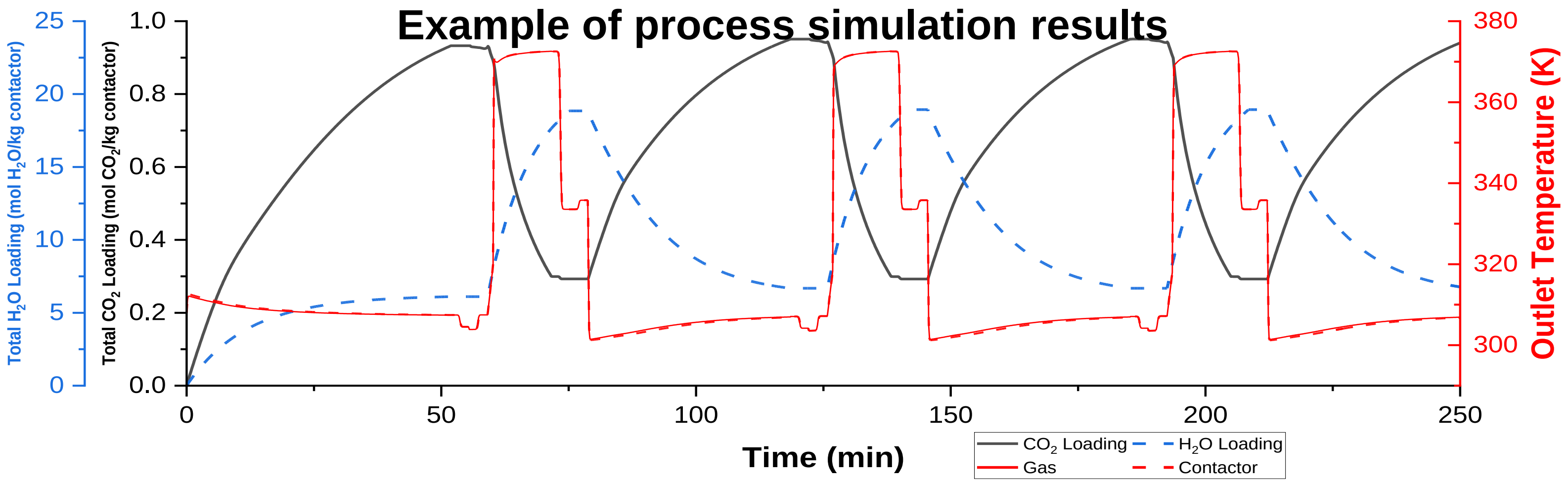
Process model for laminate contactors

1D transient mass, energy and momentum balance with mathematically derived mass transfer model



Steam-assisted temperature vacuum swing adsorption (S-TVSA) process model





Bench-scale TVSA DAC system design

Schematic process of air pretreatment system and bench-scale DAC contactor system

Air pretreatment system

Direct Air → 0.1 – 3.0 m/s, -20 – 35°C, 0 – 80 RH% →

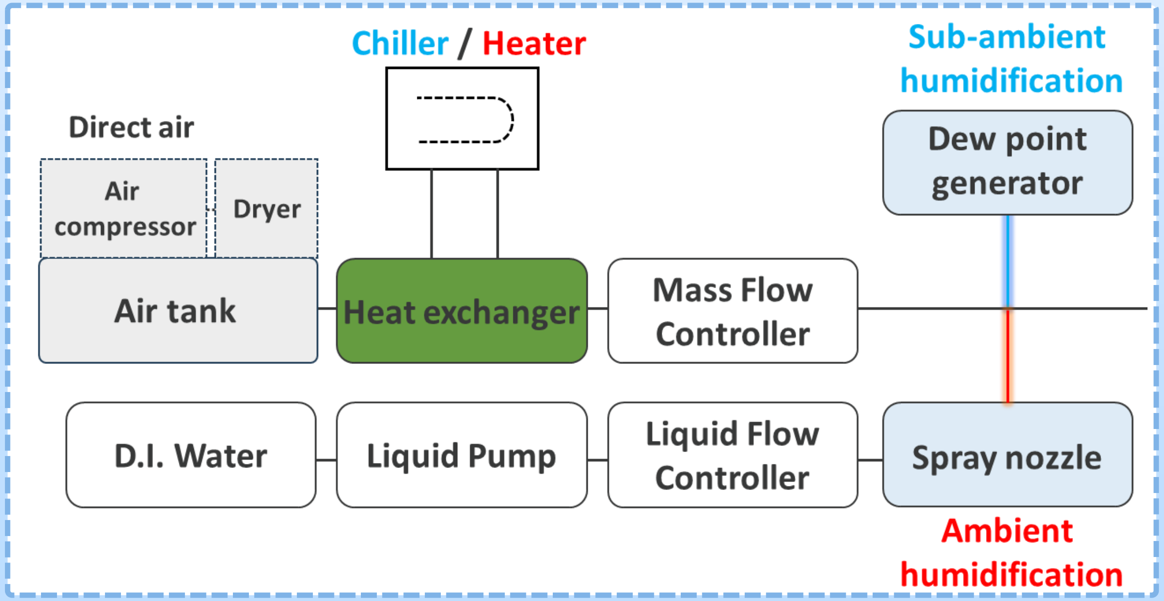
Flow rate/Temperature/Relative humidity control

Steam-TVSA DAC system

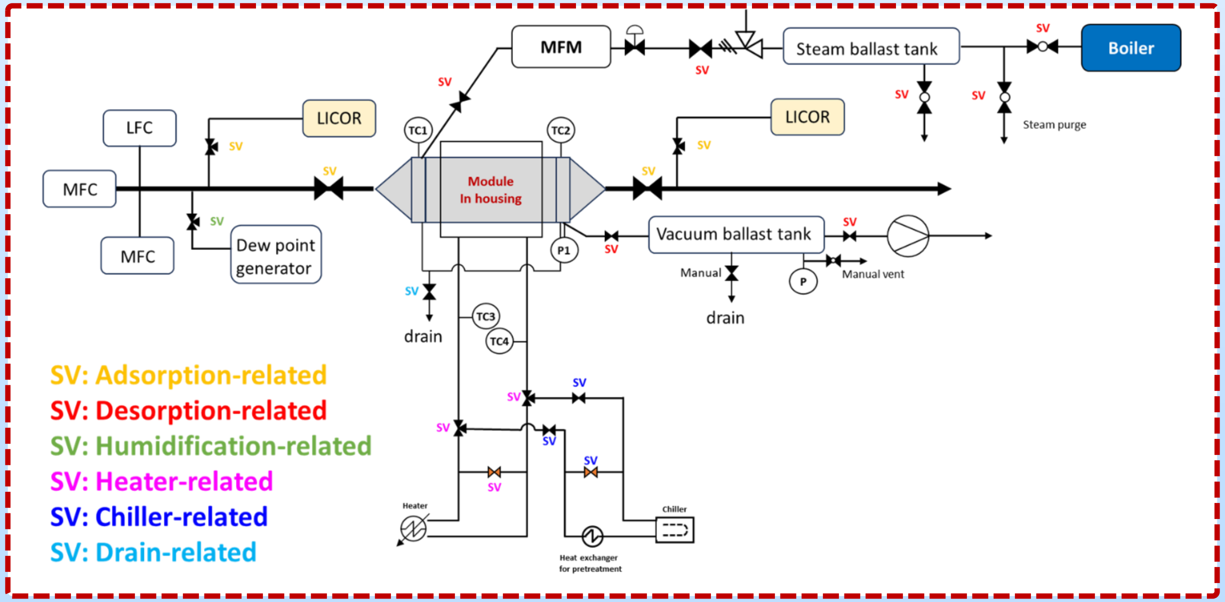
Contactor module, Housing, Detectors → CO_2 removed Air

DAC process assessment

Air pretreatment system



Steam-TVSA DAC system

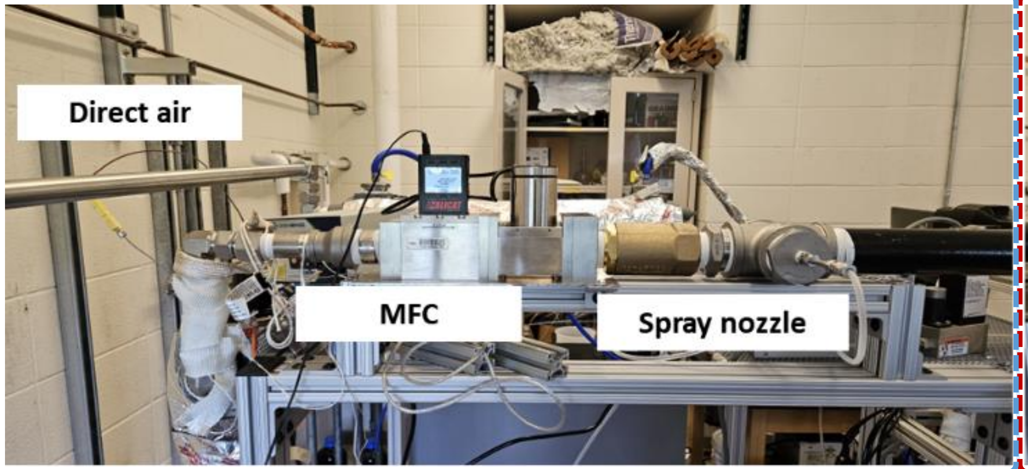


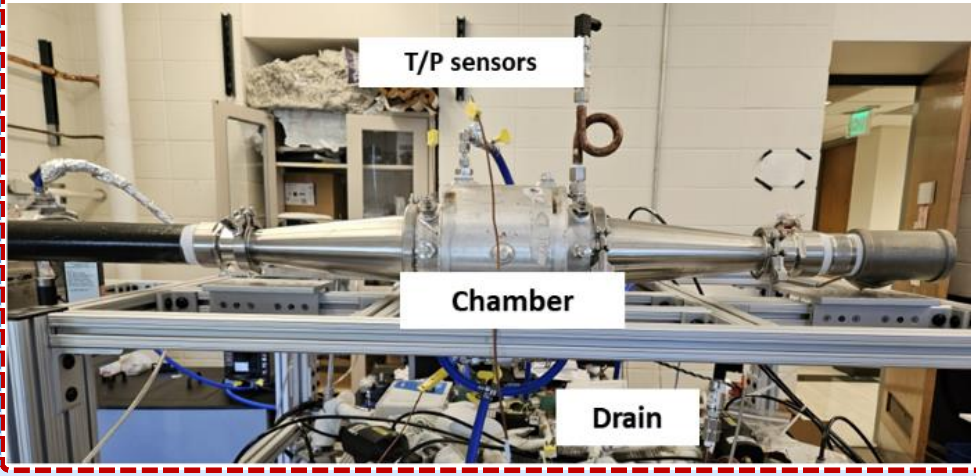
Setup of the Bench-scale DAC system

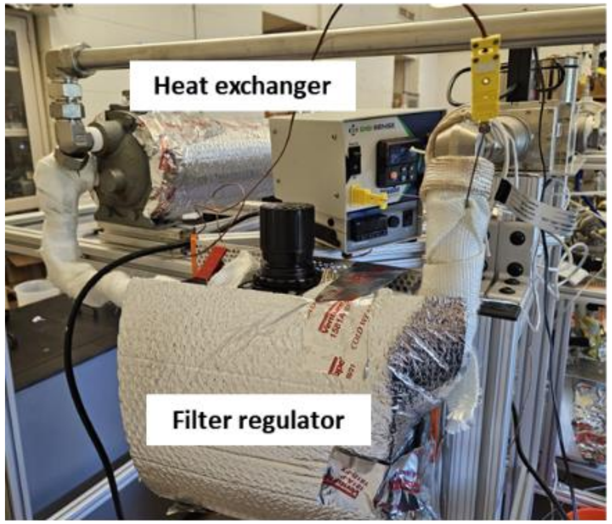
The physical setup of the DAC system in the laboratory

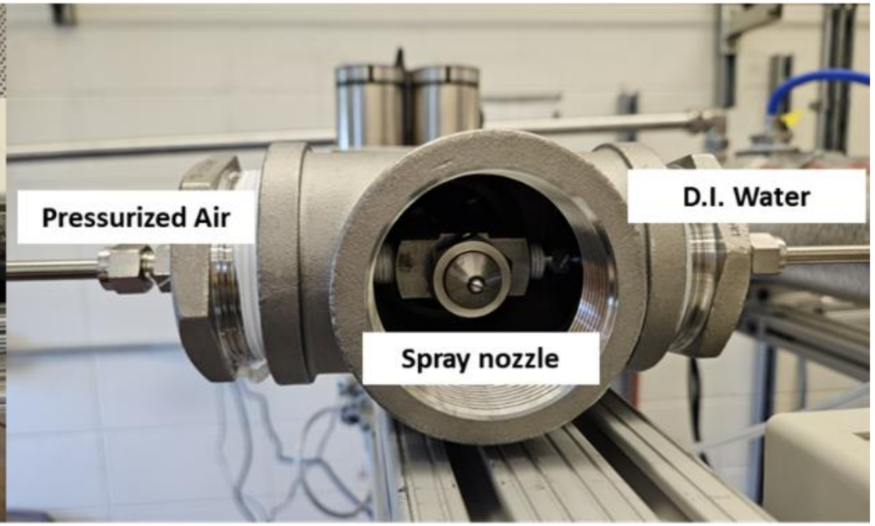
Air pretreatment system

Steam-TVSA DAC system

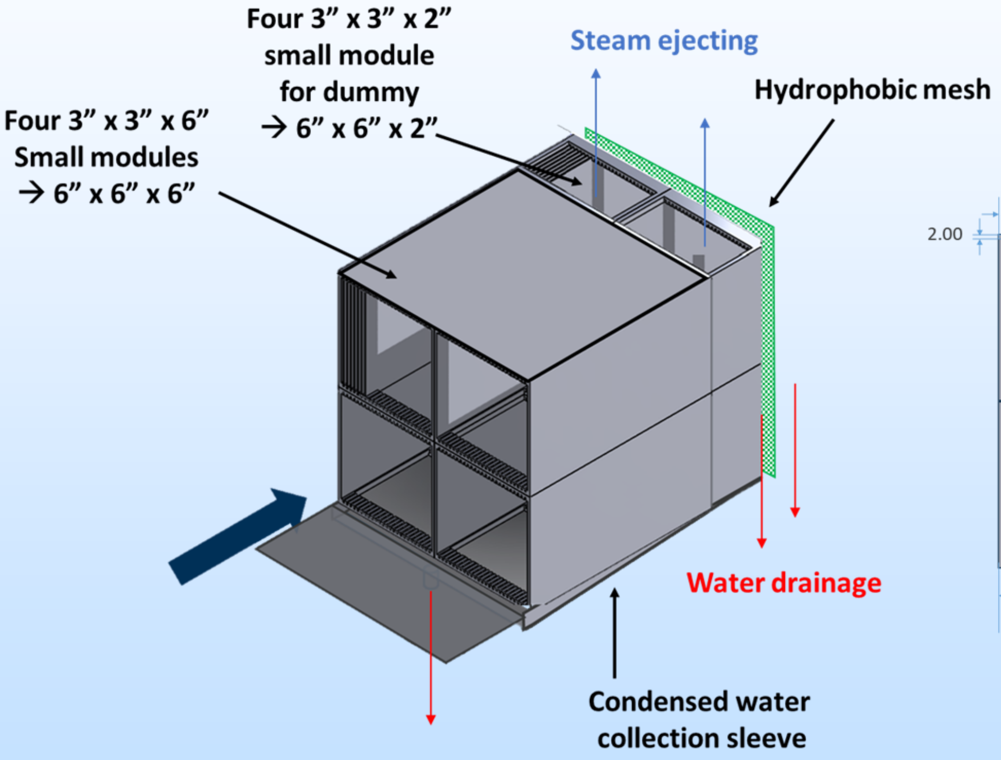




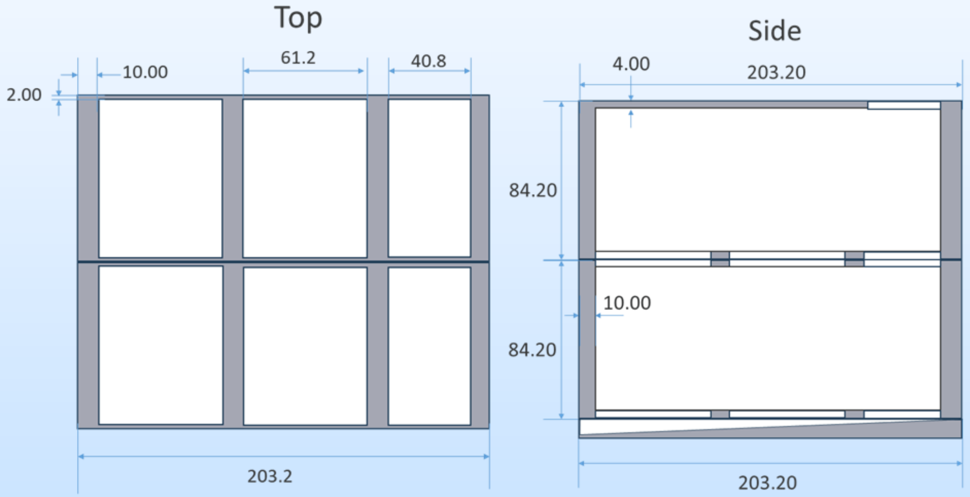




Design and dimension of contactor module



Contactor module with dummy

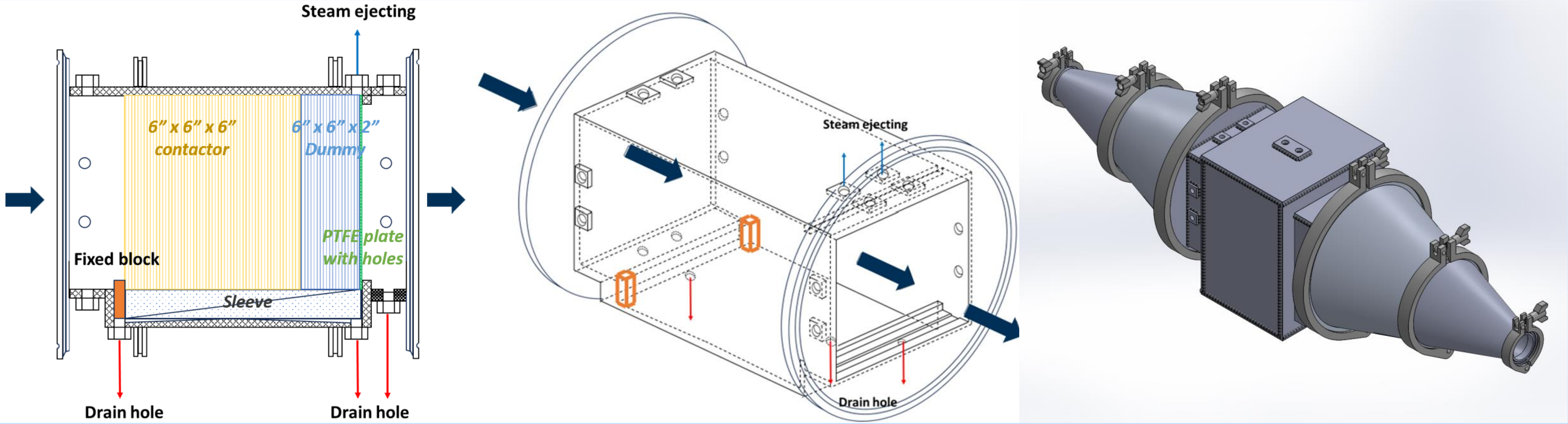


Cross sectional dimension (mm)

3d-printed laminate module to accommodate 3” height -6” length laminate sheets

Bench-scale housing

Target design and dimension of bench-scale housing (Cross-sectional, 3D view)



Quick clamp connectors are used to easily connect the housing to the air pretreatment system.

Summary

a. The evaluation of PEI-infused ePTFE/silica samples under a lab-scale fixed-bed setup for subsequent baseline bench-scale DAC system has been completed.
b. Detailed mass transfer resistance model and process model for DAC process using the laminate contactors have been successfully developed.
c. Both thermodynamics and kinetic parameters of the laminate contactor have been obtained and modeled.
d. Process model based on obtained parameters will be simulated and energy/cost of the process will be evaluated.
e. The bench-scale steam assisted –TVSA DAC system will be evaluated under ambient/sub-ambient dry/humid conditions.