Modeling and Optimization of a Rotary Packed Bed Contactor for CO_2 Capture

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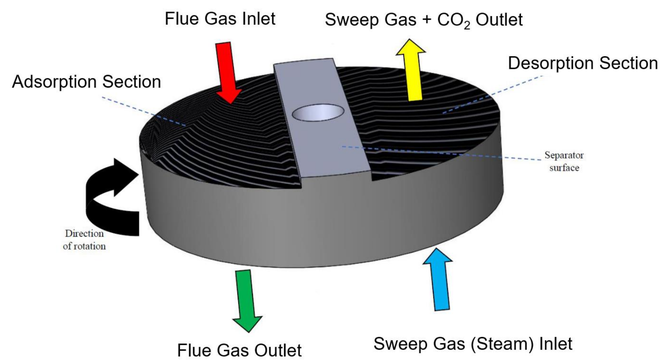
Background

- Evaluate potential alternatives to solvent capture technologies
- Non-traditional solid contactors can address mass and heat transfer limitations of fixed beds
- Worldwide use of natural gas usage expected to overtake coal in near future
- Mg_2(dobpdc)(3-4-3) is a promising sorbent for NGCC CO_2 capture[1,2]

Objectives

- Development of a rotary packed bed (RPB) contactor model
- Multi-objective optimization of energy requirement and productivity

RPB Configuration

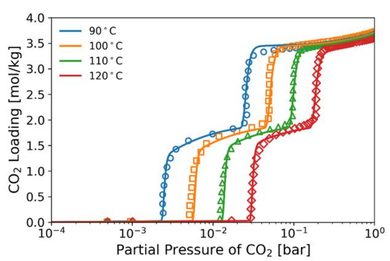


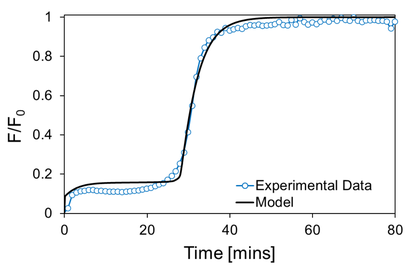
Isotherm and Kinetic Model

- Weighted Langmuir model extended to multiple adsorption steps:

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

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





Fit to Experimental Data

RPB Contactor Model

- Dynamic, non-isothermal, first-principles model developed in Pyomo[3]
- Conceptual embedded heat exchanger design to supply/remove the heat needed for regeneration/cooling

Modeling Equations

Gas phase species balance

$$\varepsilon_b \frac{\partial C_{g,i}}{\partial t} = -\frac{\partial\left(v_g C_{g,i}\right)}{\partial z} - (1-\varepsilon_b)\frac{6k_{f,i}}{d_p}\left(C_{g,i} - C_{surf,i}\right)$$

Solid phase CO_2 balance

$$\frac{\partial q_{CO_2}}{\partial t} = -\omega\frac{\partial q_{CO_2}}{\partial \theta} + k_l(q^*_{CO_2} - q_{CO_2})$$

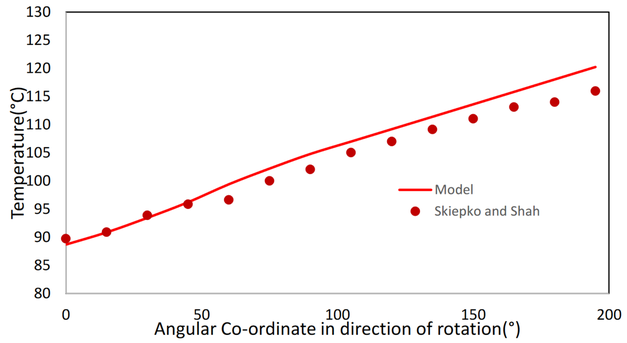
Gas phase energy balance

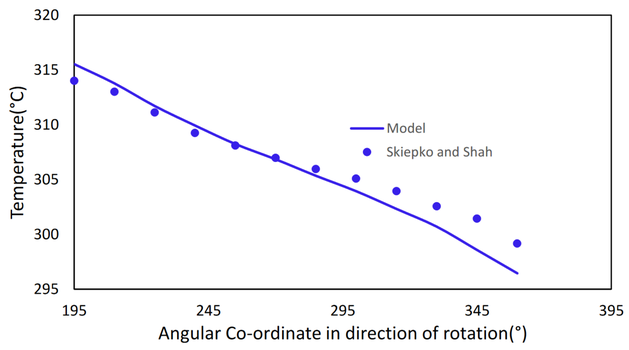
$$\rho_g C_{p,g}\varepsilon_b\frac{\partial T_g}{\partial t} = -\rho_g C_{p,g} v_g\frac{\partial T_g}{\partial z} - (1-\varepsilon_b)h_{gs}a_s\left(T_g - T_s\right) - h_{gx}a_x(T_g - T_x)$$

Solid phase energy balance

$$\rho_s C_{p,s}\frac{\partial T_s}{\partial t} = -\rho_s C_{p,s}\omega\frac{\partial T_s}{\partial \theta} - h_{gs}a_s\left(T_s - T_g\right) - \rho_s k_l(q^*_{CO_2} - q_{CO_2})(\Delta H_{CO_2})$$

Validation for non-reactive rotary air preheater system[4]





Design Optimization

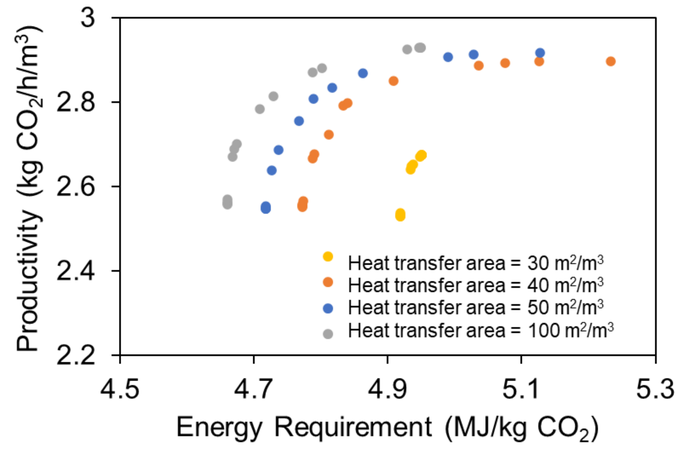
Optimization Framework

- Generation of pareto front for multi-objective optimization of energy requirement and productivity
- CO_2 capture fixed to 95%

$\min_x \ f(x)$	Multi-objective optimization with weighting parameter: α•Energy Requirement – (1-α)•Productivity
$s.t.$	
$x^L \le x \le x^U$	Decision variable bounds
$h(x) = 0$	Modeling eqs. (mass balances, energy balances, etc.)
$g(x) \le 0$	Velocity constraints, etc.

- Decisions Variables (x): Bed Length, adsorption temperature, desorption temperature, section fractions, steam flow rate

Results



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] Yancy-Caballero, D., *et. al.* Isotherm modeling and techno-economic analysis of a TSA moving bed process using a tetraamine-appended MOF for NGCC applications. *International Journal of Greenhouse Gas Control* **2023**, 128, 103957, https://doi.org/10.1016/j.ijggc.2023.103957.
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[4] C. E. Ezeobinwune, "Modeling of Rotary Packed Beds for Reactive and Non-Reactive Systems," MS, West Virginia University Libraries, **2020**. doi: 10.33915/etd.7508.

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