Novel Process That Achieves 10 mol/kg Sorbent Swing Capacity in a Rapidly Cycled Pressure Swing Adsorption Process

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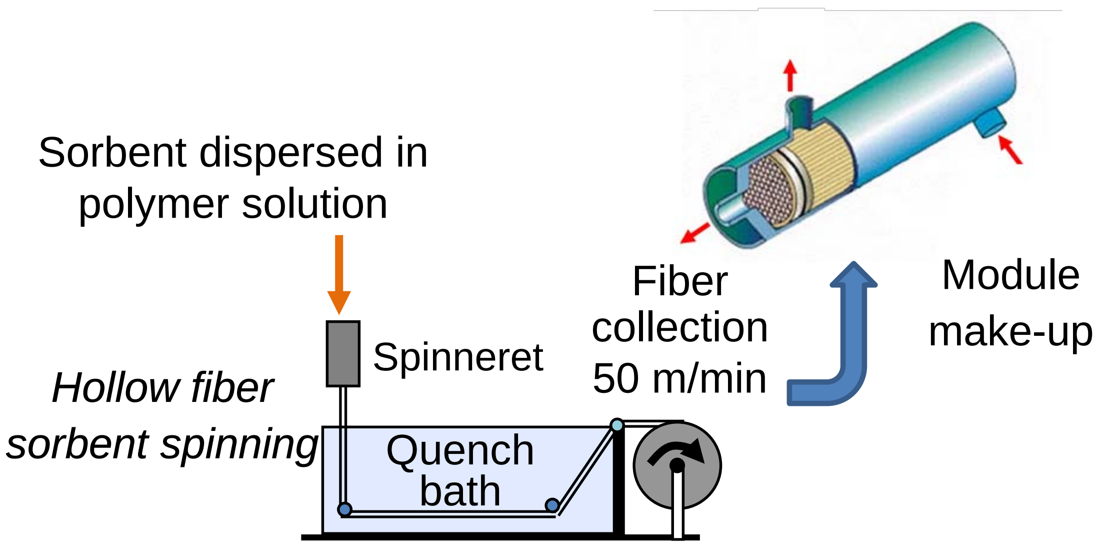
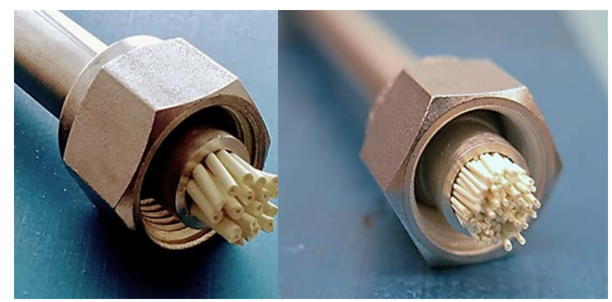
Atlanta, GA 30332





SJA DeWitt, RP Lively et al., *Ann. Rev. Chem. Bio. Eng.* **2018**

AR Sujan, RP Lively et al., *Ind. Eng. Chem. Res.* **2018**, 57(1)

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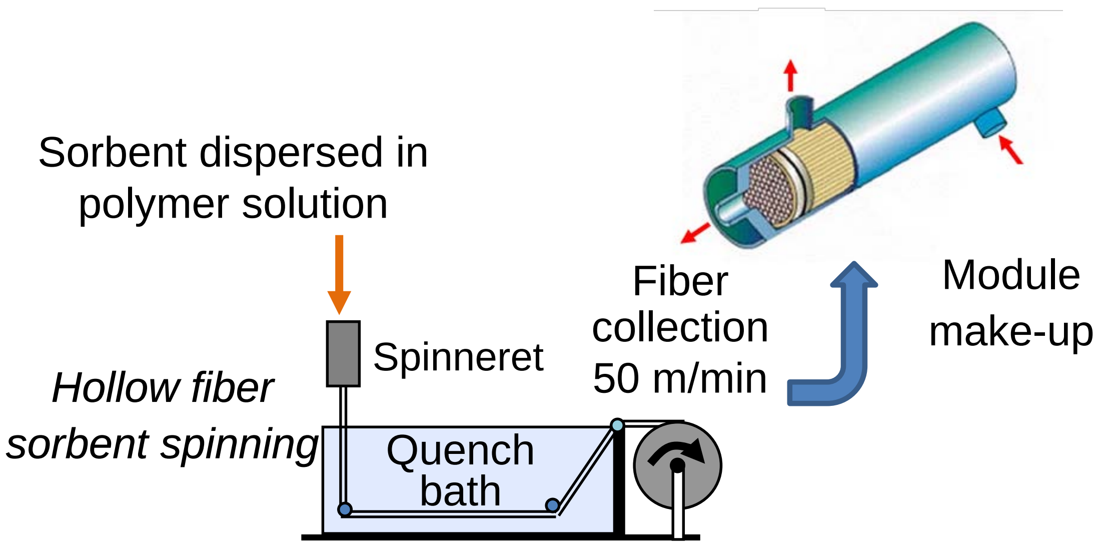
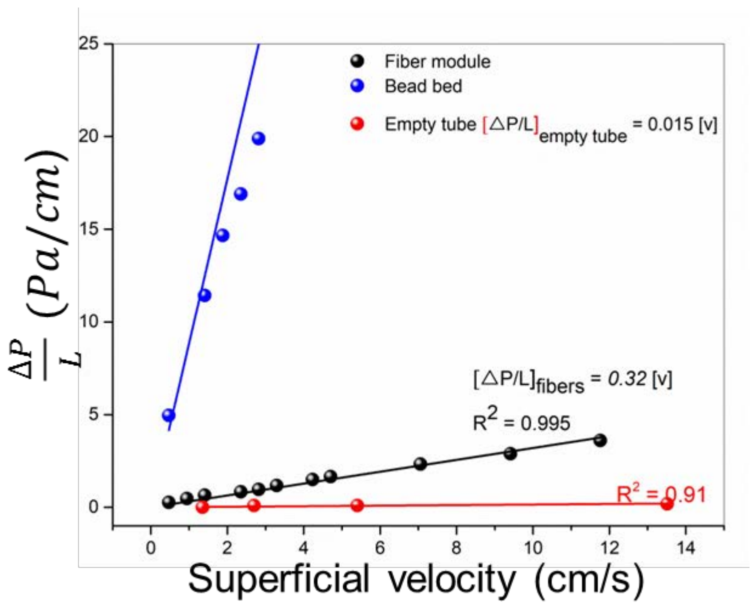
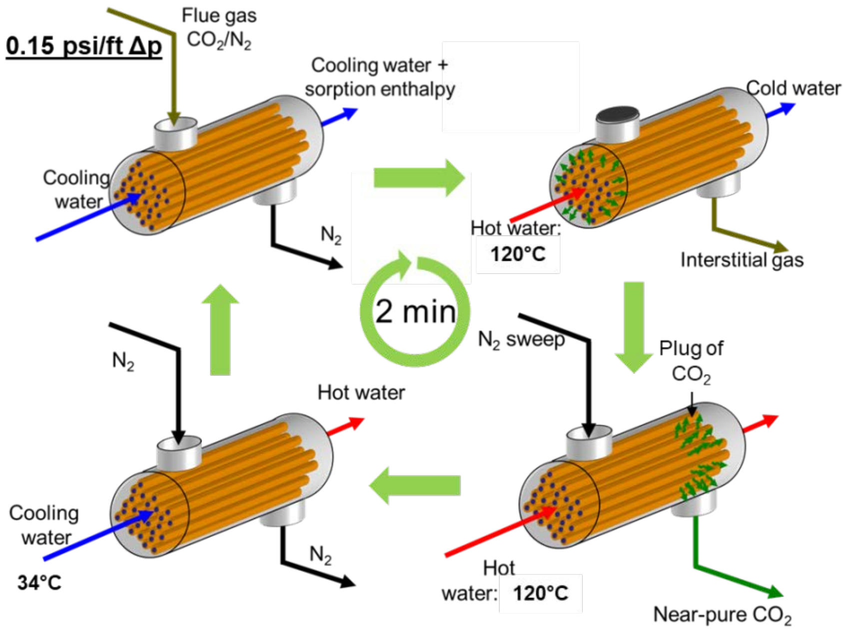


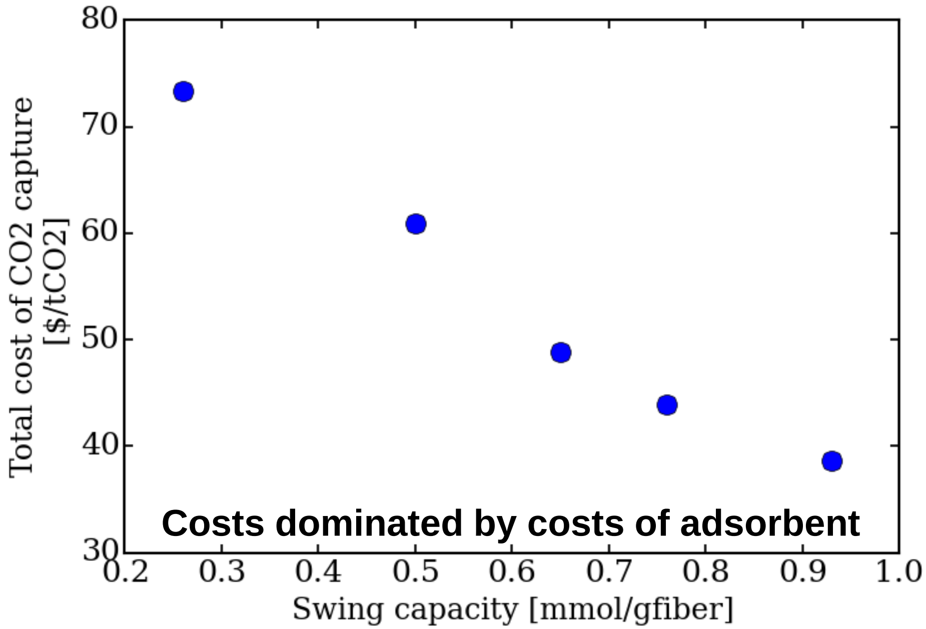


SJA DeWitt, RP Lively et al., *Ann. Rev. Chem. Bio. Eng.* **2018**

AR Sujan, RP Lively et al., *Ind. Eng. Chem. Res.* **2018**, 57(1)

Rapid thermal swing adsorption





Capital cost of RTSA system for NETL 550 MW_e baseline: ~$1B

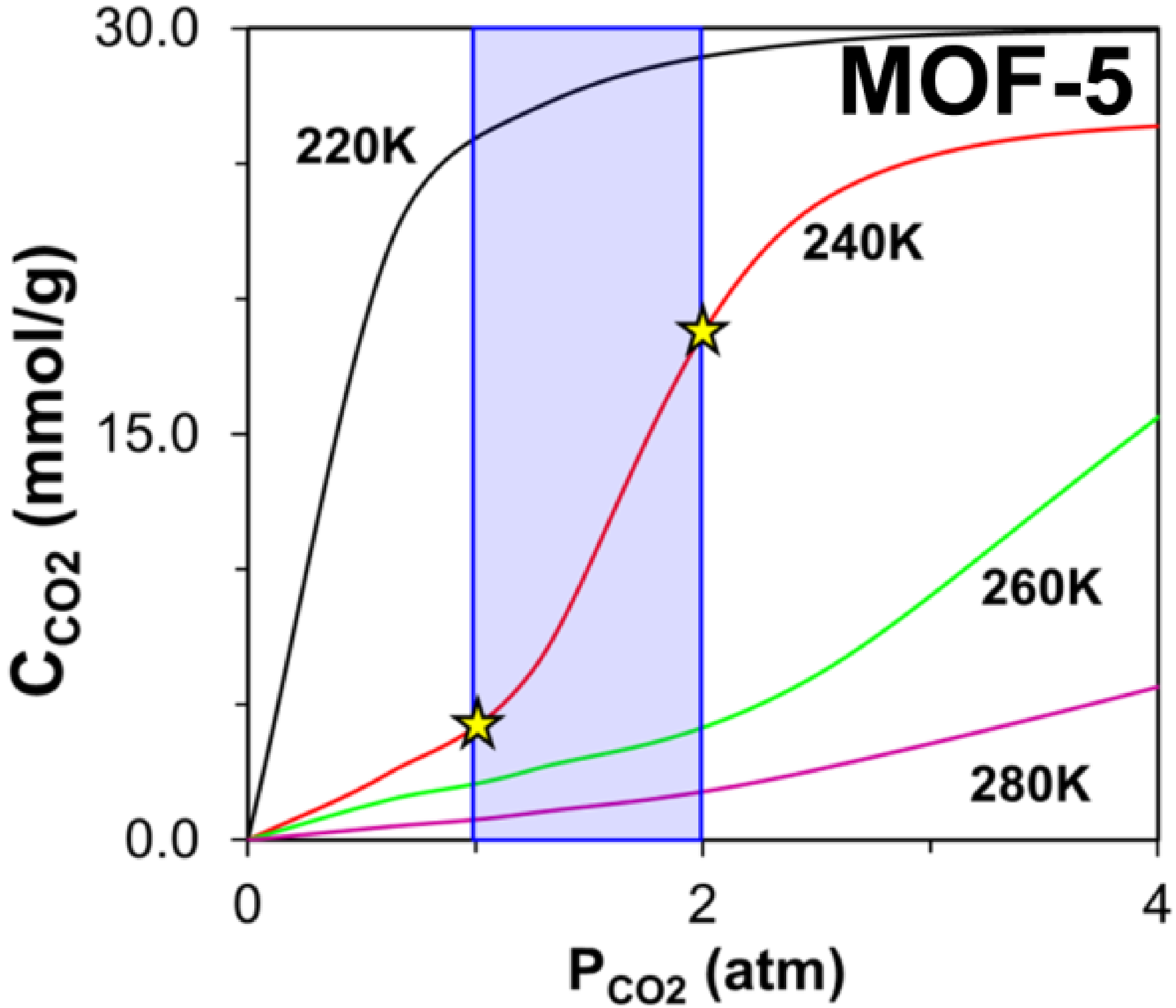
Swing capacity and cycle time are key for driving down <u>capital</u> costs of adsorption-based CO_2 capture systems!

Key question: Can we increase swing capacity by 10x and reduce cycle time by 5x to dramatically drive down adsorbent costs?

RP Lively et al., *U.S. Patent 8,409,332*   WJ Koros, *U.S. Patent 8,658,041*
RP Lively, WJ Koros et al., *Int. J. Greenhouse Gas Control* **2012**, 10(1)
Y Fan, CW Jones et al., *Int. J. Greenhouse Gas Control* 2014, 21, 61-71

Rapidly cycled pressure swing adsorption using MOFs

Cycle times of ~20 seconds are common for industrial RCPSA (>5x faster than RTSA)



JM Simmons, T Yildirim et al., *Energ. Env. Sci.*, 2011, 4(6), 2177-2185

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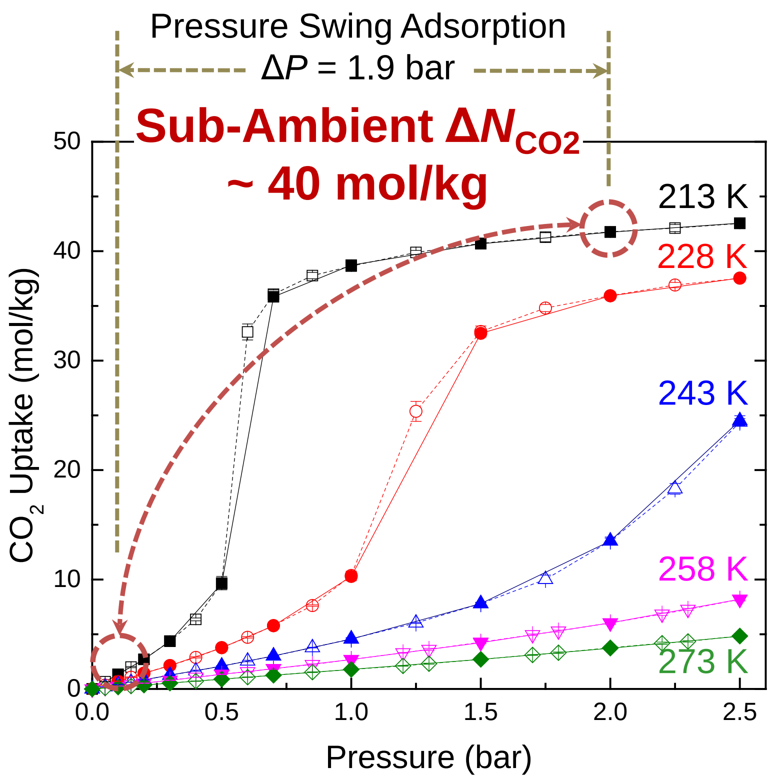

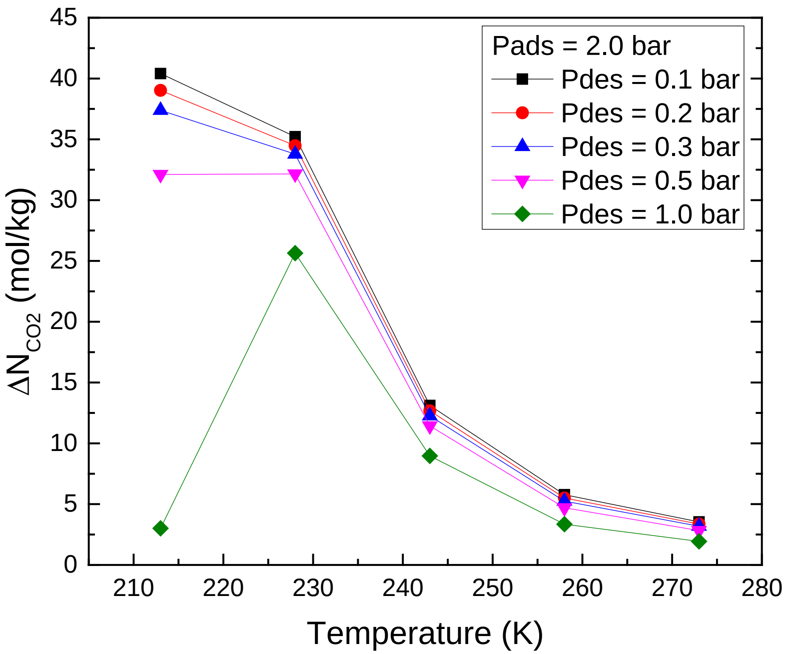

J Park, RP Lively, DS Sholl, *J. Mater. Chem. A.* 2017, 5, 12258-12265

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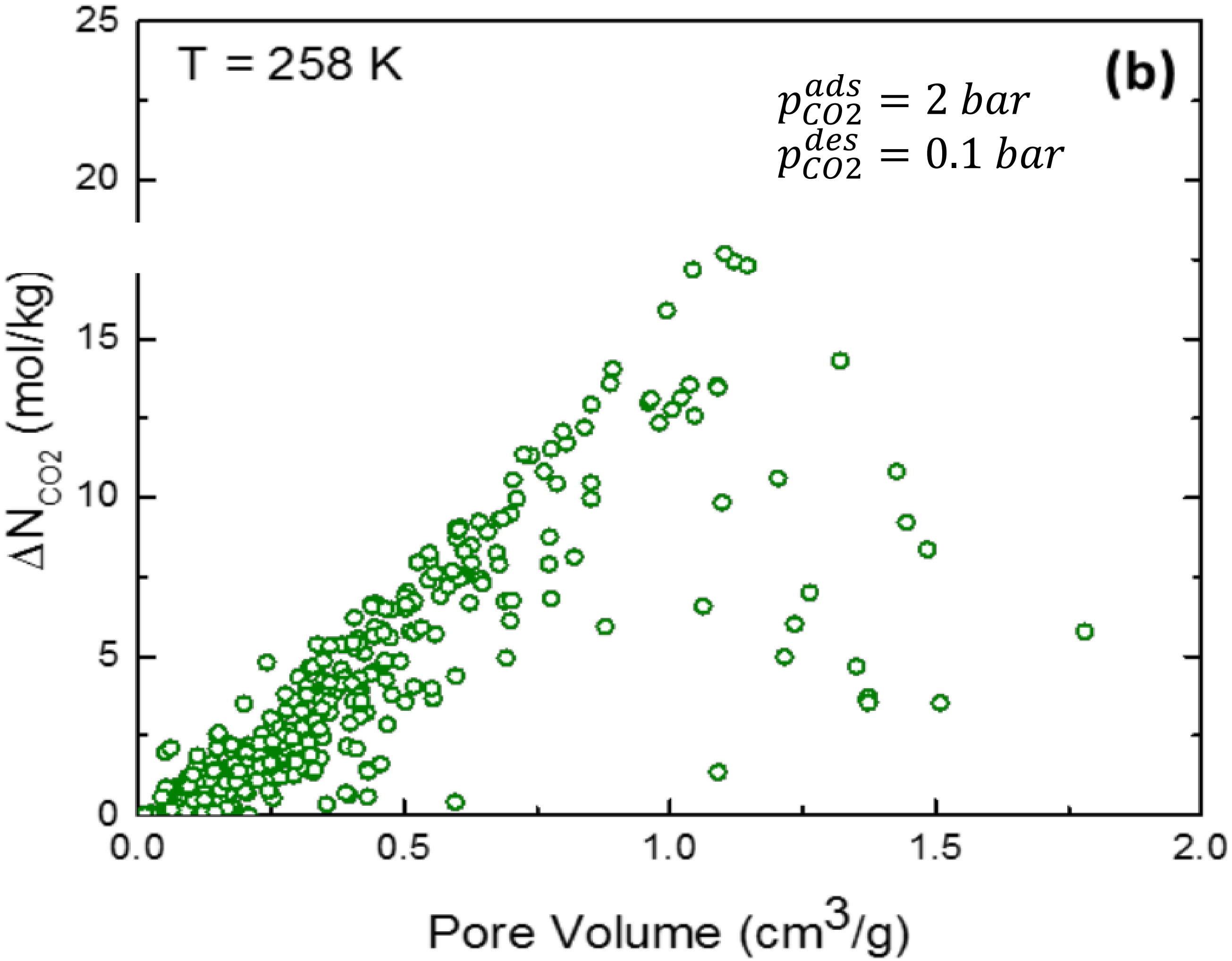
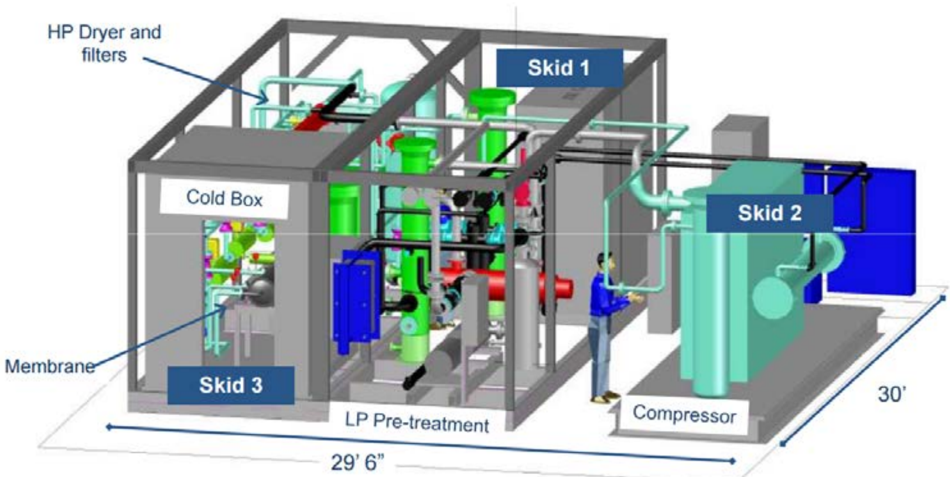


How to economically achieve these pressurized, sub-ambient conditions?

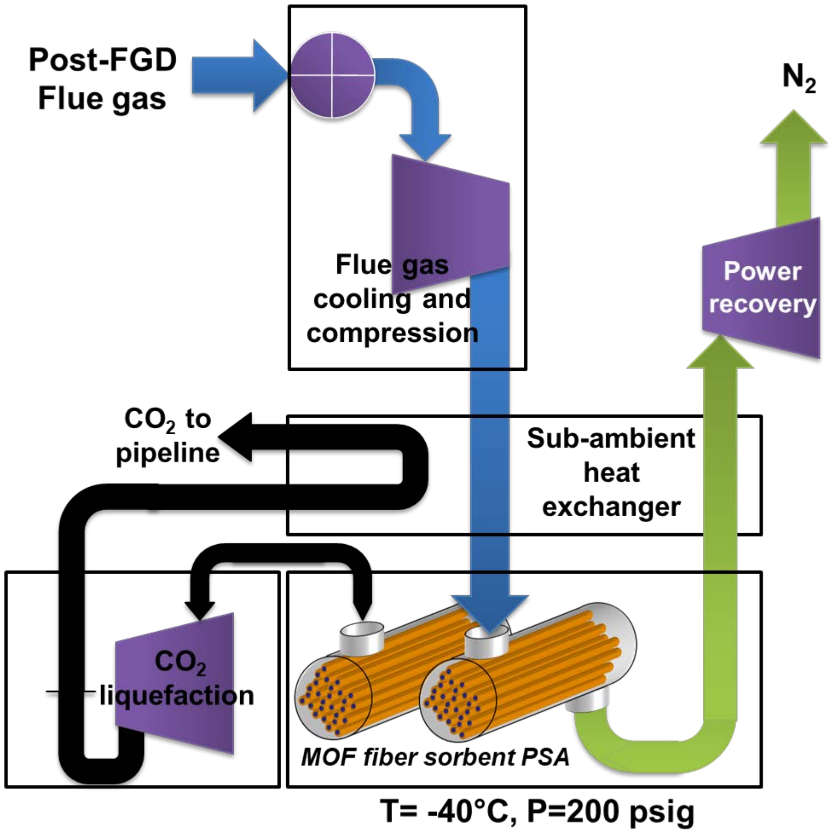
J Park, RP Lively, DS Sholl, *J. Mater. Chem. A.* 2017, 5, 12258-12265

Enabling 10 mol/kg swing capacities via flue gas pretreatment

Air Liquide Sub-Ambient Membrane System



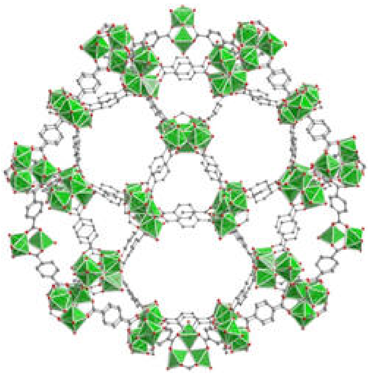
Sub-Ambient Adsorption System



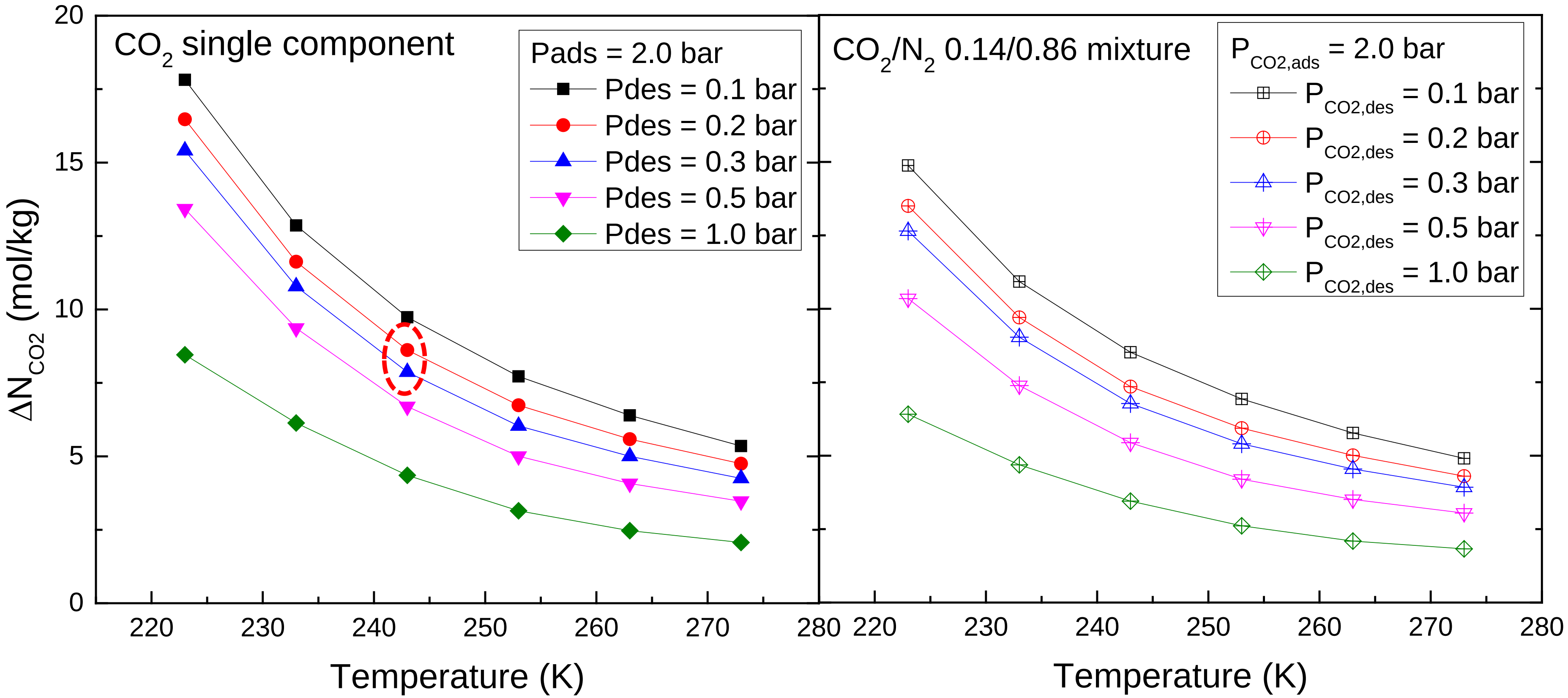
Key parameters: swing capacity & selectivity

D Hasse, S Kulkarni et al., *Energy Procedia*, 2013, 37, 993-1003

MIL-101(Cr) emerged as a promising candidate

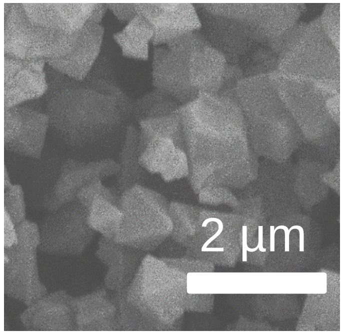


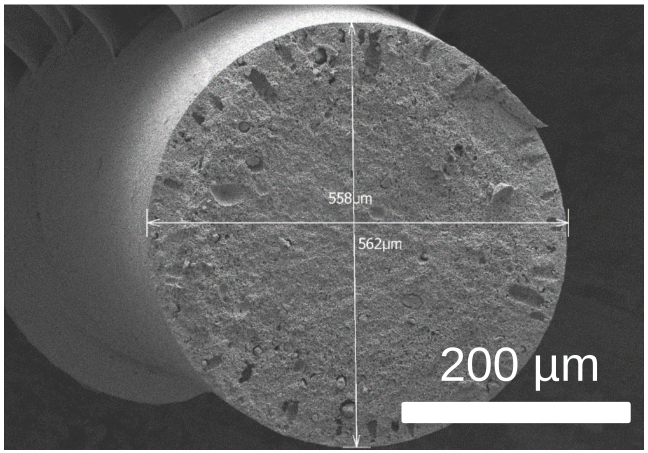
Low cost ligands (benzene dicarboxylate)
Relatively low cost metal centers (chromium nitrate)
Scale-up is straight forward (70% yield on large batches)
Water stable

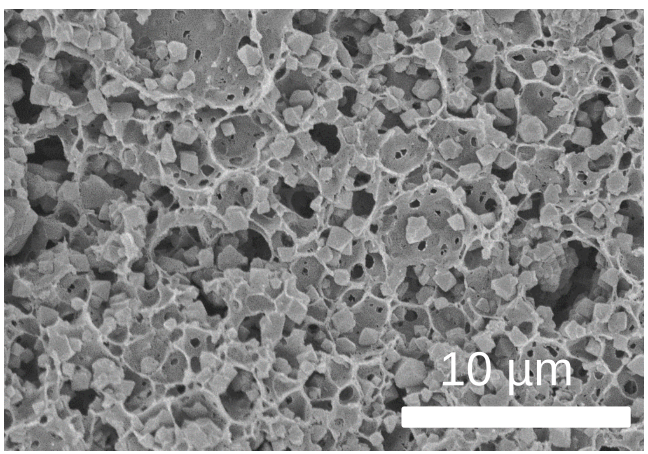


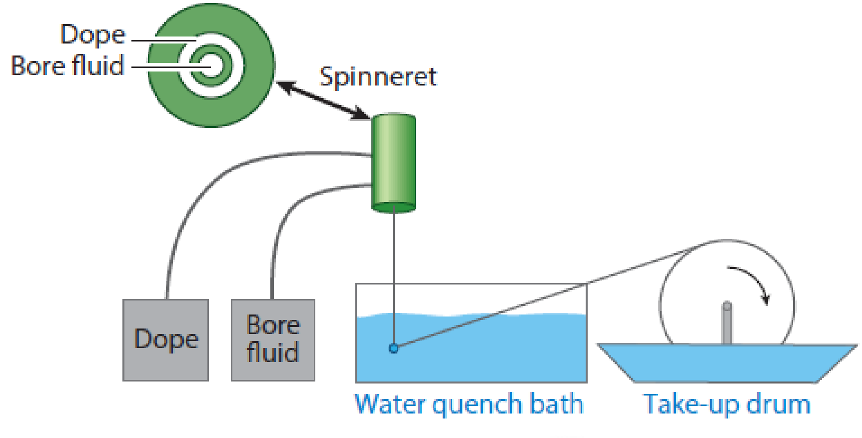
J Park, RP Lively, DS Sholl, *J. Mater. Chem. A.* 2017, 5, 12258-12265
L Hamon, GD Weireled et al., *J. Am. Chem. Soc.* 2009, 131, 8775-8777

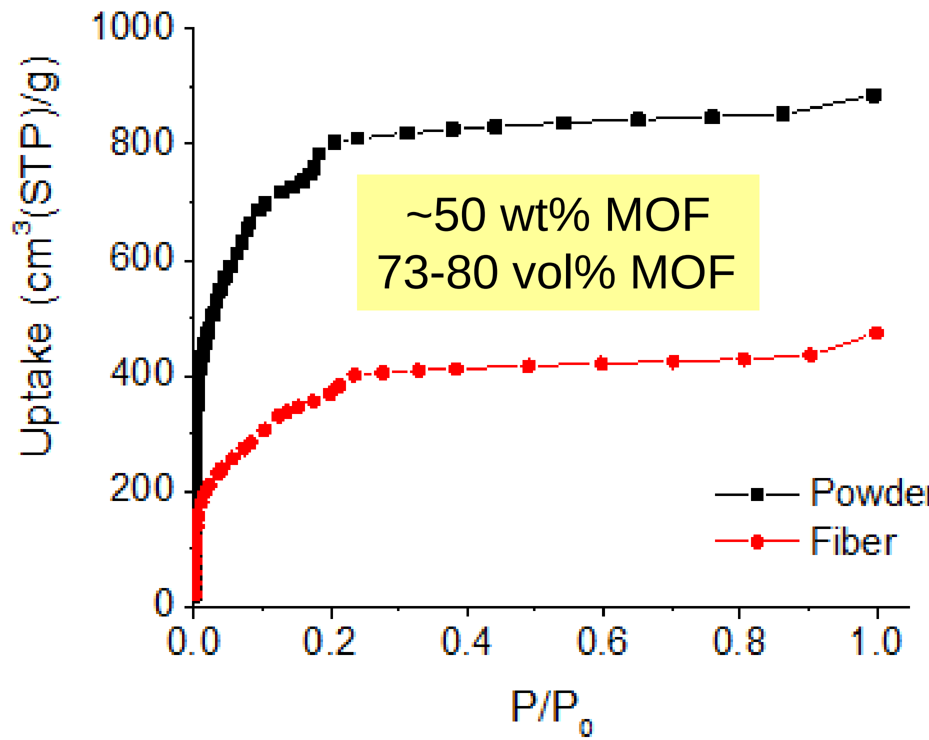
Manufacturing MIL-101(Cr) fiber sorbents



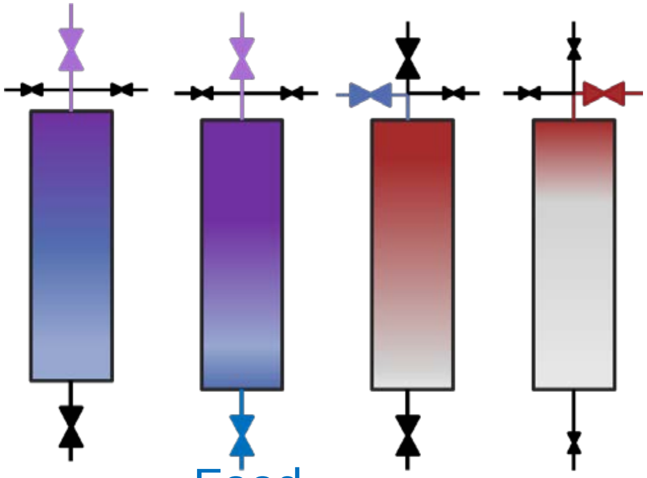








PSA separation of simulated flue gas mixtures



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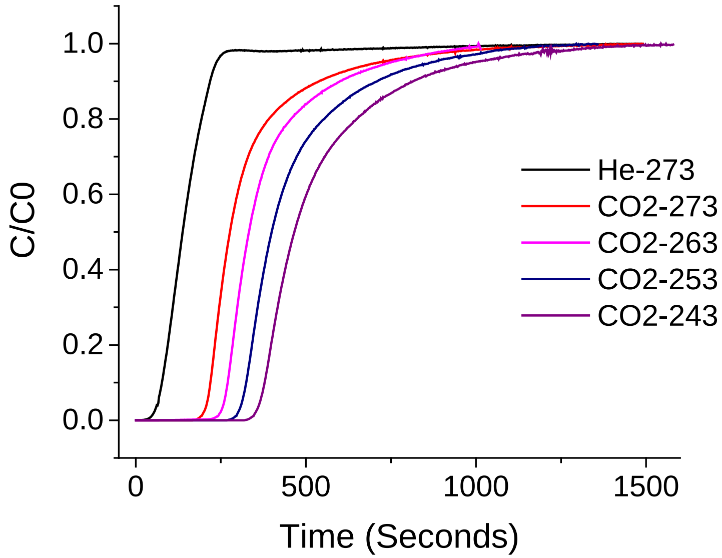
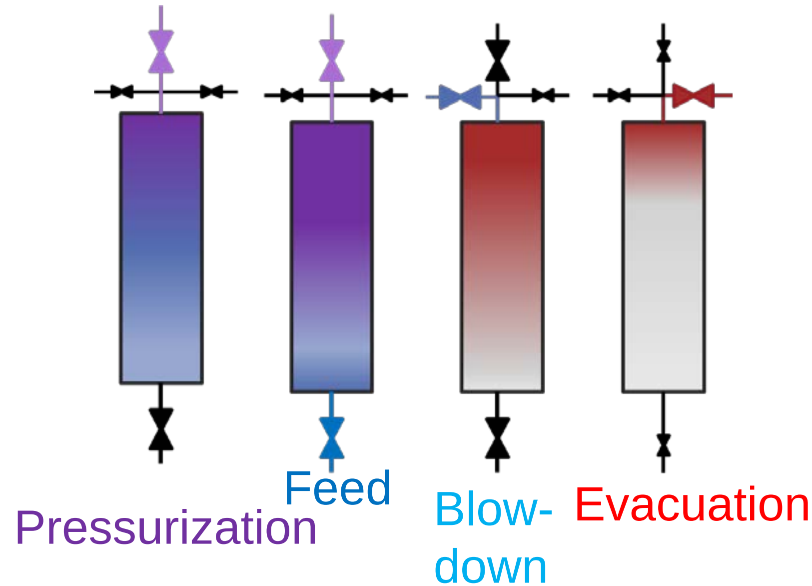
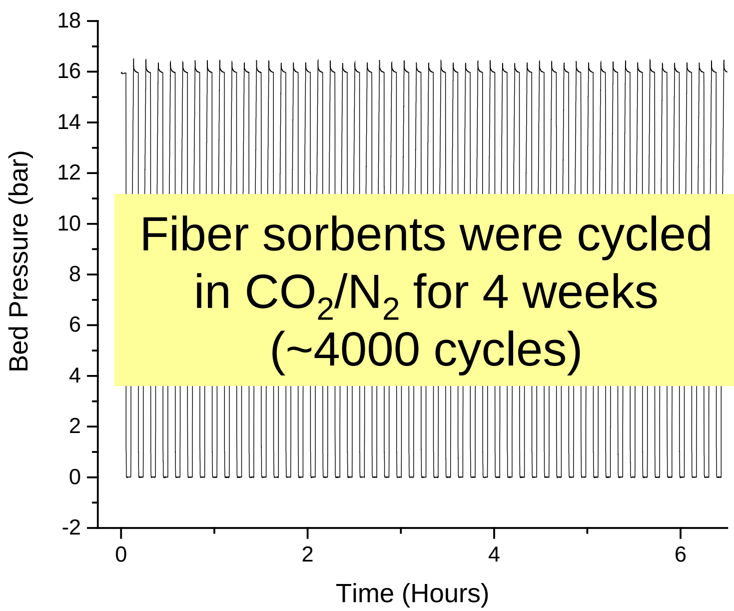
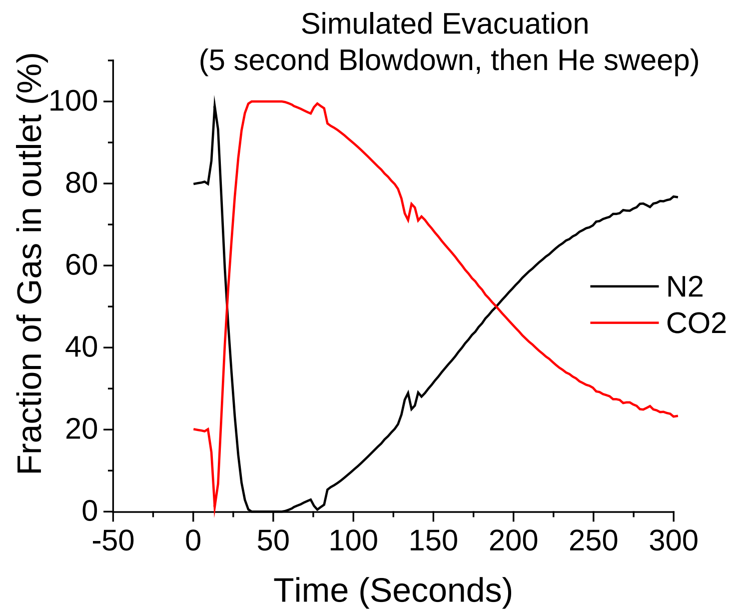
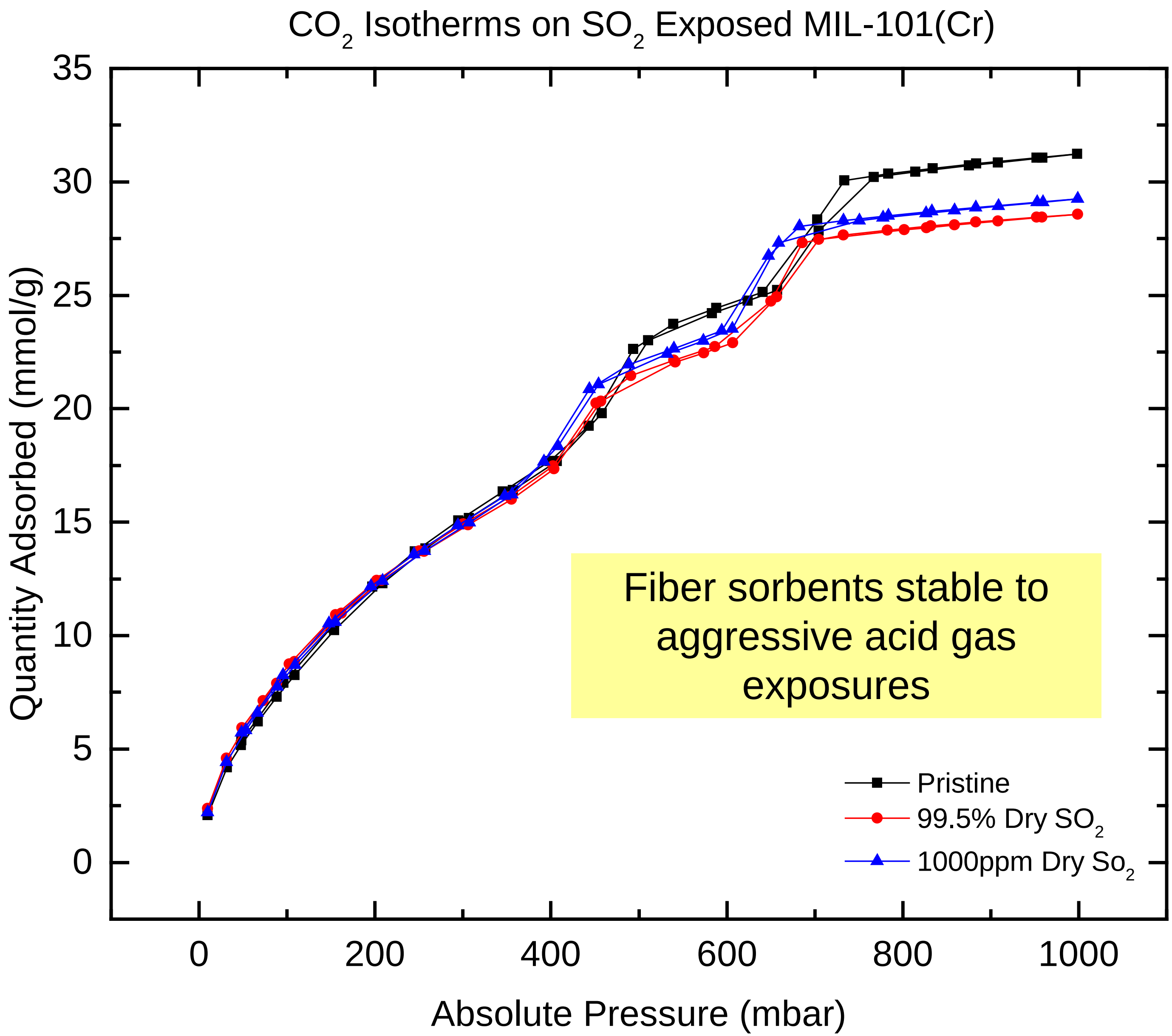








Stability to acid gases



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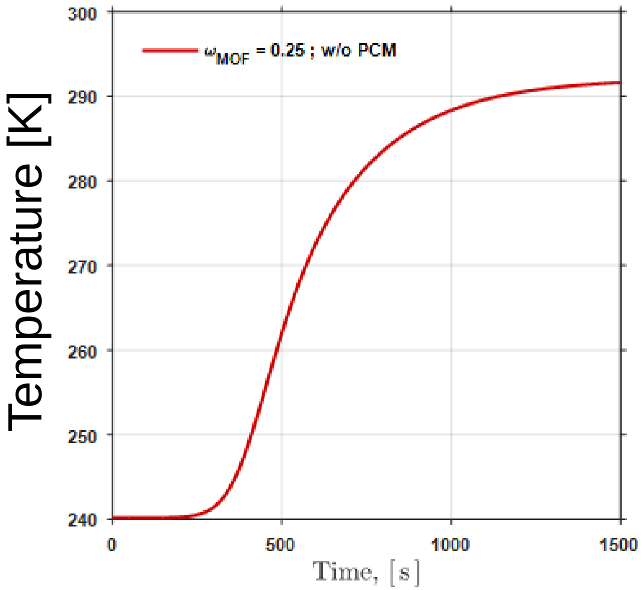
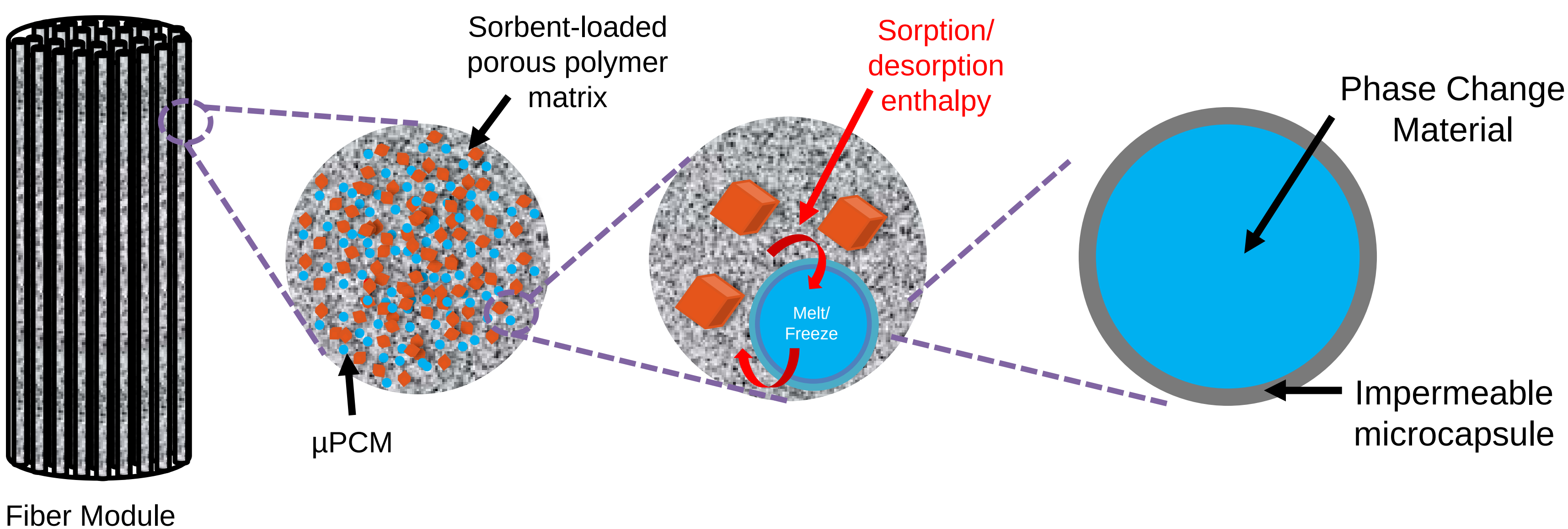
Issues with heat effects



50K increase in temperature during adsorption



SJA DeWitt, RP Lively et al., PCT US18/48110; WO 2019/09908
SJA DeWitt, RP Lively et al., *Ind. Eng. Chem. Res.* 2018, 58(15)

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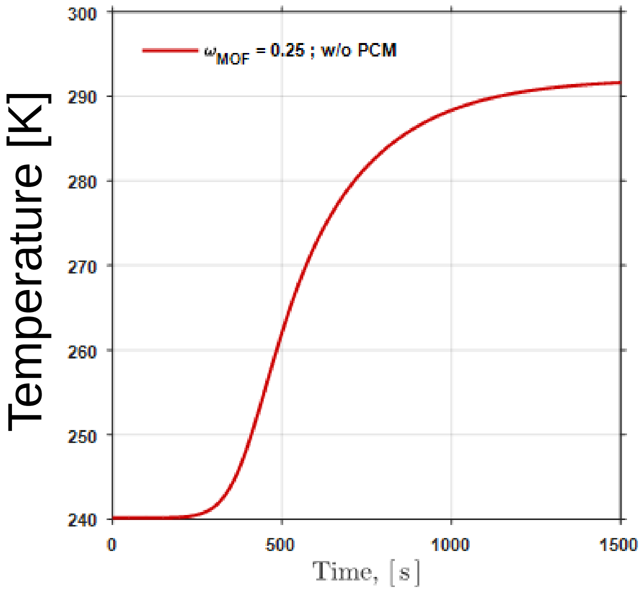

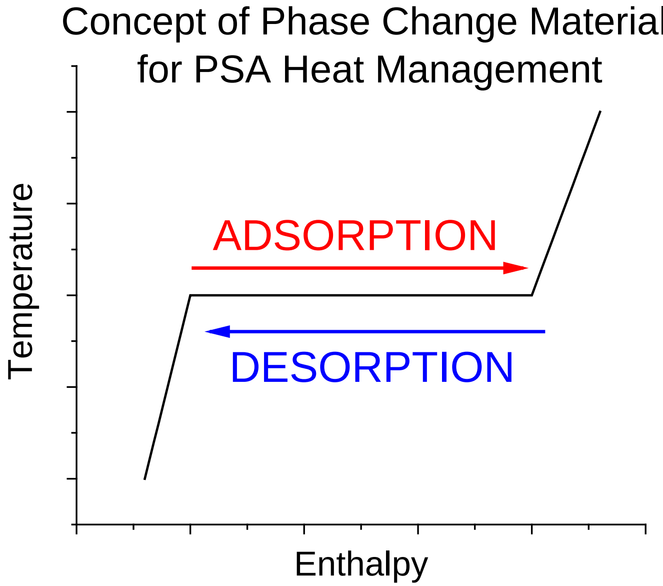

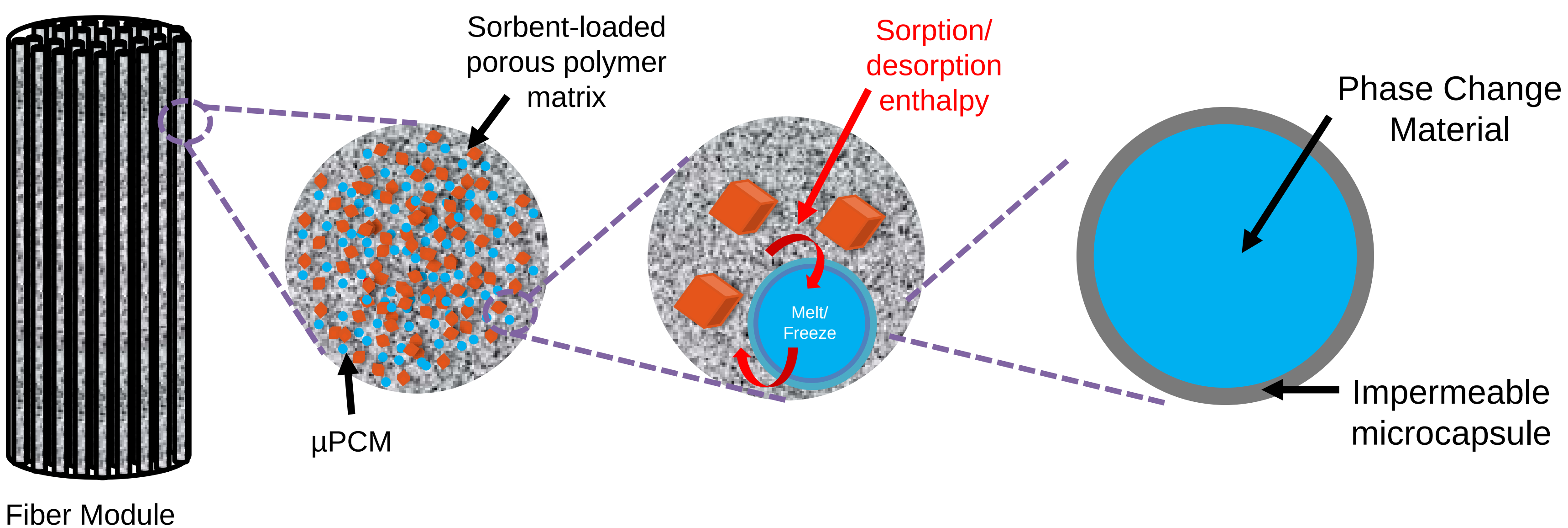

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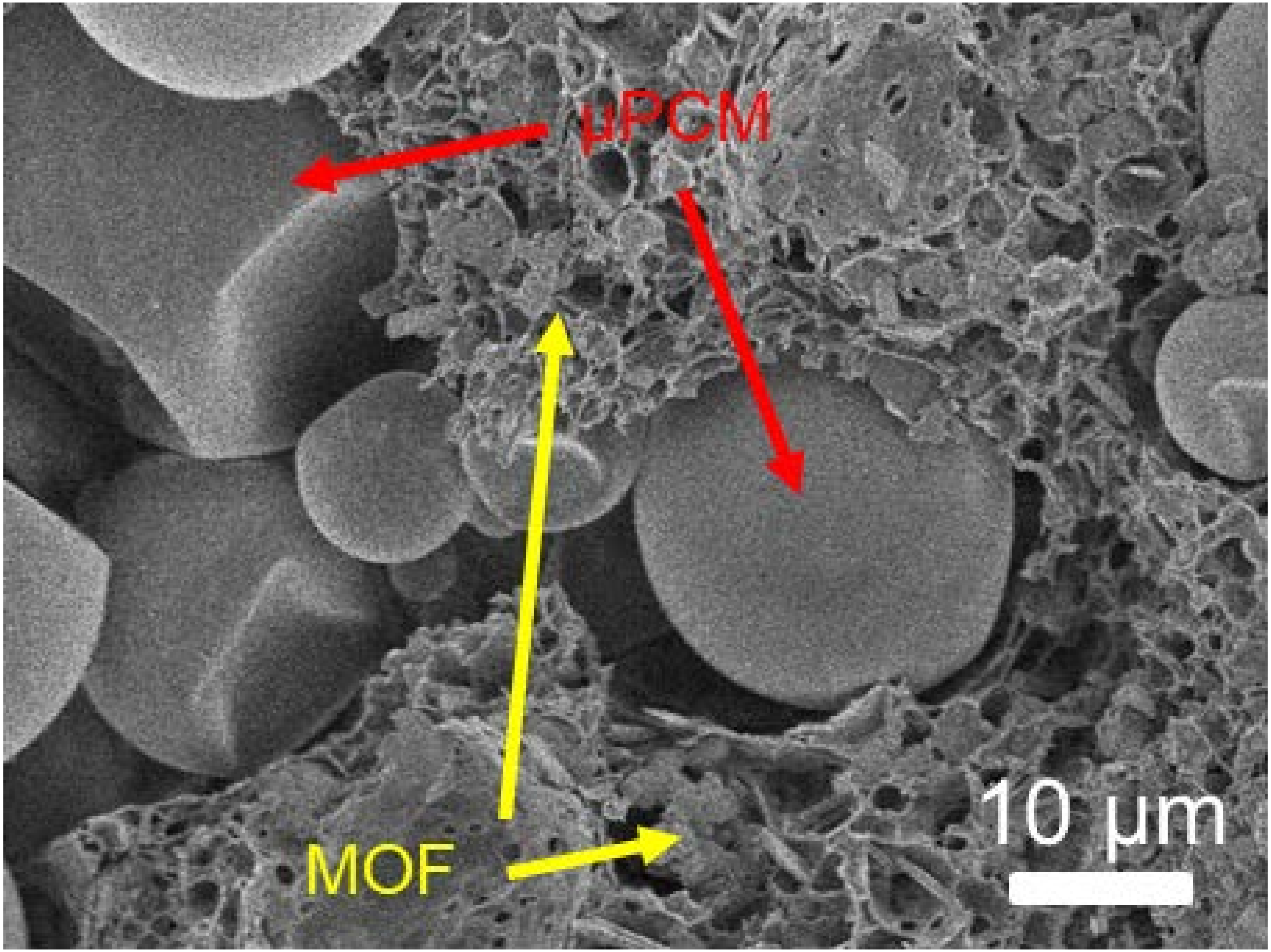
“Passive” thermal management via microPCM capsules



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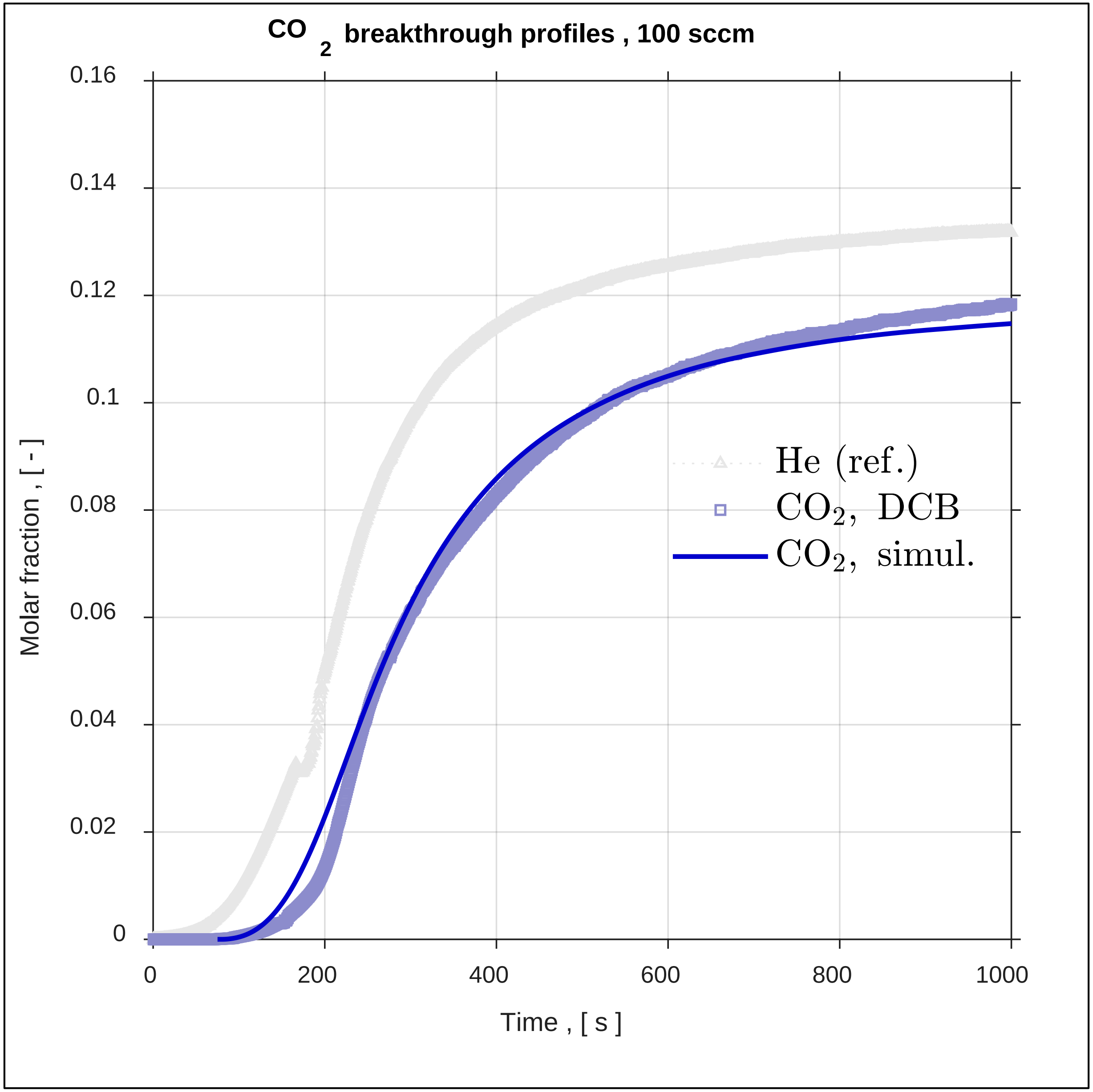

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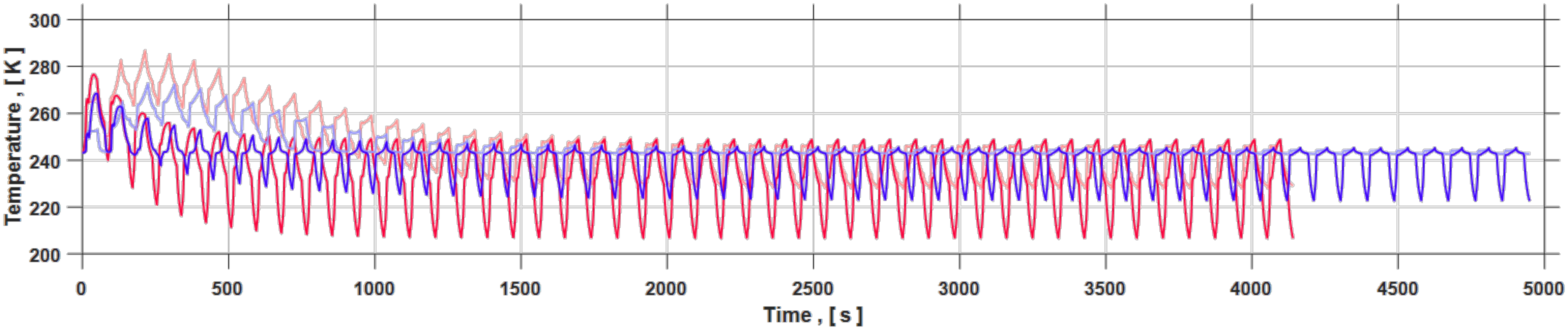
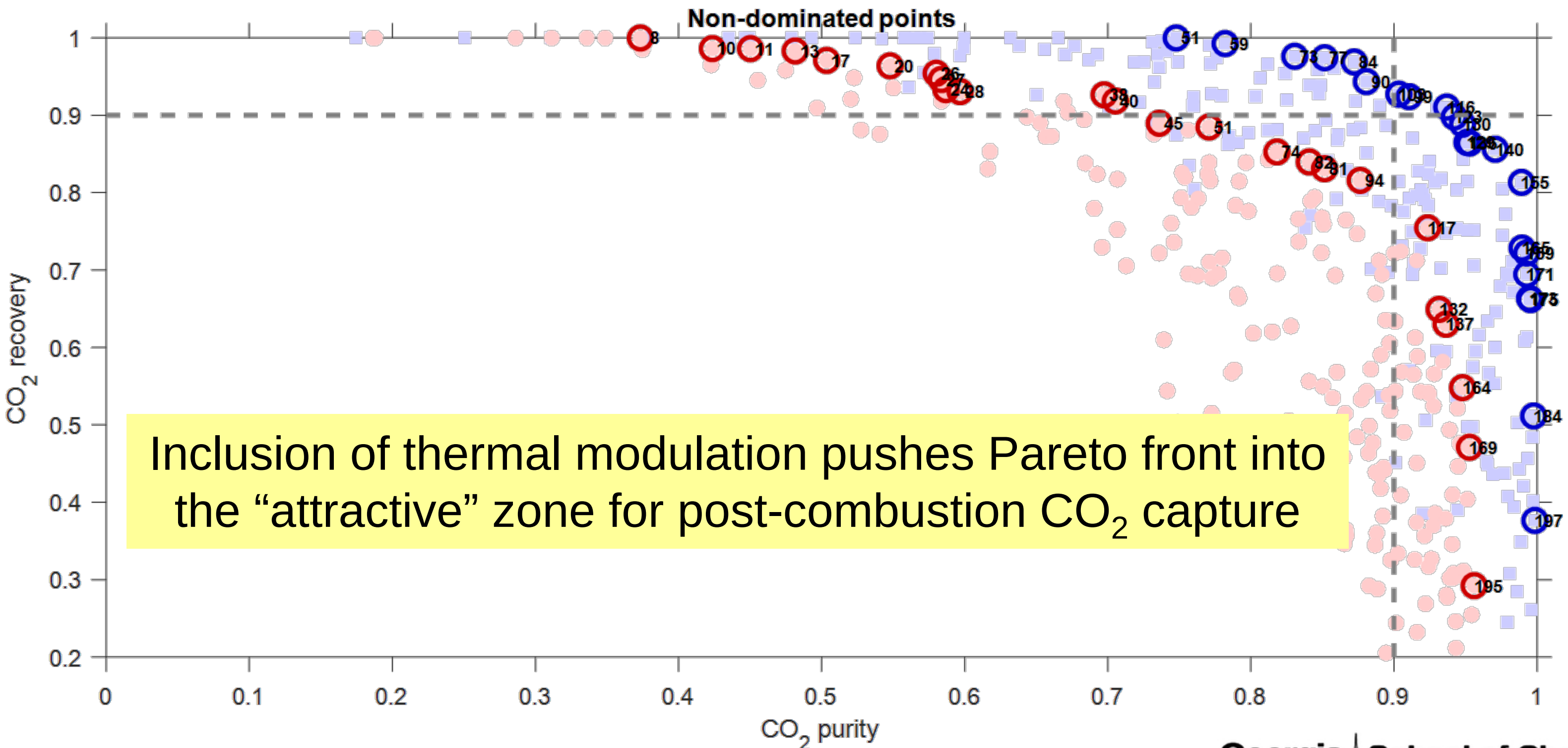
"Passive" thermal management via microPCM capsules

MIL-101(Cr) at 243 K, cyclic steady state simulations

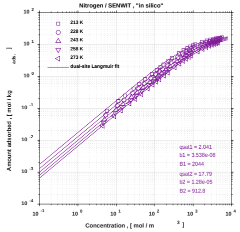


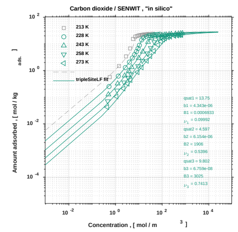


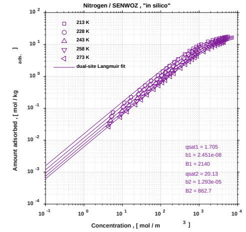
Inclusion of thermal modulation pushes Pareto front into the "attractive" zone for post-combustion CO_2 capture

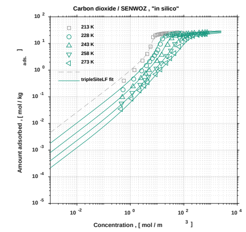
Process economics – from molecular models to PSA simulation to flowsheet analysis

Prediction of binary isotherms from CoreMOF database









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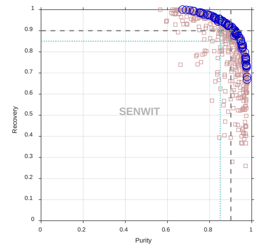
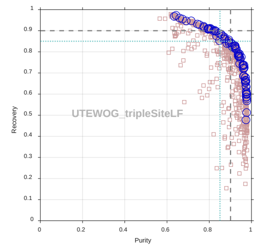
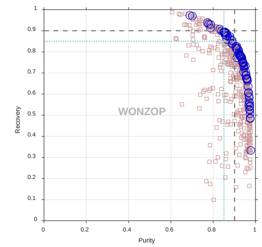
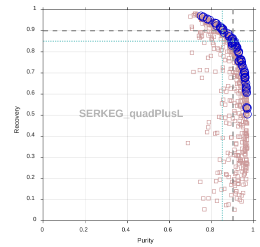
Pareto fronts from PSA optimizer









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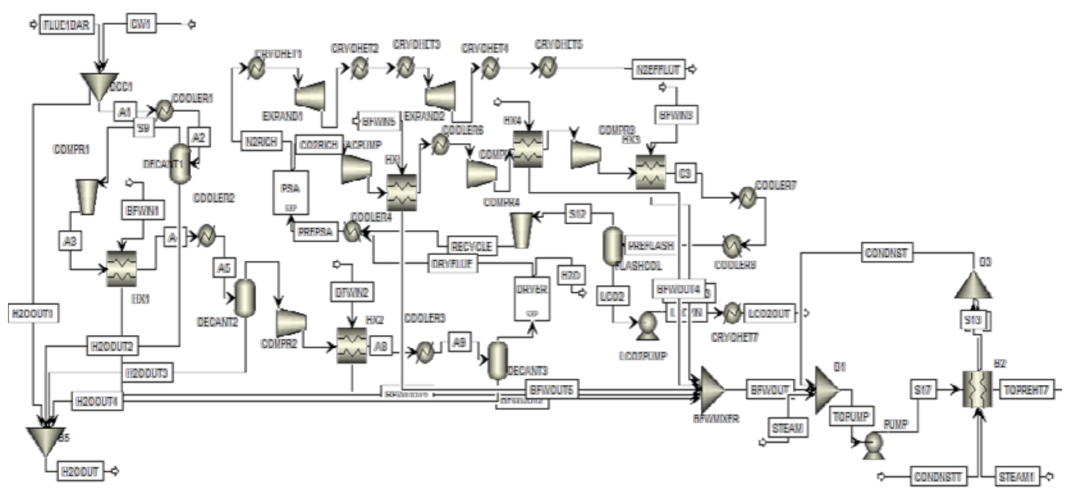
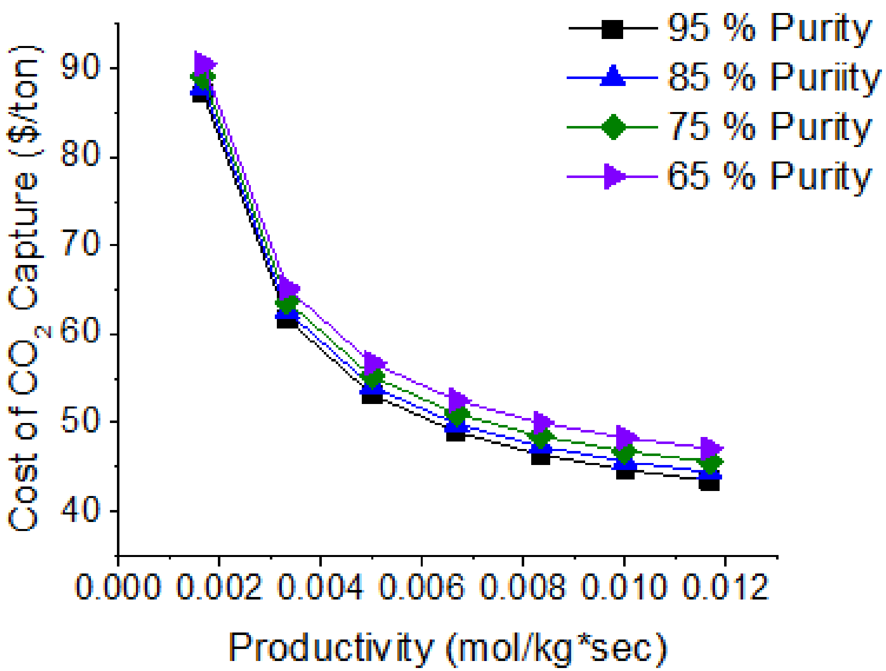
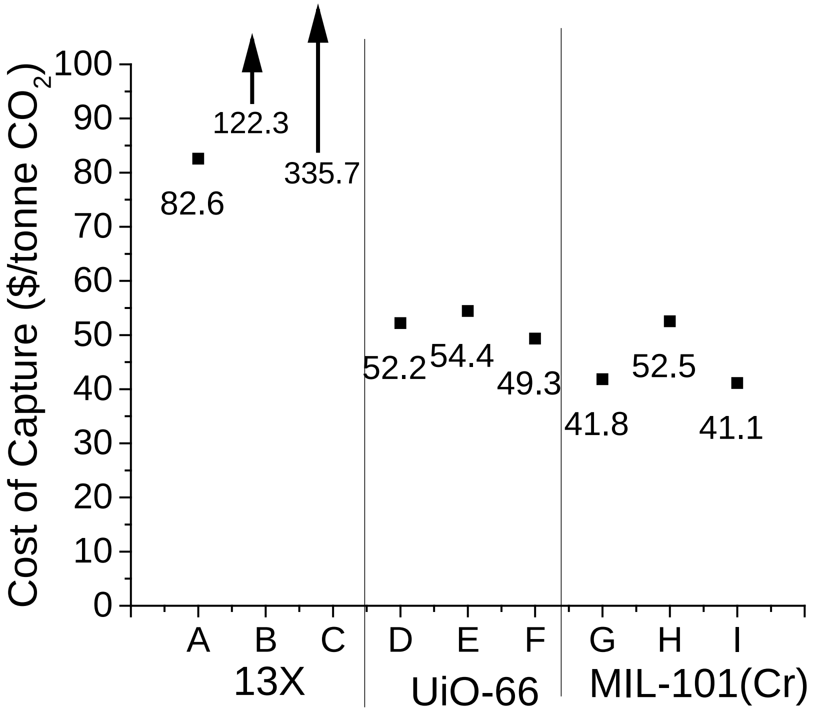
Flowsheet optimization for each material

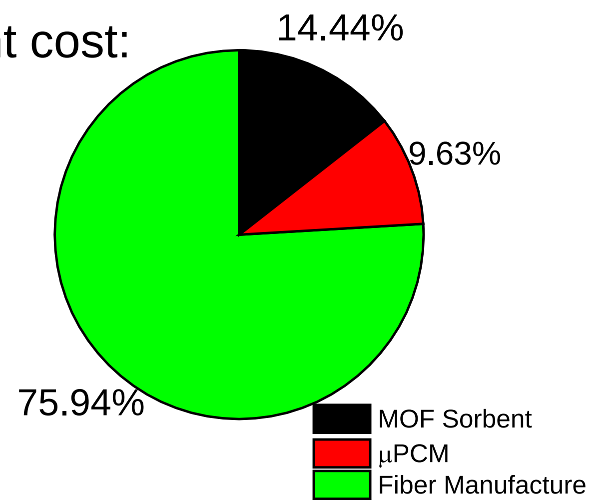


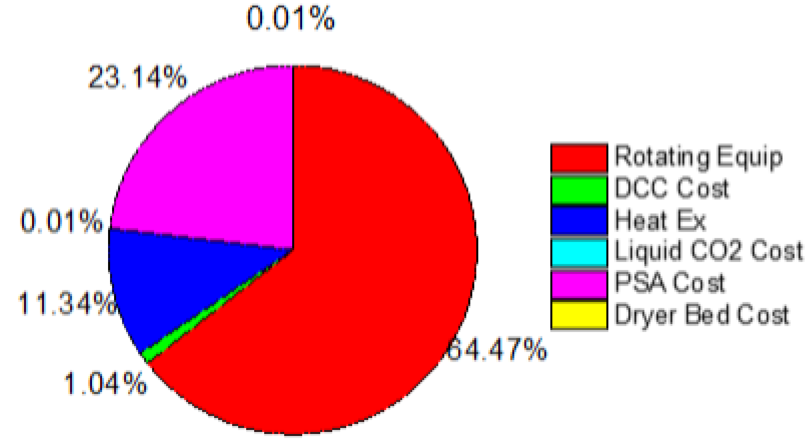
Process economics – from molecular models to PSA simulation to flowsheet analysis





Fiber sorbent cost:





Total capex: $216M (25% of RTSA)

Accomplishments and outcomes

- Developed a “template” flowsheet for any sub-ambient pressure-driven CO_2 capture process
- Created multi-scale workflow for process-driven material screening and selection for adsorption processes
- Scaled-up two different MOFs (MIL-101(Cr) and UiO-66) to >1 kg scale
- Fabricated MOF fiber sorbents with integrated, passive thermal management
- Constructed two PSA minipilot systems (~500 grams of CO_2/day productivity)
- Humid acid gas stability of MOFs, PSA, and fiber sorbents demonstrated
- Capital and operating cost estimation for sub-ambient PSA CO_2 capture

Papers and Patents

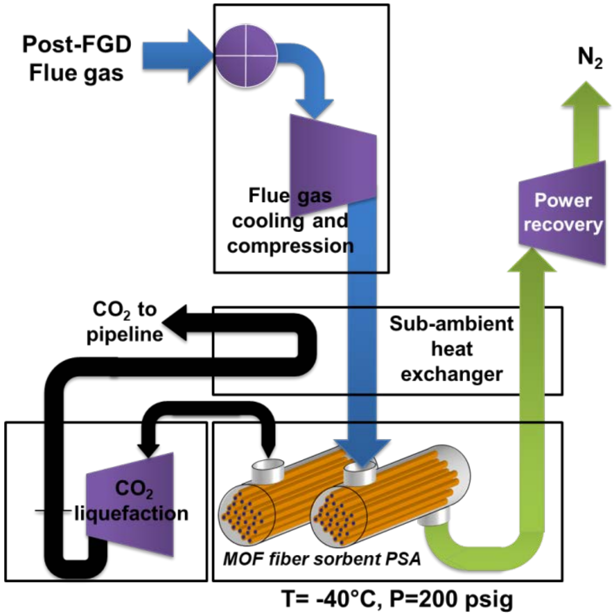
1. J Park, RP Lively, DS Sholl, ″Establishing upper bounds on CO2 swing capacity in sub-ambient pressure swing adsorption via molecular simulation of metal-organic frameworks″, *J. Mater. Chem. A* 2017, 5, 12258-12265.
2. J Park, JD Howe, DS Sholl, ″How Reproducible Are Isotherm Measurements in Metal-Organic Frameworks?″, *Chem. Mater.* 2017, 29, 10487-10495
3. SJA DeWitt, HO Rubiera Landa, Y Kawajiri, MJ Realff, RP Lively. “Development of Phase-Change-Based Thermally Modulated Fiber Sorbents”, *Ind. Eng. Chem. Res.* 2019, 58, 155, 768-5776
4. SJA DeWitt, A Sinha, J Kalyanaraman, F Zhang, MJ Realff, RP Lively. “Critical Comparison of Structured Contactors for Adsorption-Based Gas Separations” *Annu Rev Chem Biomol Eng*. 2018 Jun 7;9:129-152.
5. SJA DeWitt, Y Kawajiri, HOR Landa, MJ Realff, RP Lively. “Incorporation of microencapsulated phase change materials into wet-spin dry jet polymer fibers”. PCT US18/48110; WO 2019/09908
6. BR Pimentel, AW Fultz, KV Presnell, RP Lively, “Synthesis of water-sensitive metal-organic frameworks within fiber sorbent modules”, *Ind. Eng. Chem. Res.* 2017, 56, 17, 5070-5077

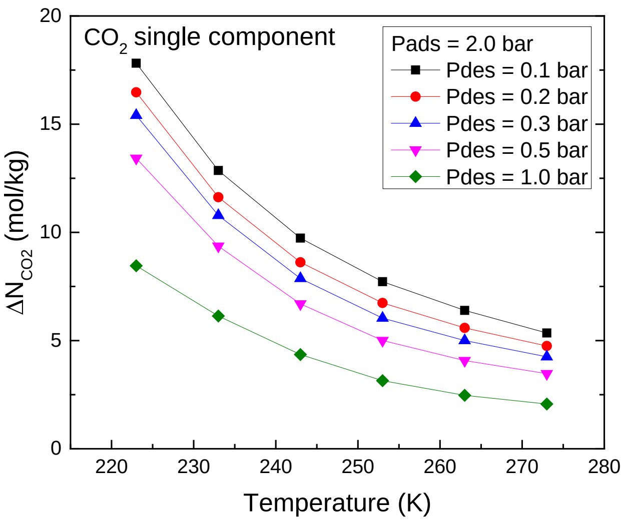
1 submitted, 5 to be submitted Fall 2019

Conclusions and perspectives

Key question: Can we increase swing capacity by 10x and reduce cycle time by 5x to dramatically drive down adsorbent costs?

- Combining RCPSA cycles with appropriate metal-organic frameworks in sub-ambient conditions results in highly productive adsorption systems (i.e., ~30 tonne CO_2/tonne adsorbent-day)





- Significant “real world” complexities exist, but hollow fiber sorbent platform provides solutions to many of these (scalability, transport limitations, etc.)

- Costs in the range of **<u>$40-$50/tonne CO_2</u> at sequestration pressures** may be achievable using these materials in this process concept, but significant work remains. Advantages of small size, material stability to flue gas conditions, and modularity are important.

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