Modeling and Analysis of Climate Variation Effects on Fixed-Bed Direct Air Capture Systems

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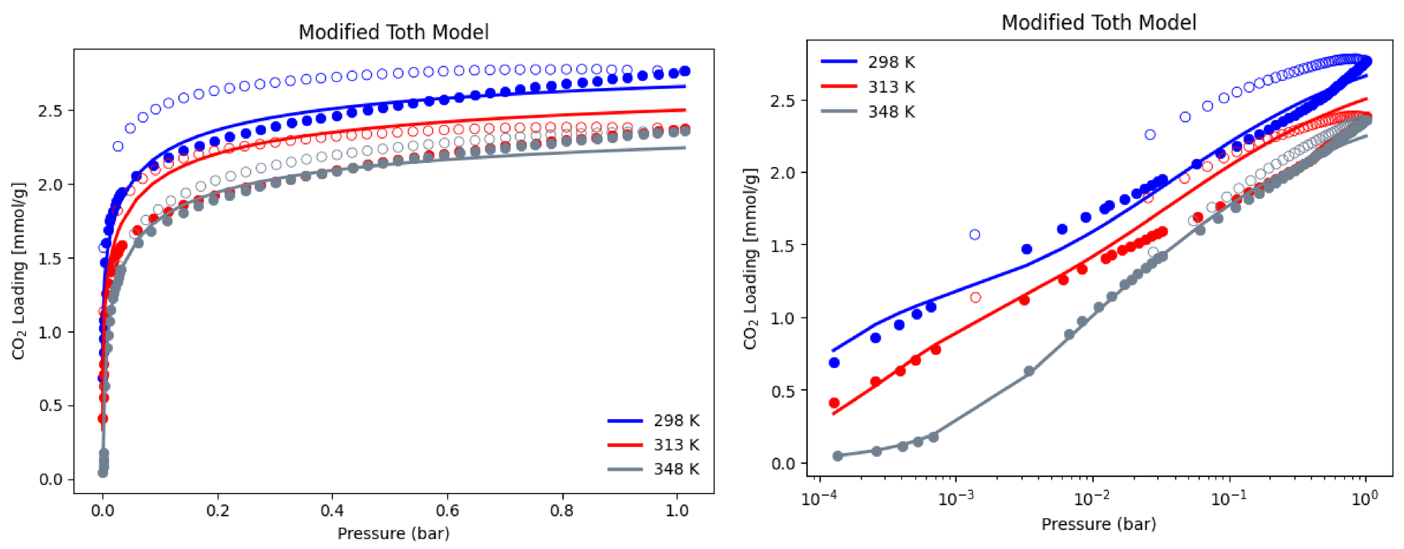
Background

- Direct air capture (DAC) may be significantly impacted by climate and shifting ambient conditions
- Understanding the economic impacts of shifting ambient conditions is critical in determining optimal site locations and control strategies to minimize negative impacts
- This work demonstrates tool development that can be implemented with first-principles models to better understand these impacts

Modeling of NETL DAC PIM Sorbent

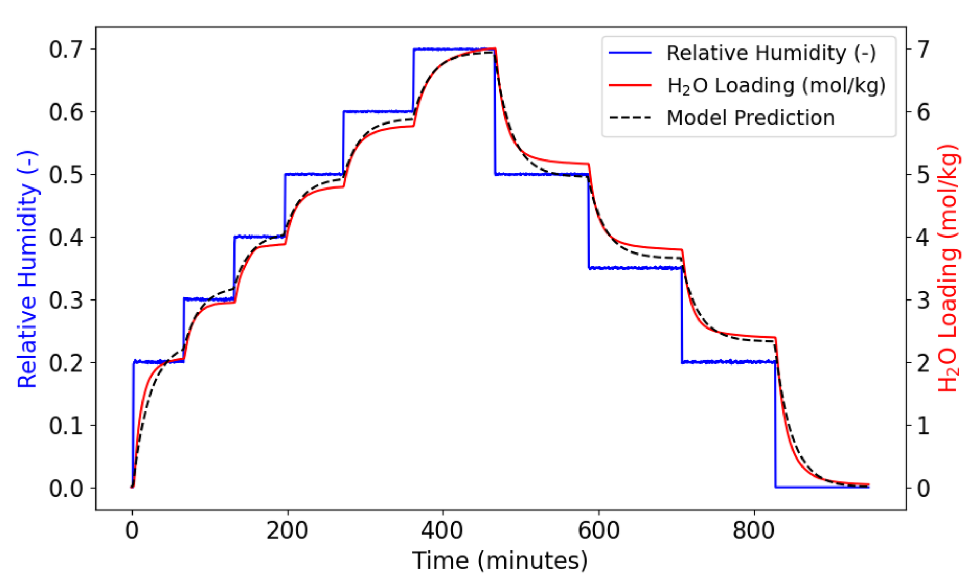
CO_2 Isotherm Model: Modified Toth[1]

$$q_{CO_2} = \left[\frac{q^{\infty} bP}{(1+(bP)^t)^{1/t}}\right]_{chem} + \left[\frac{q^{\infty} bP}{(1+(bP)^t)^{1/t}}\right]_{phys}$$

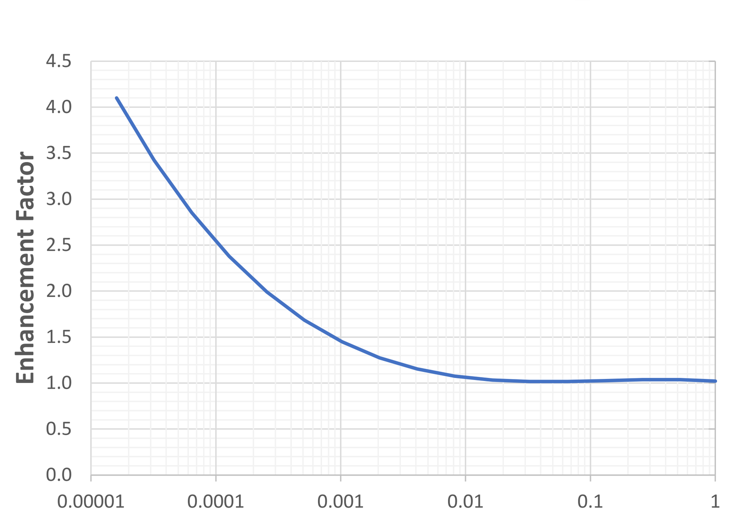


H_2O Isotherm Model: GAB Model[2]

$$q^*_{H_2O} = q_m \frac{K_{ads} C_G x_{RH}}{(1 - K_{ads} x_{RH})(1 + (C_G - 1) K_{ads} x_{RH})}$$



Effect of Humidity on CO_2 Adsorption:



Assumption: The limited availability of data was addressed by combining the sorbent PIM-1-AO-TAEA CO_2 isotherm with available enhancement factor models for other materials (Lewatit VP OC 1065[2])

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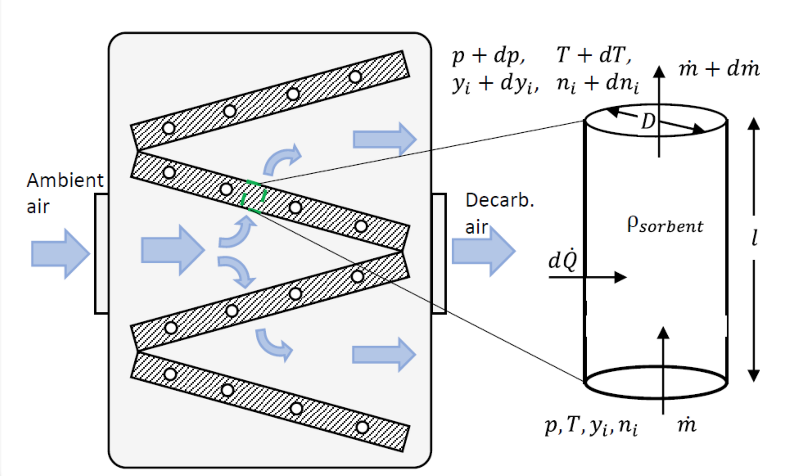
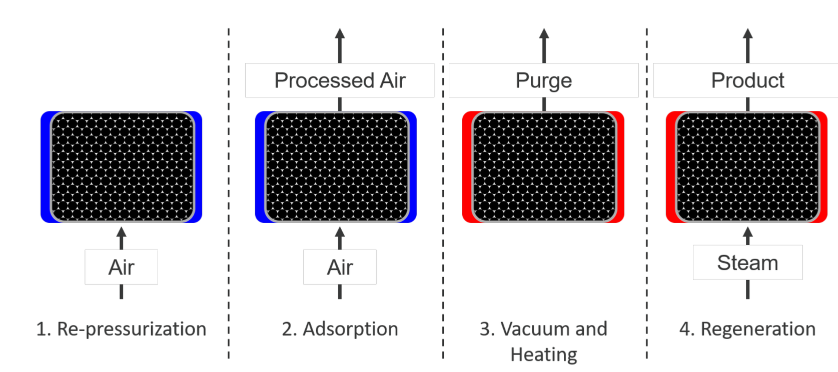
Vacuum-Assisted Temperature Swing Adsorption

Modeled Fixed-Bed Design with Low Pressure Drop:

- Assumption of a flat bed[2] to mimic a differential segment of the plates containing the solid sorbent in the Climeworks contactor
- First-principles vacuum-assisted temperature swing adsorption model developed in Aspen Adsorption



Cycle configuration of Aspen model



Techno-economic Optimization

IDAES Costing Framework

- Uses NETL Quality Guidelines for Energy System Studies methods and implemented as IDAES library[3]
- Costing information obtained from NETL DAC Sorbent Report[4]

Derivative-Free Optimization Using CCSI² Toolset (FOQUS)

$$\min_x \; f(x) \quad \text{Cost of capture (\$/tonne)}$$

$$s.t.$$

$$x^L \le x \le x^U \quad \text{Decision variable bounds}$$

$$h(x) = 0 \quad \text{Modeling eqs. (mass balances, energy balances, etc.)}$$

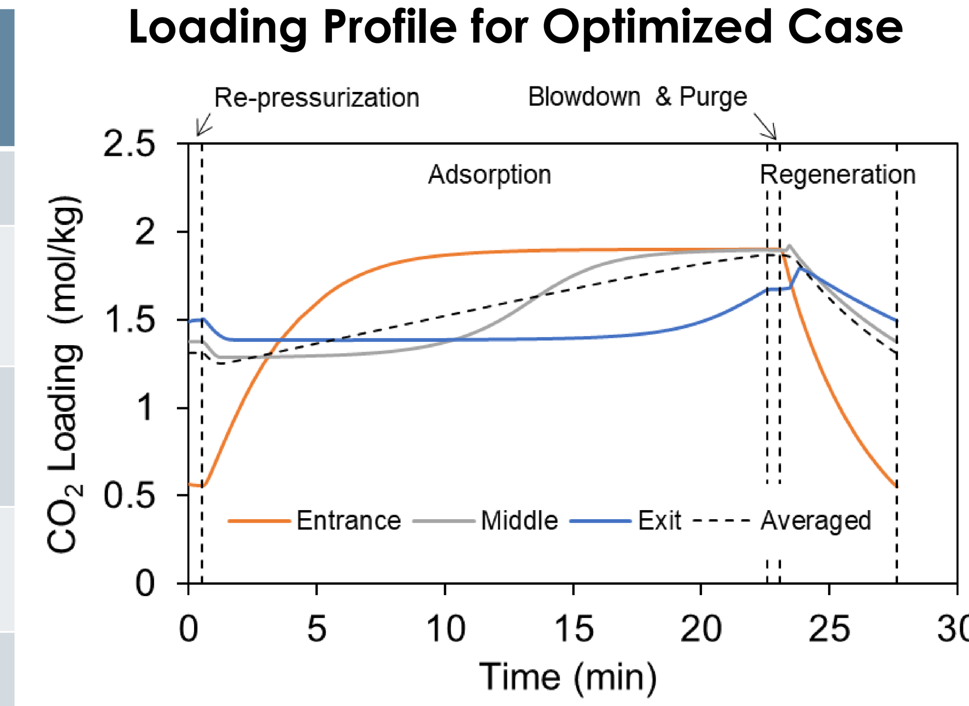
$$g(x) \le 0 \quad \text{Process constraints}$$

Results

Metric	Optimized Value
Recovery	0.73
CO_2 product purity (water-free basis)*	0.95
Energy requirement [MJ/kg CO_2]	14.71
Productivity [kg CO_2/h/m^3]	15.67
Cost of capture [$/tonne]*	268.2

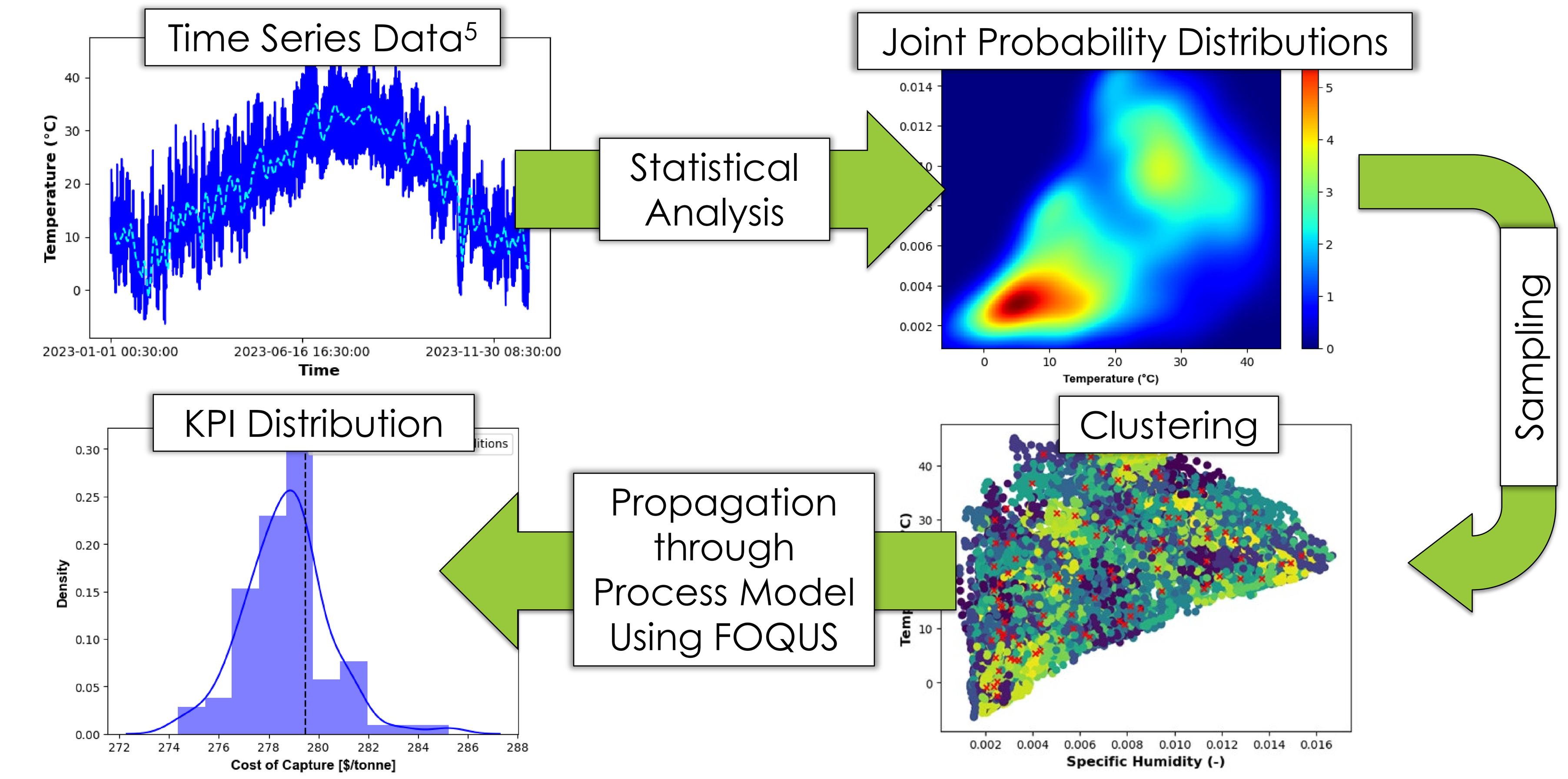
*Costs are preliminary, DO NOT CITE

Loading Profile for Optimized Case

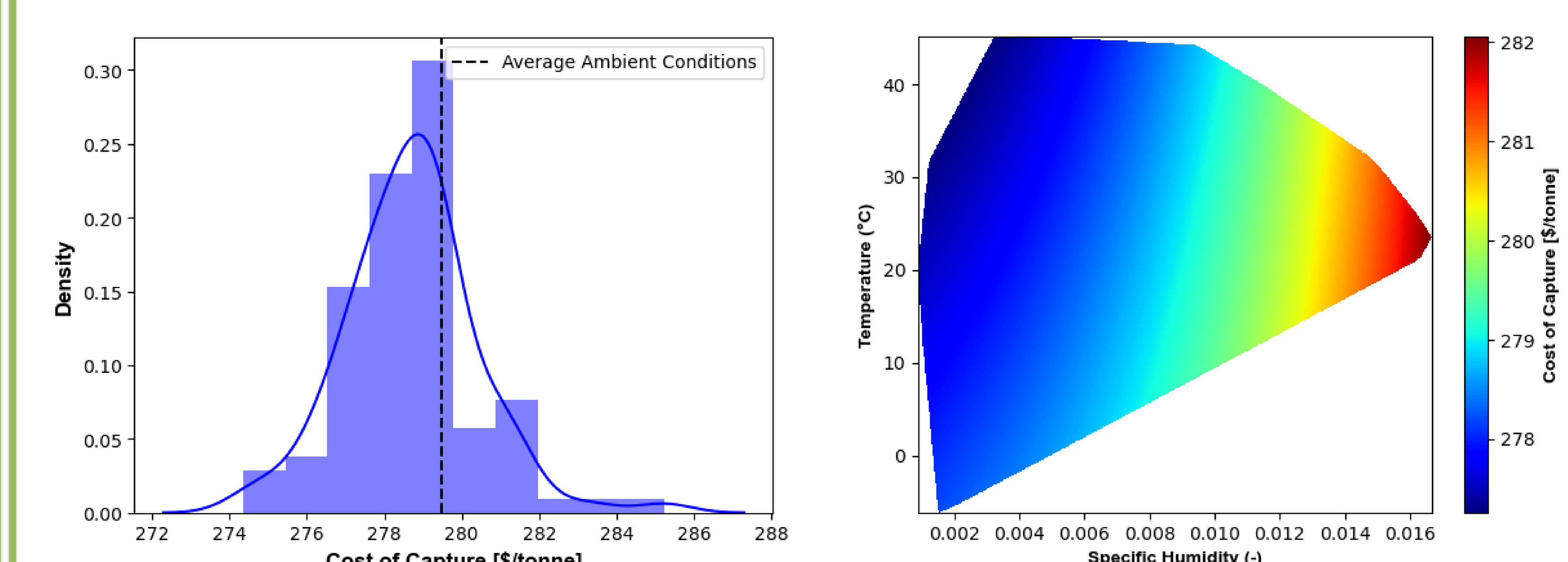


Ambient Conditions: 25 °C, 50% relative humidity, 1 atm

Ambient Conditions Performance Analysis



Analysis of Candidate Site (Odessa, TX)



- Cost of capture increases at higher temperatures and specific humidities
- Cost of capture is most sensitive to specific humidities

Conclusions

- Modeling tools available in IDAES and CCSI² open-source software were used to model PIM sorbent technology for DAC applications
- The FOQUS tool enables the propagation of conditions through process models
- Critical analysis is needed to determine the robustness of the process to ambient conditions and to identify needed control strategies to transition from one condition to another

References

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