Process Modeling and Analysis of a Novel Sorbent Material for Direct Air Capture Applications

Research & Innovation Center

NATIONAL ENERGY TECHNOLOGY LABORATORY

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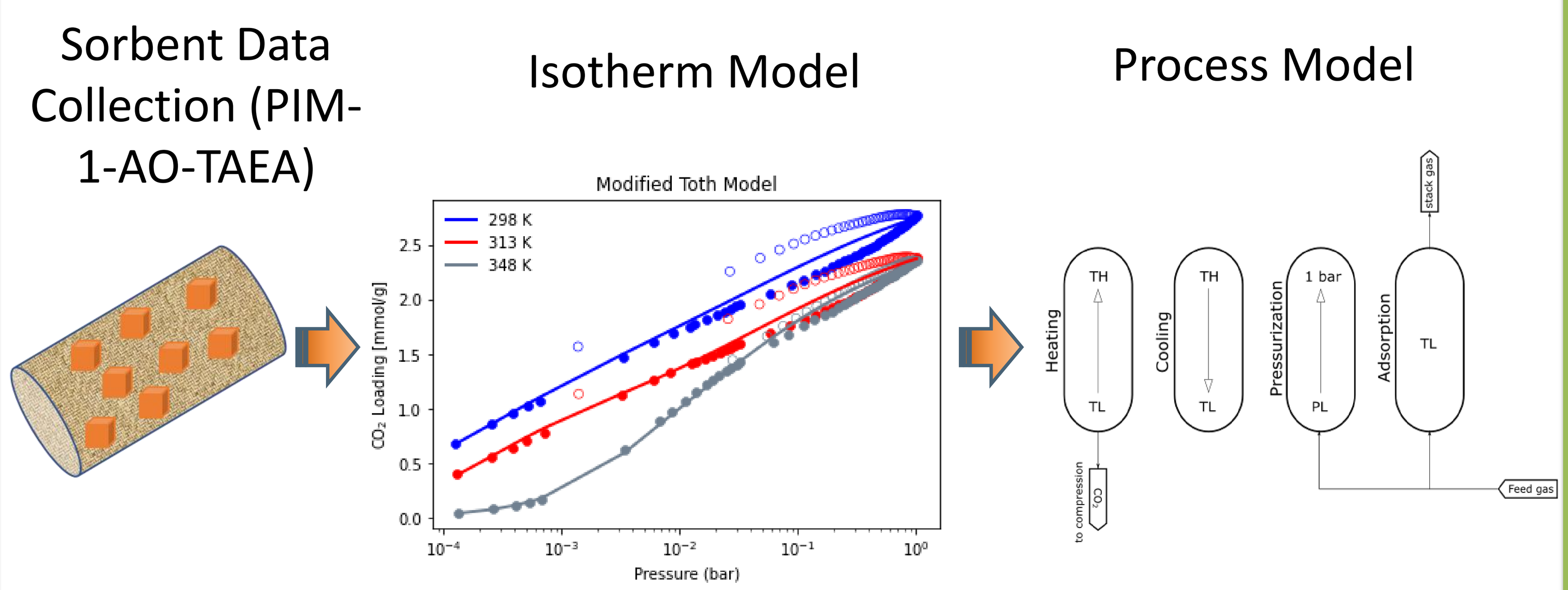
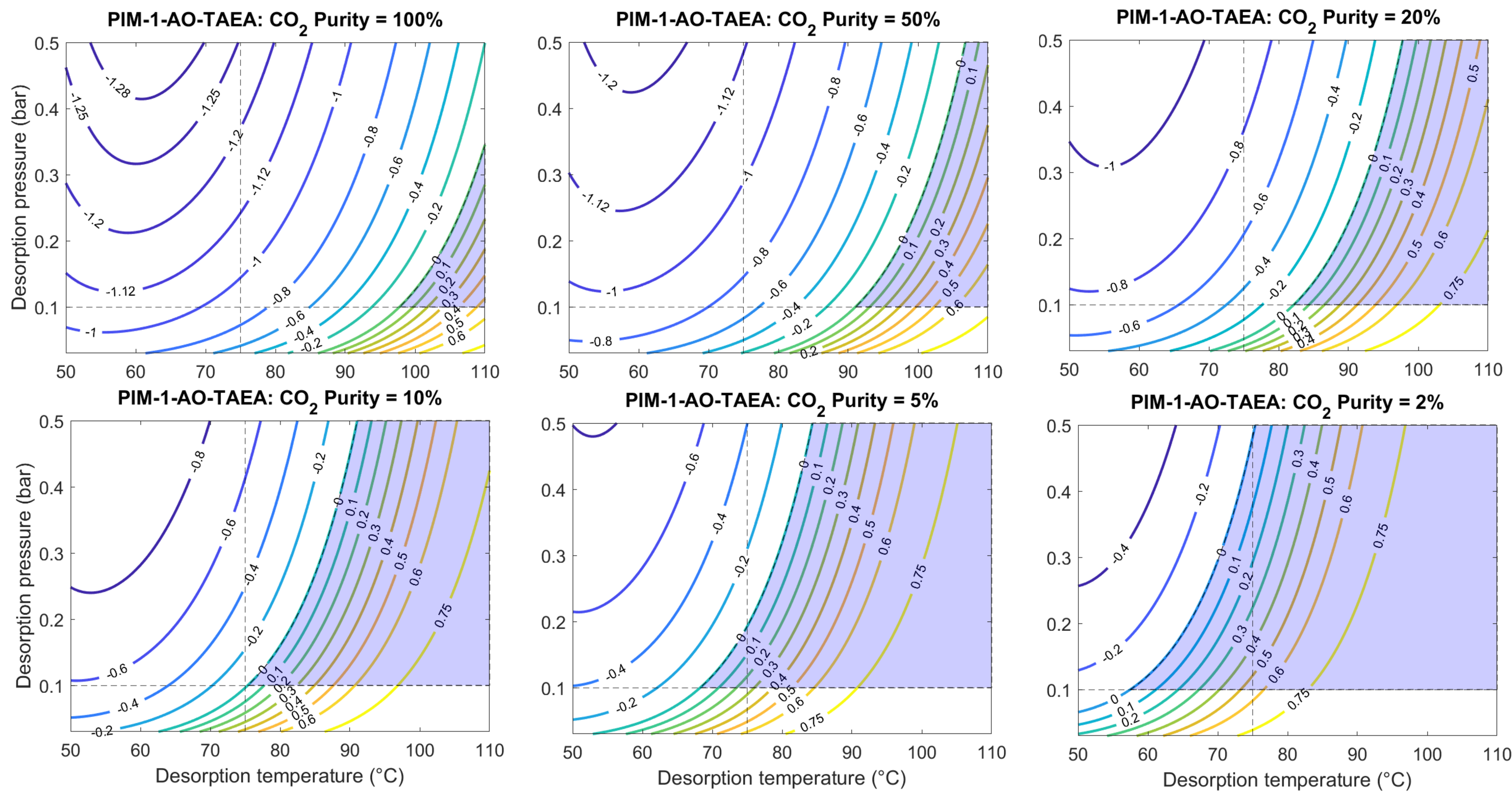
Objectives

- Develop property models for NETL's sorbent (PIM-1-AO-TAEA) for direct air capture (DAC) conditions
- Develop and optimize process configurations for DAC applications of PIM-1-AO-TAEA sorbent
    - Temperature vacuum swing adsorption (TVSA)
    - Sweep gas/steam for regeneration
- Account for the effect of humidity on CO_2 adsorption process

PIM-1-AO-TAEA Sub-models



CO_2 Cyclic Working Capacity



Adsorption conditions	Desorption conditions
T = 25 °C	T = 50–110 °C
P = 1 bar	P = 0.00001–0.5 bar
y_{CO_2} = 400 ppm	y_{CO_2} = 0.02–1 → purity = 2–100%

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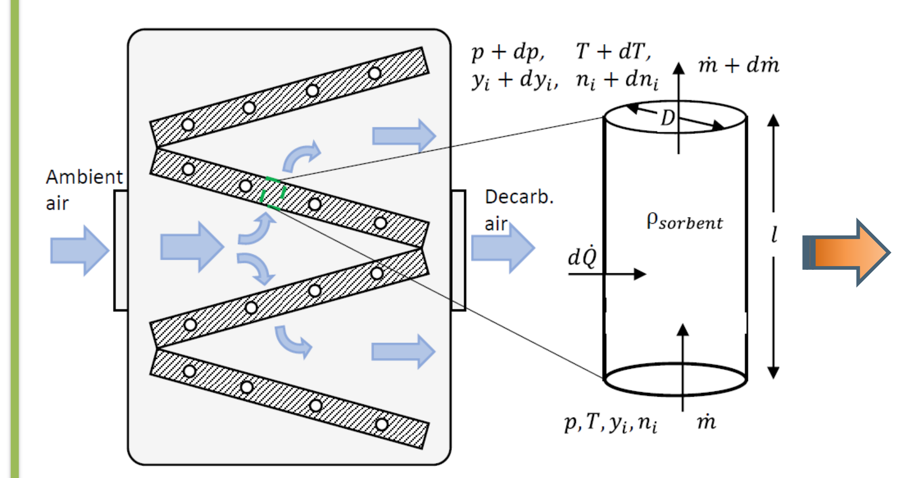
Vacuum-Assisted Temperature Swing Adsorption

Modeled fixed-bed design with low pressure drop:

- Assumption of a flat bed[1] to mimic a differential segment of the plates containing the solid sorbent in the Climeworks contactor.

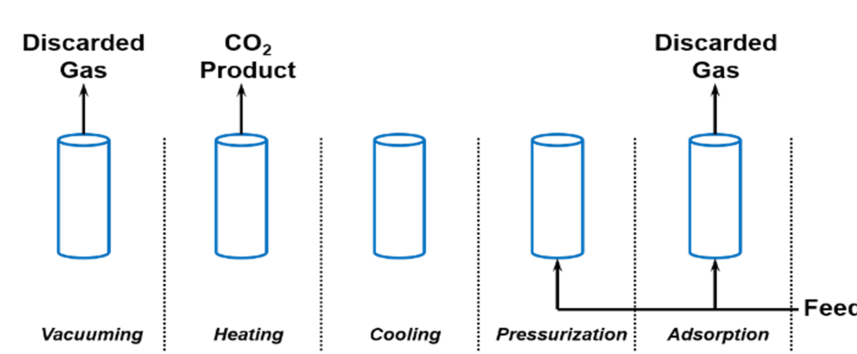


Dimension	IDAES/Aspen Models
Bed Diameter (m)	0.1
Bed Height (m)	0.01

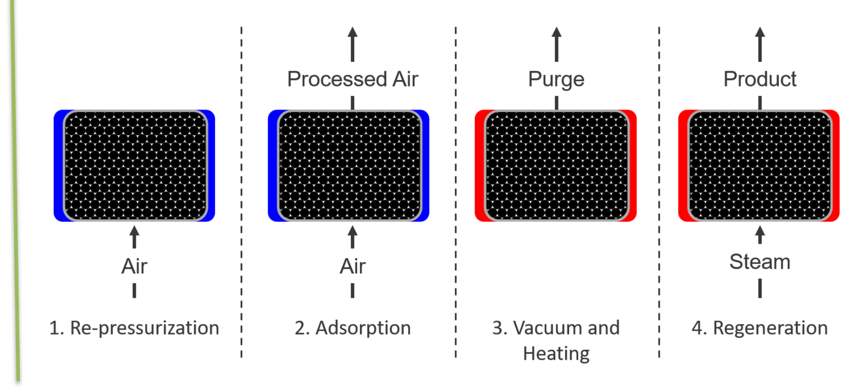
Fixed-bed process models developed:

- Simplified TVSA model developed in the IDAES framework (0D equilibrium-based model) – no sweep gas
- Rigorous TVSA model developed in Aspen Adsorption (1D model) – sweep gas (steam)

Cycle configuration of IDAES model

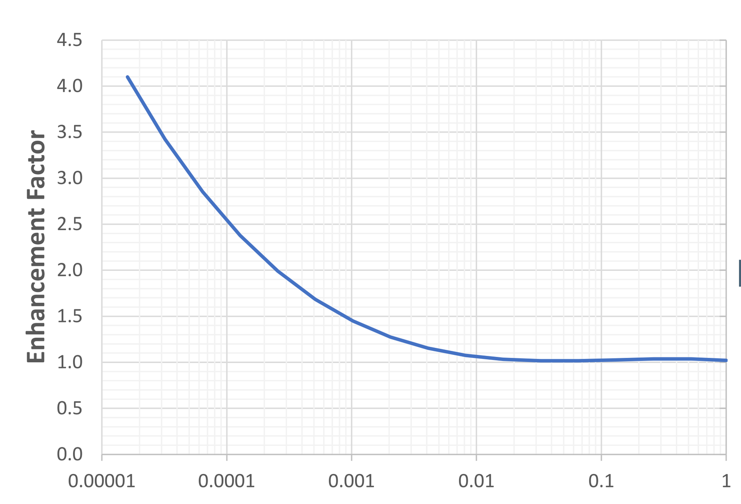


Cycle configuration of Aspen model

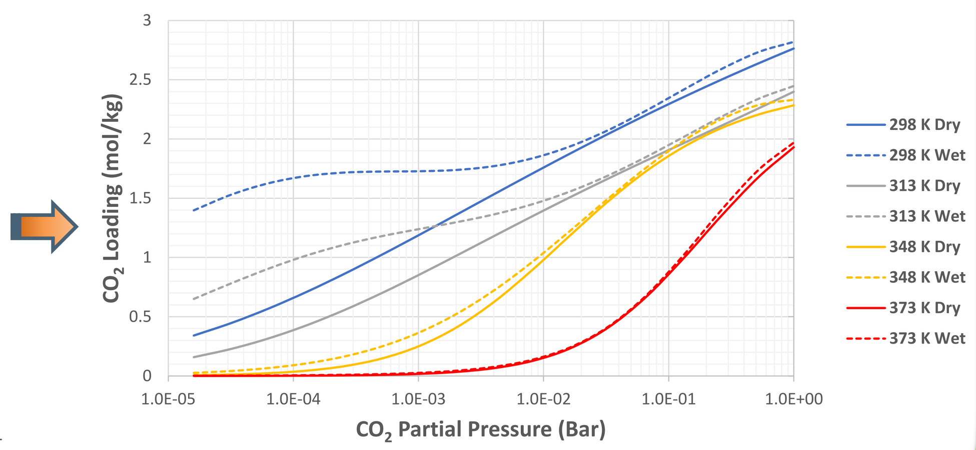


Effect of humidity on CO_2 adsorption:

Enhancement factor of water impact



Isotherm model for PIM-1-AO-TAEA sorbent with enhancement factor for wet CO_2/H_2O co-adsorption



Assumption: We cope with the limited availability of data by combining the sorbent PIM-1-AO-TAEA CO_2 isotherm with available H_2O isotherm for other materials (Lewatit VP OC 1065 [1])

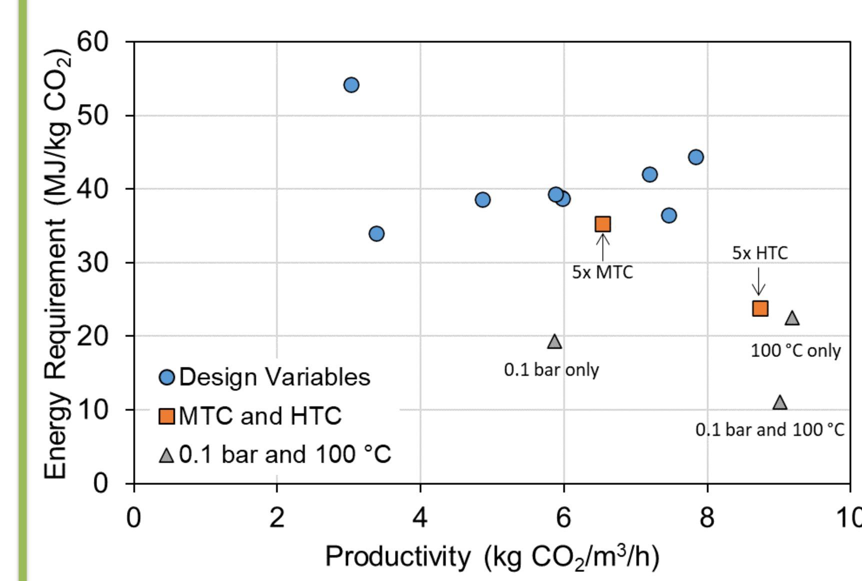
TVSA Process Results

Metric/Cases	1	2	3	4	5
CO_2 Capture %	0.8	83.2	81.5	99.0	13.3
CO_2 Purity %	3.1	12.7	17.7	24.6	2.4
CO_2 Purity % (H_2O-free)	10.3	96.2	87.2	98.0	87.8
Specific Energy (MJ/kg)	1707	20.6	33.7	9.3	38.8

Cases tested:

1. 75 °C, humid air, no enhancement factor, no sweep gas (IDAES)
2. 100 °C, humid air, no enhancement factor, no sweep gas (IDAES)
3. 75 °C, humid air, enhancement factor, no sweep gas (IDAES)
4. 100 °C, humid air, enhancement factor, no sweep gas (IDAES)
5. 75 °C, humid air, no enhancement factor, sweep gas (Aspen)

Sensitivity Study (Aspen Model)



- Design variables adjusted by +/- 50% (step times, pressure drop, flowrate)
- MTC and HTC increased to 5x
- Regeneration conditions of 0.1 bar and 100 °C

Conclusions

- Enhancement of CO_2 loading due to water in humid air helps the performance of the TVSA process
- TVSA at 0.2 bar vacuum pressure and 75 ₵ desorption temperature does not achieve high enough CO_2 purity or a high enough recovery percentage
- Productivity is in a range consistent with literature studies while the energy requirement is higher

References

[1] J. Young, E. García-Díez, S. Garcia, and M. van der Spek, "The impact of binary water–CO2 isotherm models on the optimal performance of sorbent-based direct air capture processes," *Energy Environ. Sci.*, vol. 14, no. 10, pp. 5377-5394, Aug. 2021.

Acknowledgements: We graciously acknowledge funding from the U.S. Department of Energy, Office of Fossil Energy and Carbon Management, through the Carbon Dioxide Removal Program.