Techno-Economic Analysis and Optimization for MOF-Based CO_2 Capture from NGCC Applications

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Background

- Amine-appended metal organic frameworks (MOF) have shown promising attributes for post combustion capture (long-term stability, CO_2 selectivity, maintained performance under humid conditions) accompanied by a unique step-shaped adsorption isotherm.
- Unique isotherms and dynamic sorbent processes present difficult modeling and optimization challenges.

Objectives

- Development of an isotherm model for a tetraamine-appended MOF.[1]
- Development of fixed-bed contactor and moving-bed contactor models.
- Techno-economic optimization of post-combustion capture processes from natural gas combined cycle (NGCC) flue gas.

Isotherm Model

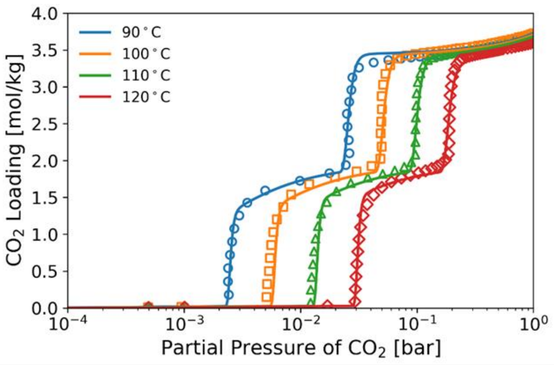
- Weighted Langmuir model extended to multiple adsorption steps.

$$q^*_{CO_2} = (1-\omega_1)q^*_1 + (\omega_1-\omega_2)q^*_2 + \omega_2 q^*_3$$

- Parameter Estimation.

θ: Set of isotherm parameters

$$\min_{\theta} \left(\frac{q^*_{CO_2,exp} - q^*_{CO_2,model}(\theta)}{q^*_{CO_2,exp}}\right)' \Sigma^{-1} \left(\frac{q^*_{CO_2,exp} - q^*_{CO_2,model}(\theta)}{q^*_{CO_2,exp}}\right)$$

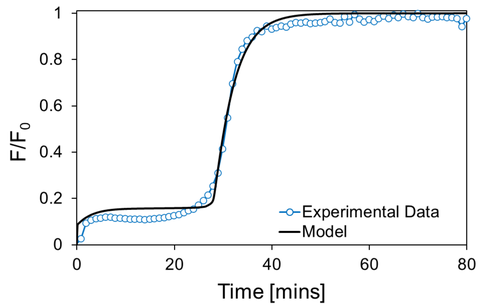


Fit to Experimental Isotherm Data

Contactor and TSA Process Models

- Dynamic, non-isothermal, first-principles contactor models (Aspen Custom Modeler).
- Mass transfer model developed using experimental fixed-bed breakthrough data.

Linear driving force equation: $\frac{dq_{CO_2}}{dt} = k_l\left(q^*_{CO_2} - q_{CO_2}\right)$

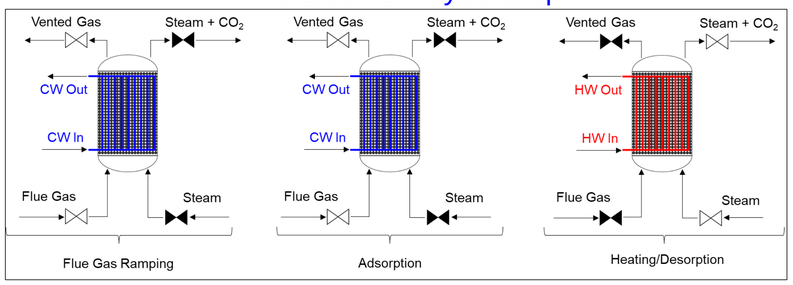


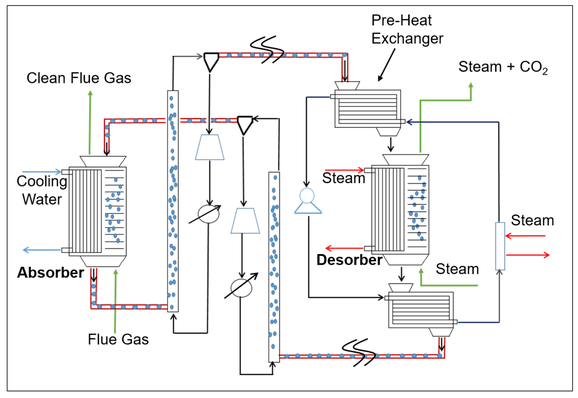
Fit to Fixed Bed Experimental Breakthrough Data

Process Models

- Sized to capture CO_2 from a 650 MW NGCC plant.[2]
- Designed for 90% CO_2 capture.
- Embedded heat exchangers used to aid in thermal management.

Fixed Bed TSA Cycle Steps





Moving Bed TSA Process

Techno-Economic Optimization

Cost Model

- Closely follows the NETL costing guidelines.[2]
- Main costing components:
  - Annualized capital cost.
  - Fixed O&M.
  - Variable O&M (utilities such as steam and electricity).

Optimization Framework

- Connection to derivative-free optimization algorithms within the FOQUS tool.[3]

$\min_x \ f(x)$	Total annualized cost ($MM/y)
$s.t.$	
$x^L \le x \le x^U$	$x \rightarrow$ Decision variables
$h(x) = 0$	Rigorous, first principles models in ACM
$g(x) \le 0$	CO_2 capture, velocity constraints, etc.

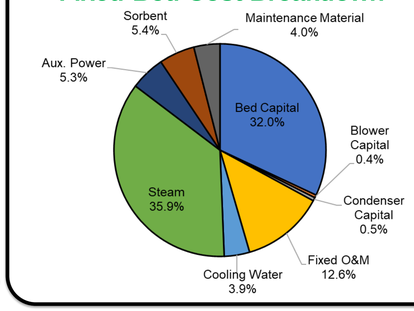
- Decisions Variables (x).
  - Fixed Bed: *L, D, tube pitch, F_{FG}, F_{steam}, step times.*
  - Moving Bed: *L_{ads}, D_{ads}, L_{des}, D_{des}, tube pitch, lean sorbent loading.*

Results

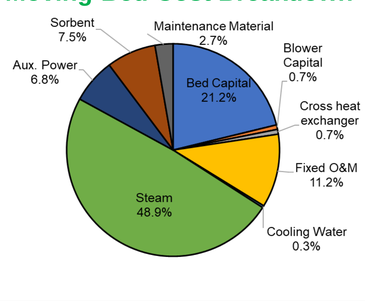
- Enhanced driving forces due to counter-current flow pattern in the moving-bed process reduces sorbent/reactor volume and results in lowest cost of capture.

	Fixed Bed Process	Moving Bed Process	MEA Reference[4]
Total Annualized Cost ($MM/y)	193.1	118.2	-
Cost of Capture ($/tonne CO_2)	109.4	67.4	73.9

Fixed-Bed Cost Breakdown



Moving-Bed Cost Breakdown



References

[1] Kim, E.J., *et al*. Cooperative Carbon Capture and Steam Regeneration with Tetraamine-Appended Metal–Organic Frameworks. *Science* **2020**, No. 369, 392–396. https://doi.org/10.1126/science.abb3976.

[2] James, III, R., *et al. Cost and Performance Baseline for Fossil Energy Plants Volume 1: Bituminous Coal and Natural Gas to Electricity*; 2019; NETL-PUB-22638, 1569246. https://doi.org/10.2172/1569246.

[3] Miller, D., *et al.* "Innovative computational tools and models for the design, optimization and control of carbon capture processes," *26th European Symposium on Computer Aided Process Engineering – ESCAPE 26,* pp. 2391-2396, 2016.

[4] Du, Y., *et al.* "Zero- and negative-emissions fossil-fired power plants using CO2 capture by conventional aqueous amines," *International Journal of Greenhouse Gas Control,* vol. 111, p. 103473, 2021.

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