Process driven engineering of sorbents for optimal CO_2 capture from air

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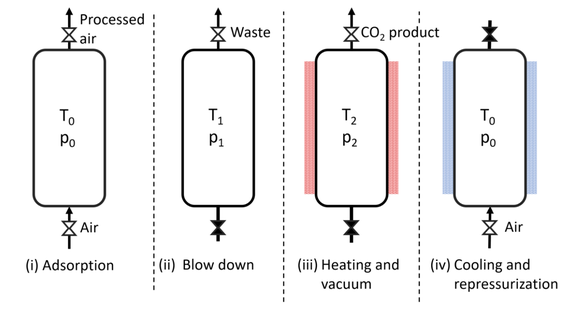
1 Introduction

- There exist hundreds of thousands of solid sorbent materials, both real and hypothetical, mainly developed to capture CO_2 from point sources.
- In this study, we first scan existing materials to assess their suitability to capture CO_2 from diluted sources, e.g. direct air capture (DAC).
- In a second step, we carry out a theoretical exercise and optimize the parameters of different isotherm models, representing different isotherm shapes.
- By doing so, we can investigate the limits of CO_2 adsorption from dilute feed streams, in terms of process performance as well as costs.
- Furthermore, we can compare these optimal isotherms with existing materials.

2 Modeling tools

Methodology

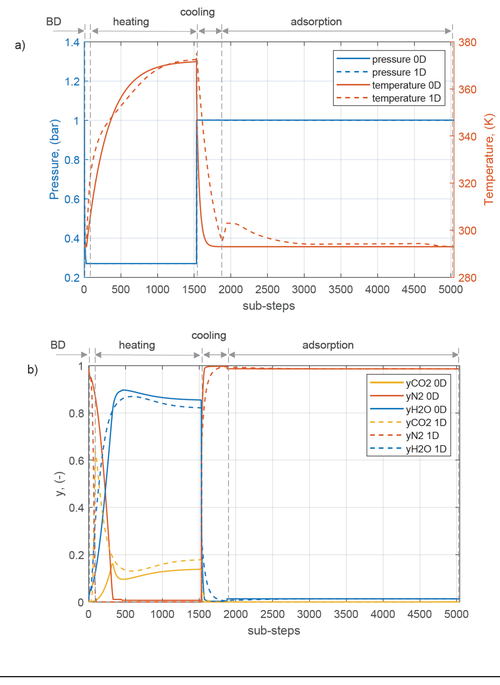
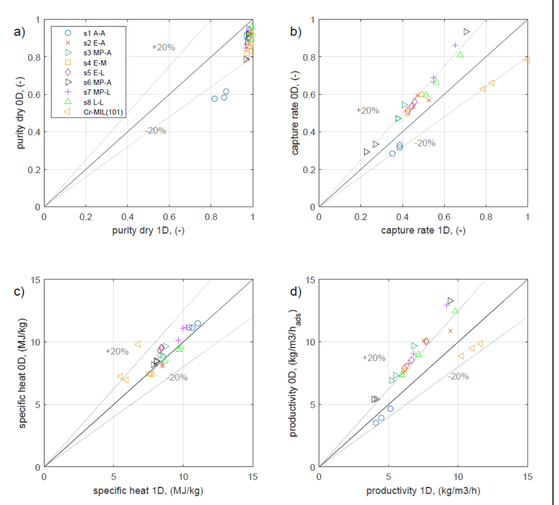
- Simplified 0D model of a four-step temperature vacuum swing (TVSA) adsorption system.
- The model is based on a batch system and each step is modeled by assuming adsorption equilibrium.



- Extended by incorporating a neural network, trained with a rate-based model, to include productivity as a performance parameter, besides the specific thermal energy consumption, the purity as well as the recovery.
- In addition, we consider saturation levels in the bed during adsorption below 100%.
- Considering a ternary mixture as feed, where CO_2 is not necessarily the most retained gas, i.e. we add H_2O adsorption.
- Including multiple CO_2 isotherm types in the model, i.e. Toth, extended Toth model (Toth-cp), Langmuir-Freundlich, Dual-Site-Langmuir (DSL) and s-shaped isotherm model.

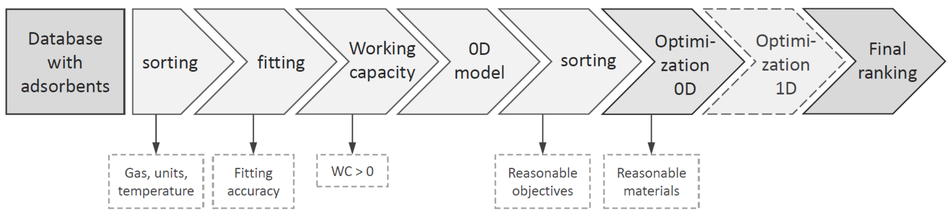
Model validation

- Validation using a rate-based model[1]
- Two steps:

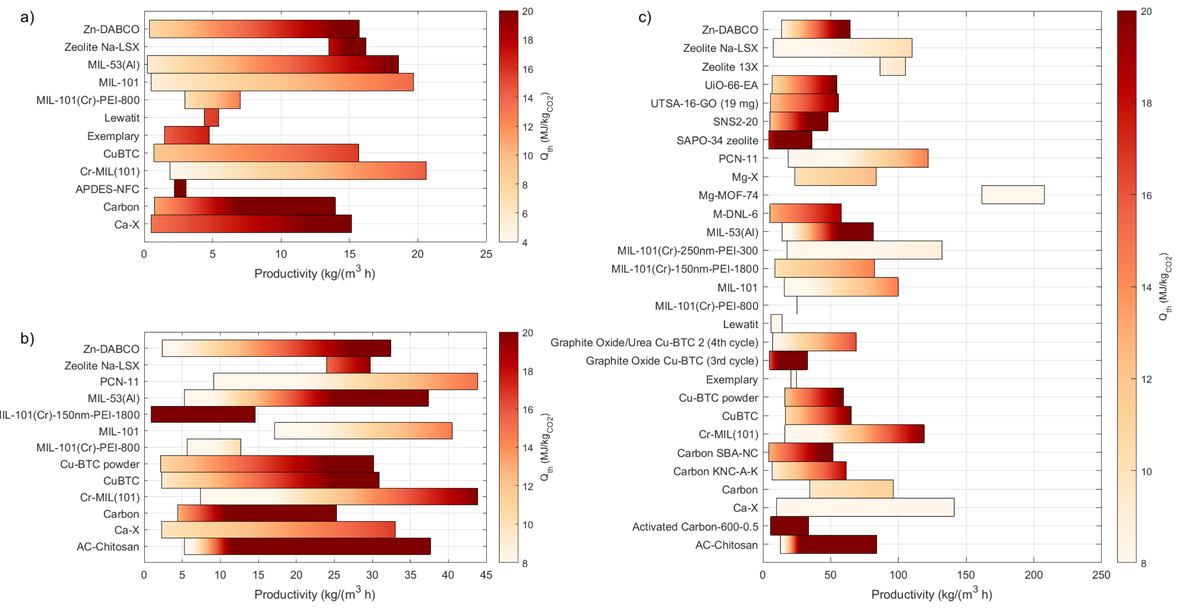
Performance of a specific cycle	Process-optimization
	*minimize(-Pr,e_{th}), subject to* $\phi \geq \phi_{spec}$ 

3 Sorbent screening

- Screening of the NIST/ARPA-E database (around 2500 materials) and 80 additional adsorbents added by hand[2-4].
- Approach:



- Varying the CO_2 concentration in the feed (0.04%, 0.1%, 1.0%).
- For y_{CO2}>0.04%, the capture rate is constrained to >90%.
- Resulting ranking:



4 Sorbent isotherm optimization

Optimization variables

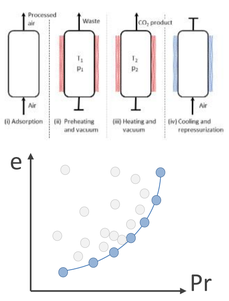
Sorbent

- Fitting **coefficients** for Toth, Toth-cp, DSL, Langmuir-Freundlich, and S-shaped isotherm model
- Physical **properties**: density, void fraction, particle diameter

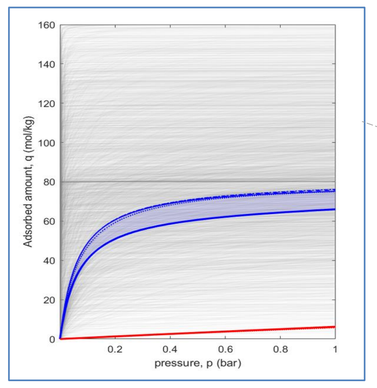
Process

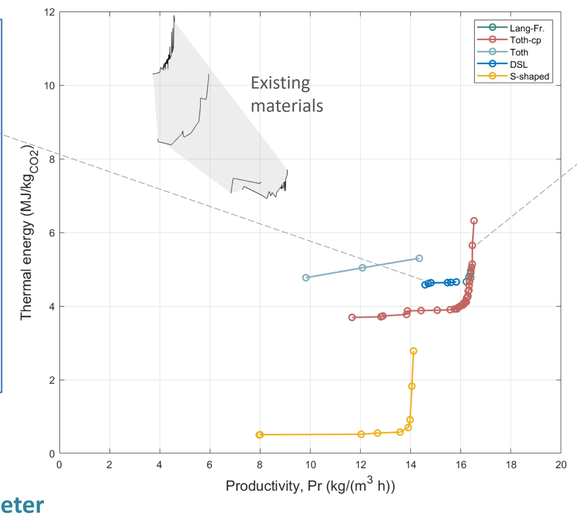
- Desorption temperature T_{des}
- Vacuum pressure p_{vac}
- Feed stream $\dot{V}_{feed}$

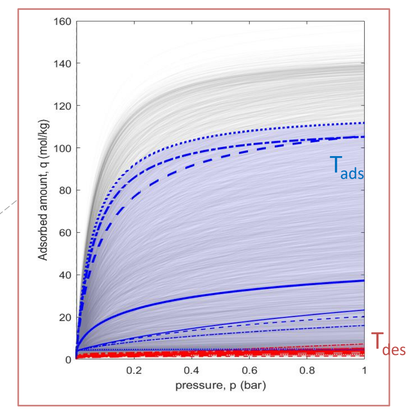
Process modeling + optimization



Isotherm **models** + **metrics**







+ density, **void** fraction, particle **diameter**

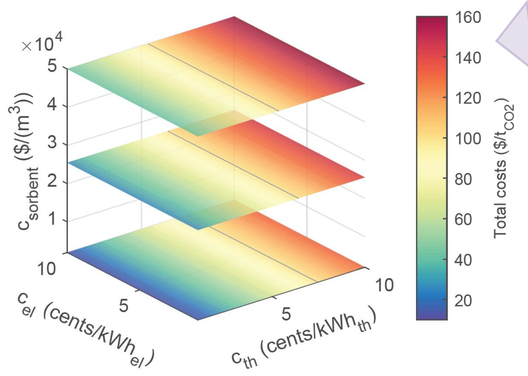
Sensitivity analysis concerning the costs:

As an example, for one Pareto point using the Toth-cp isotherm model, with:

c_{el} = 1-20 cents/kWh$_{el}$

c_{th} = 1-20 cents/kWh$_{th}$

$c_{contactor}$ = 2000-50000 $/m^3



Comparing the simulated isotherms with respect to isotherm metrics (working capacity, equilibrium loading, initial slope, heat of adsorption,…).

Carrying out a sensitivity analysis concerning kinetics using the rate-based model:

k_{LDF}=0.0001-0.1 s^{-1}.

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[1] N. Casas et al., *A parametric study of a PSA process for pre-combustion CO2 capture,* 2013.
[2] *J. Elfving, Direct capture of CO2 from air using amine-functionalized resin - Effect of humidity in modelling and evaluation of process concepts. 2021.*
[3] *M. Khurana; S. Farooq, Adsorbent Screening for Postcombustion CO2 Capture: A Method Relating Equ. Isotherm Characteristics to an Optimum VSA Process Performance, 2016.*
[4] *F. Sabatino et al., A comparative energy and costs assessment and optimization for direct air capture technologies, 2021.*