A Multiscale Modelling Approach to Large-Scale Screening of Porous Materials

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Introduction

Highlights:

- A multi-scale approach for large-scale screening of porous materials proposed.
- The key characteristics of the materials examined in the molecular scales.
- The actual ranking of materials carried out based on the results obtained from process simulations.
- A process modelling and optimization toolbox is under development in which molecular simulations provide equilibrium and transport data, while the materials ranking is performed in the process scale where effects of process configuration, materials stability and process cycle parameters are taken into account.

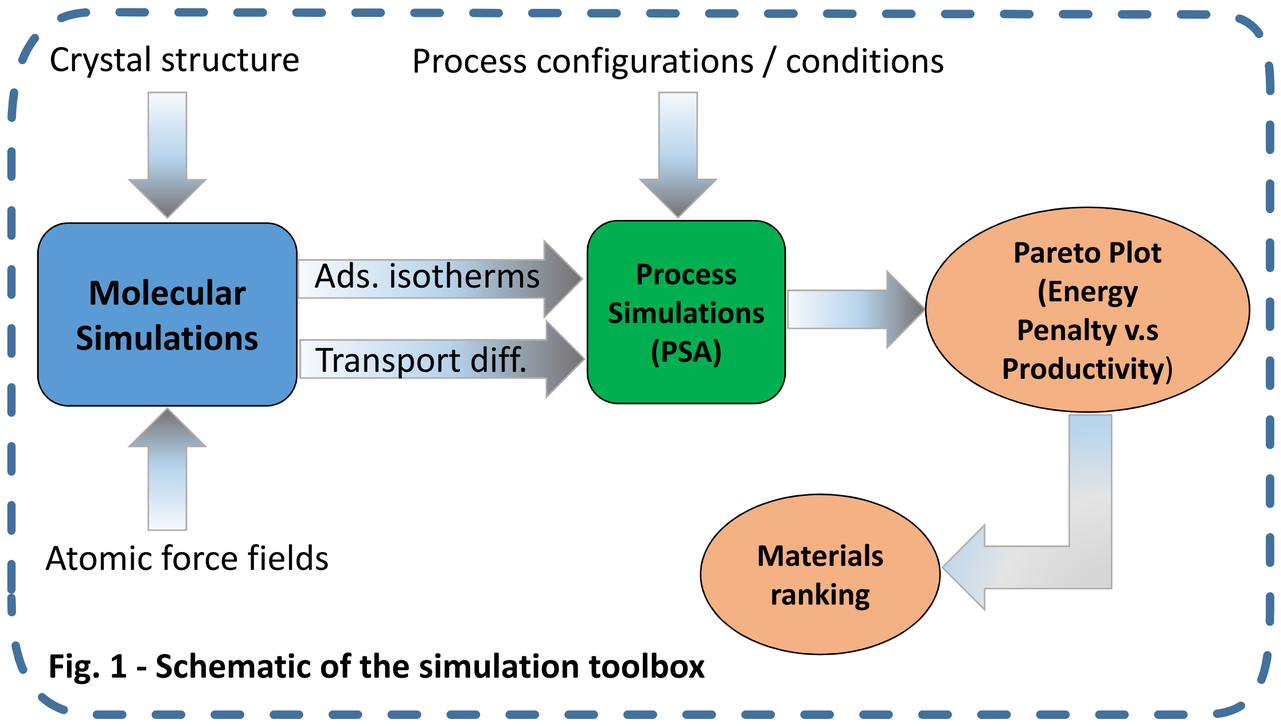


Fig. 1 - Schematic of the simulation toolbox

Post-combustion CO_2 Capture

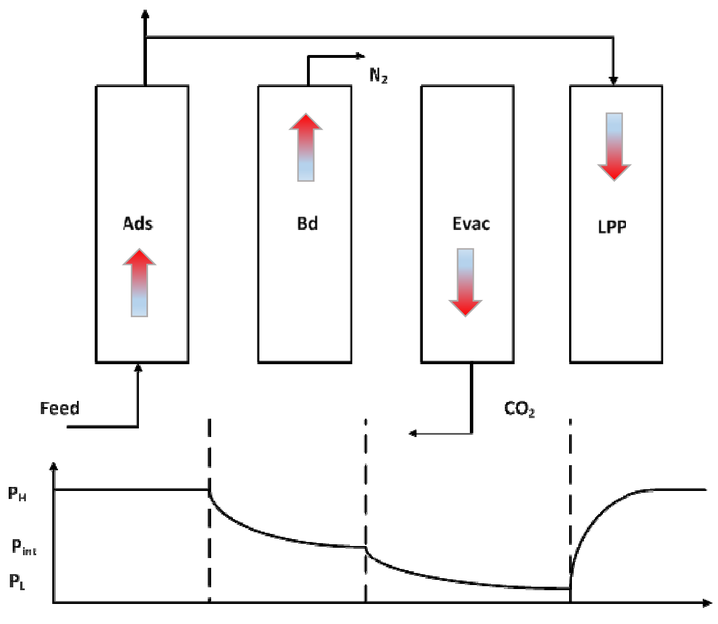


Fig. 2 - Schematic of the 4-step Cycle with LPP

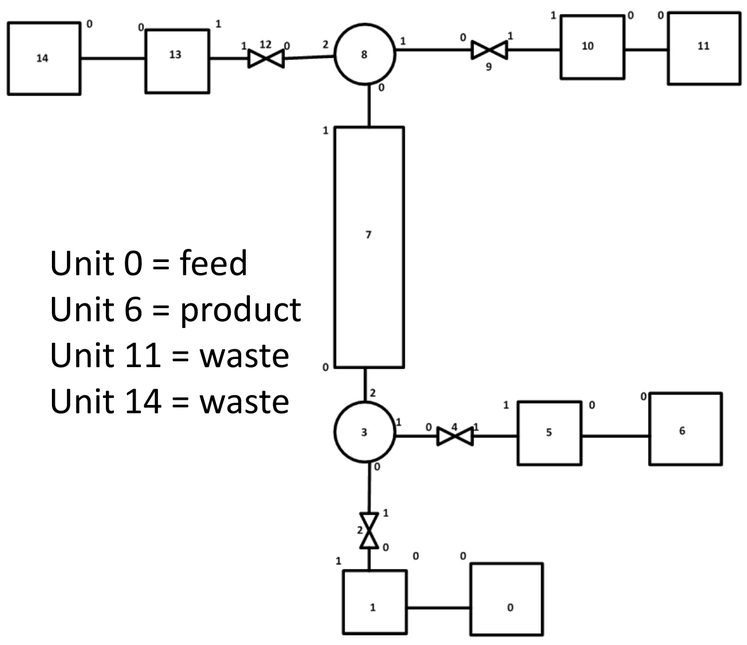


Fig. 3 - Schematic of the 4-step cycle with LPP

Four-step PSA Cycle with LPP for Post-combustion CO_2 capture:

- Adsorption at high pressure with the feed
- Co-current blowdown to an intermediate pressure to remove nitrogen
- Counter-current evacuation to remove the product
- Counter-current pressurizing with the light product to high pressure

Process conditions:

T = 298.15 K
n_{N2} = 85%
n_{CO2} = 15%
Column length = 1 m
Column radius = 0.15 m

Optimization using a multi-objective genetic algorithm:

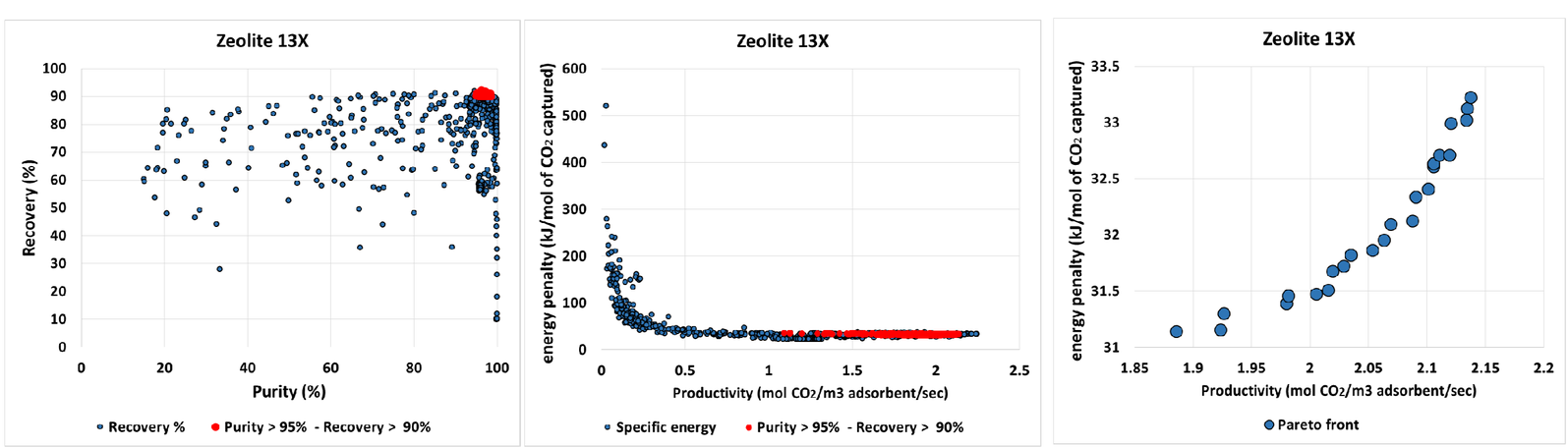
Objectives:

- Purity > 95%
- Recovery > 90%
- Minimized energy penalty
- Maximized productivity

Optimization parameters:

- Adsorption step time
- Blow down step time
- Evacuation step time
- Blow down pressure
- Evacuation pressure
- Feed flowrate

Materials Screening



Future work:

- Detailed process study of PSA cycle based on simulation data.
- Improvement of the computational performance of the simulation modules (GCMC, MD and Process simulations).
- Materials screening based on the results obtained from process simulation.
- Validation of the results against experiment-based process simulation data.

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