Utrecht University

Screening materials for removal of CH_4 from air and non-fossil diluted sources by cyclic adsorption process

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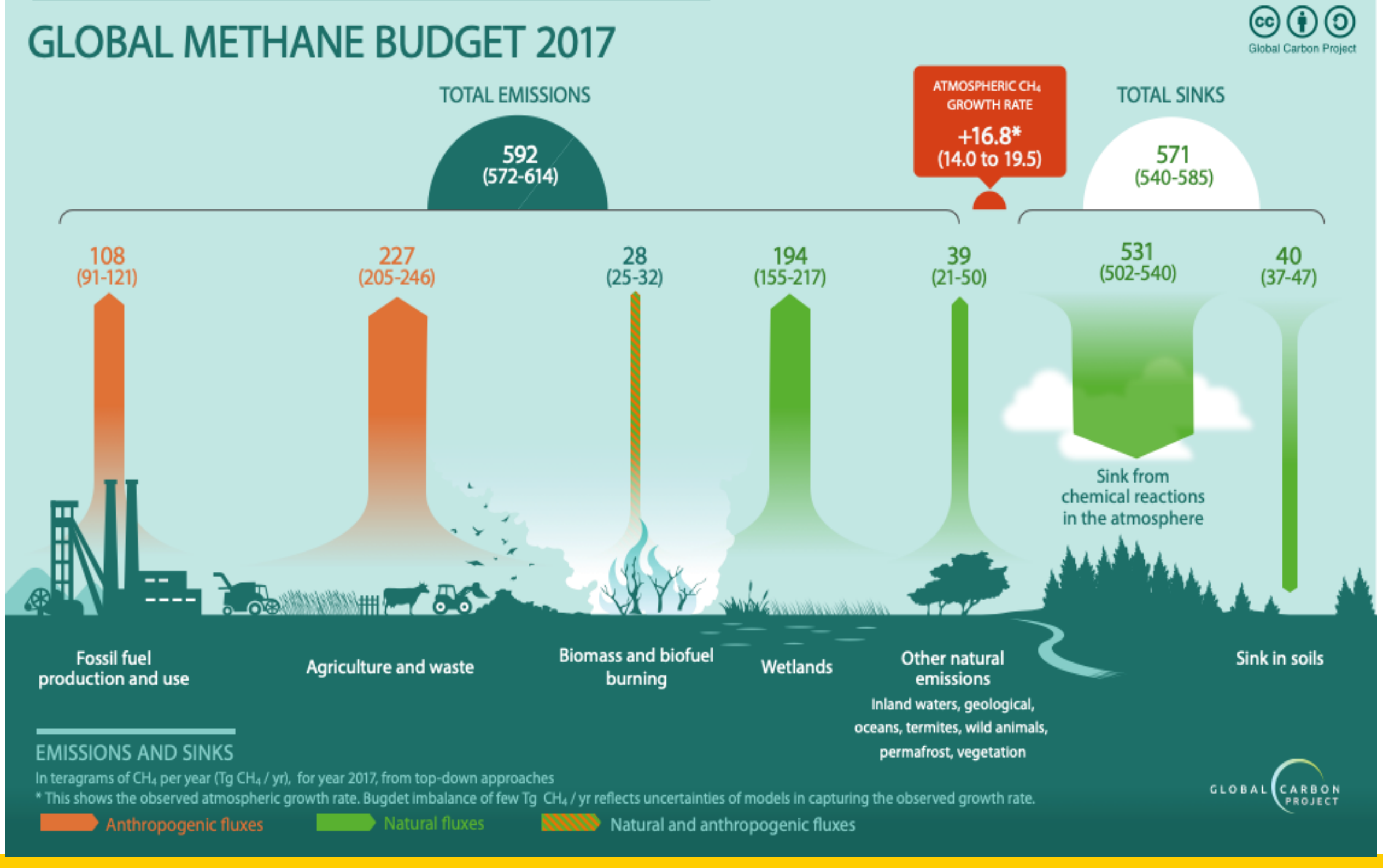
Overview

Motivation

- Methane is a strong short-living greenhouse gas, responsible for 0.5 ° C of the current global warming
- 60% of methane emissions are from anthropogenic sources
- Methane removal could help to lower the peak temperature, and minimize the risk of natural feedback and tipping elements

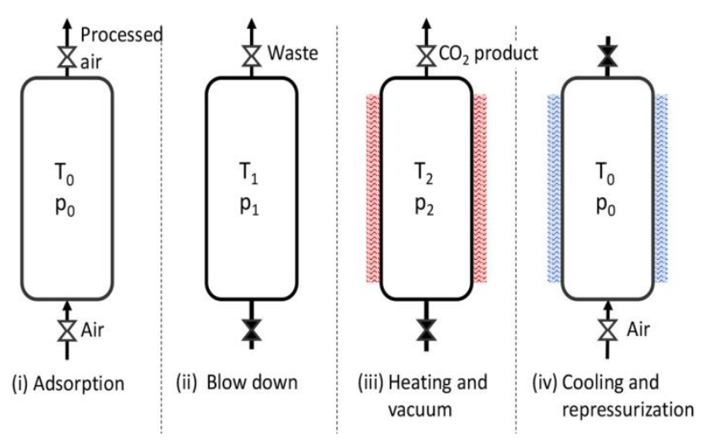
Aim

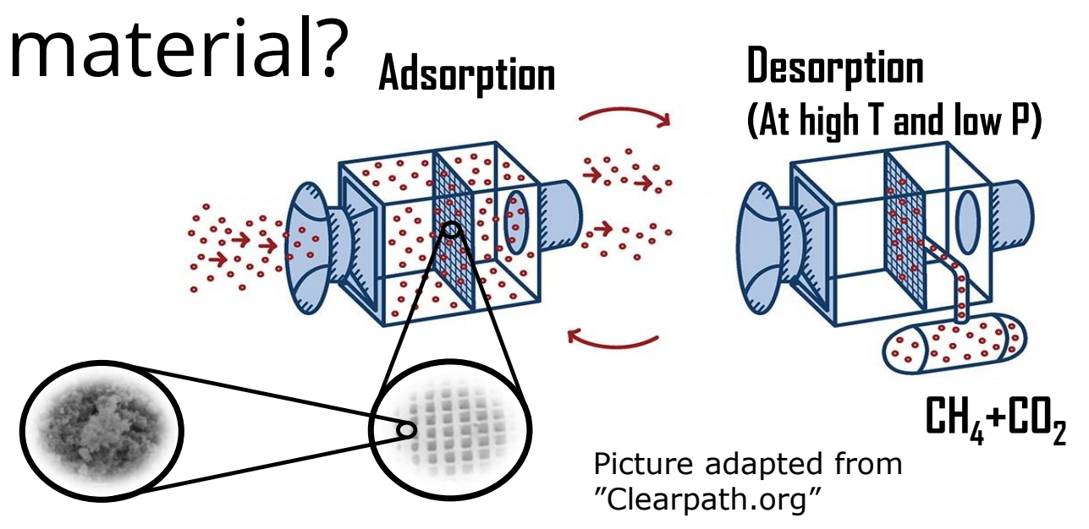
- Investigate the potential of adsorption process for CH_4 capture
- Find suitable sorbents for methane capture from non-fossil, diluted sources (<1% CH4) by screening large material database



Cyclic Adsorption process Design

- Vacuum Temperature Swing Adsorption (VTSA)
- Collector?
  Radial
  Monolith
  Layered bed
- Operating conditions?
- Sorbent material?





Picture adapted from "Clearpath.org"

Screening Methodology

Modelling method: Shortcut equilibrium model (0D)

- Fully mixed reactor, no spatial gradient
- Ternary mixture of N_2, CH_4 and CO_2, where all components can adsorb
- Including multiple isotherm types in the model, i.e. Toth, Langmuir-Freundlich and s-shaped isotherm model

Energy and material balances:

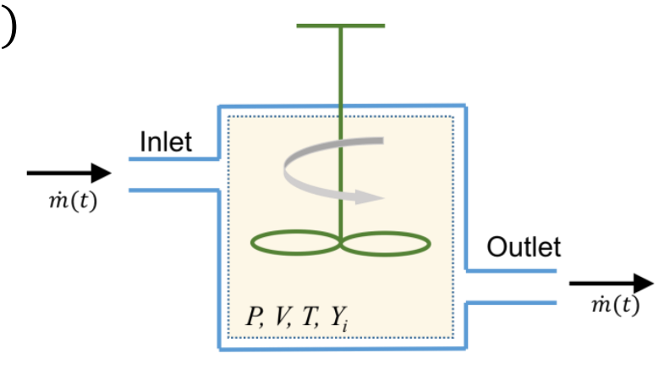
$$\sum_i N_{i,total}(t_f) - \sum_i N_{i,total}(t_0) = \int_{t_0}^{t_f} \dot{N}_{in} dt - \int_{t_0}^{t_f} \dot{N}_{out} dt$$

$$N_{i,total}(t) = N_{i,s}(t) + N_{i,f}(t)$$

$$N_{i,s}(t) = m_s q_i^*(y_i, p, T)$$

$$q_i^* = f(y_i, p, T)$$

$$N_{i,f}(t) = \frac{p y_i V_c \epsilon}{RT}$$



$$m_s c_{p,s}\left(T(t_f) - T(t_0)\right) = \int_{t_0}^{t_f} \dot{Q} dt + (N_{i,s}(t_f) - N_{i,s}(t_0)) \sum_i^n |\triangle H_{ads,i}|$$

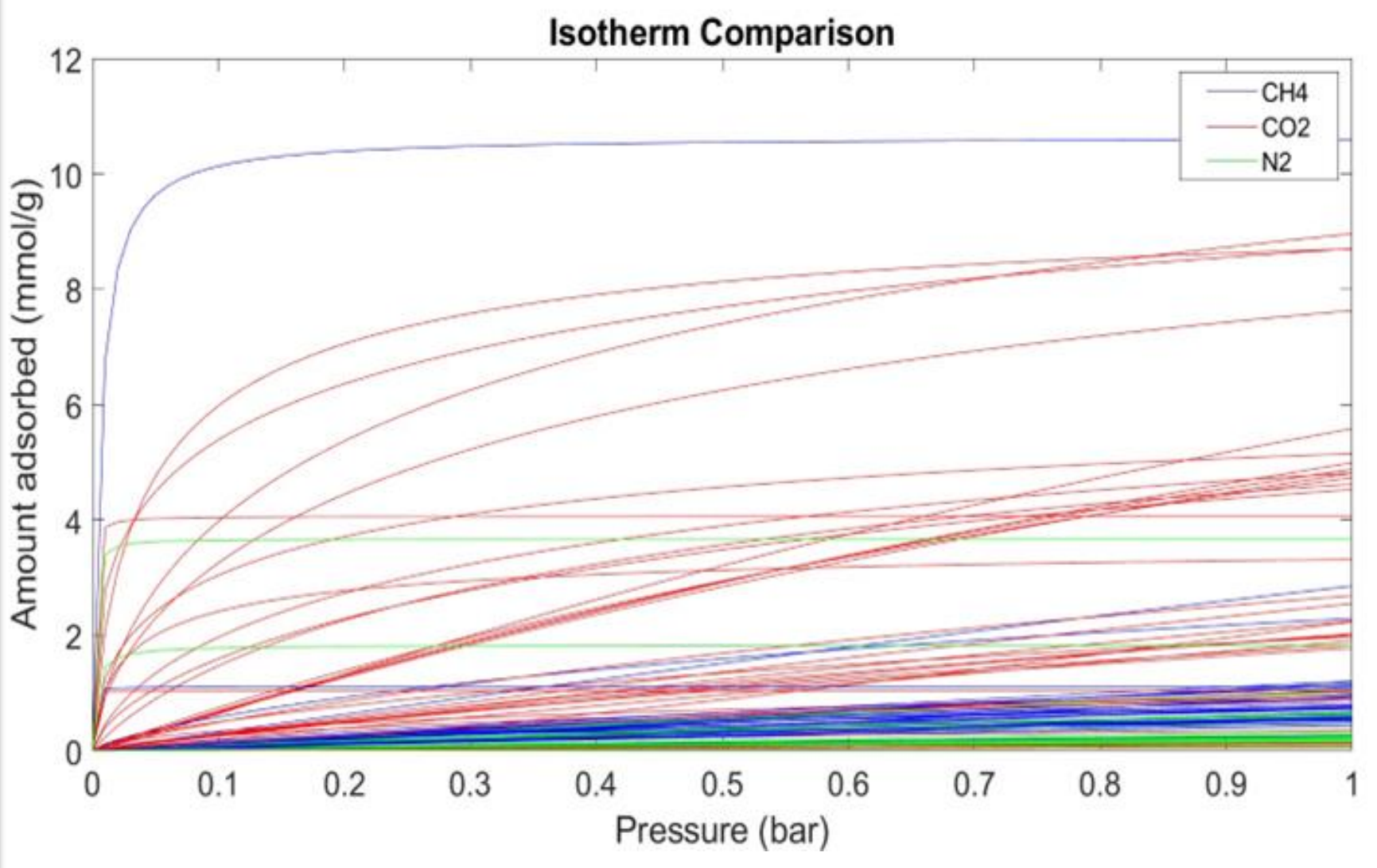
$$\left(\frac{\partial ln p_i}{\partial T}\right) = \frac{-\triangle H_{ads,i}}{RT^2}$$

Step 1: Sorbent data and isotherms

Database

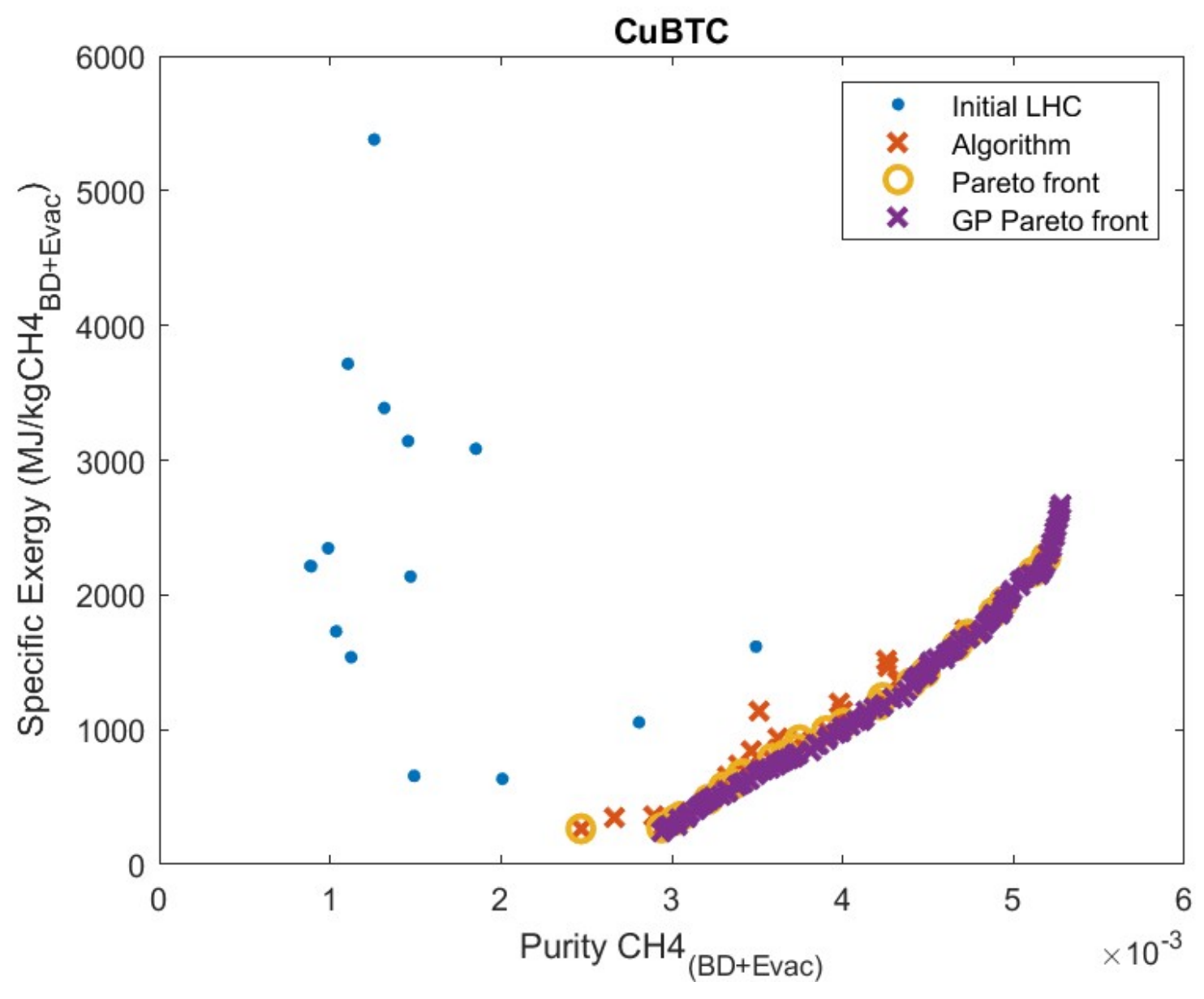
- **NIST/ARPA-E** Database of Novel and Emerging Adsorbent Materials
- More than 8000 materials

Sorting and isotherm fitting



Step 2: 0D optimization

- Algorithm:
  Thompson Sampling Efficient Multiobjective Optimization (TSEMO)
- Decision variables:
  Desorption and Adsorption Temperature, Vacuum Pressure
- Objectives:
  Min (-Purity, specific exergy)

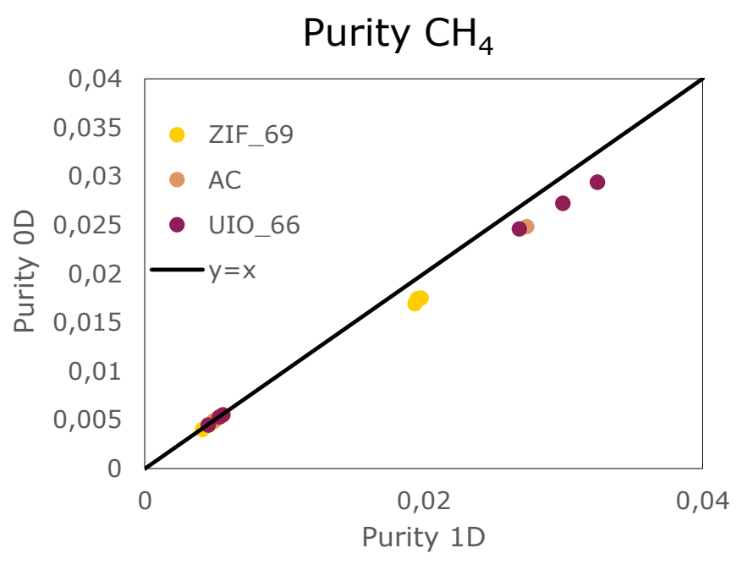


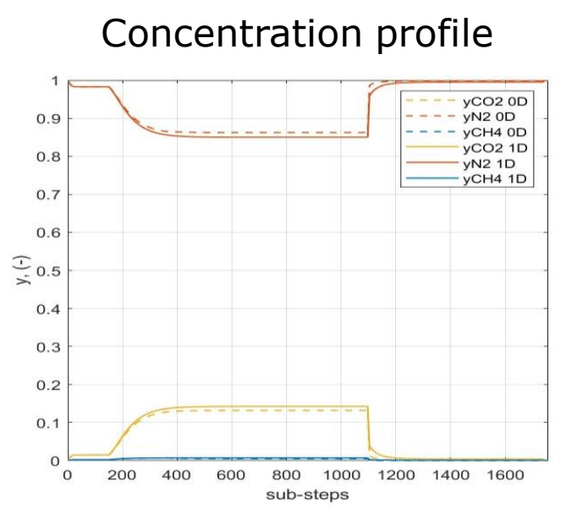
Step 3: Rate-based model optimization (1D)

- Algorithm:
  Multi-Objective Multi-Coordinate Search (MO-MCS)
- Decision variables:
  Adsorption time, Adsorption T, Feed flowrate, Vacuum P, Preheat T, Preheat time, Heating T, Heating time
- Objectives:
  Min(-Prodcutivity, specific exergy)

0D validation against 1D

- Process performance and Concentration profile

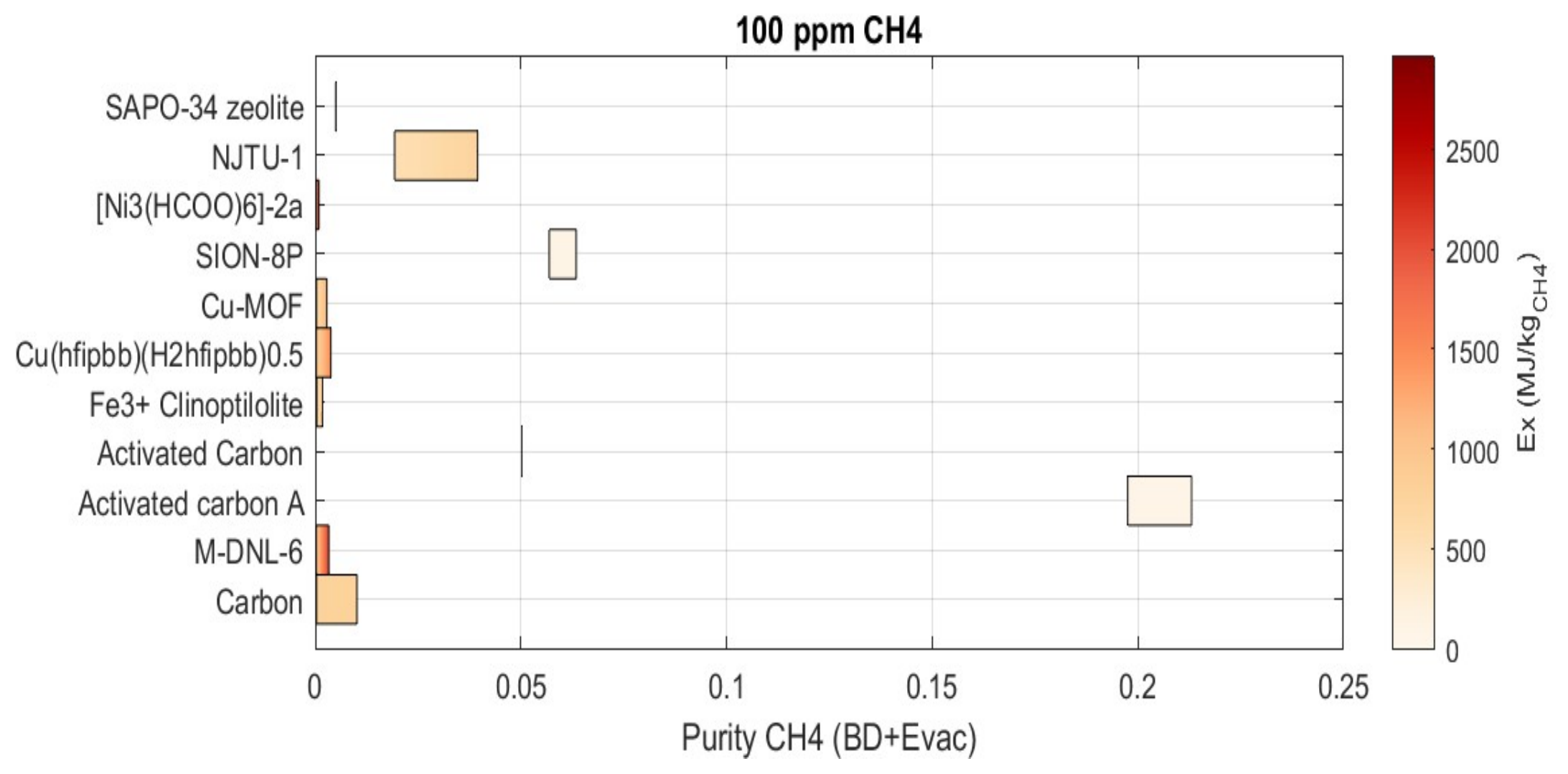




Results

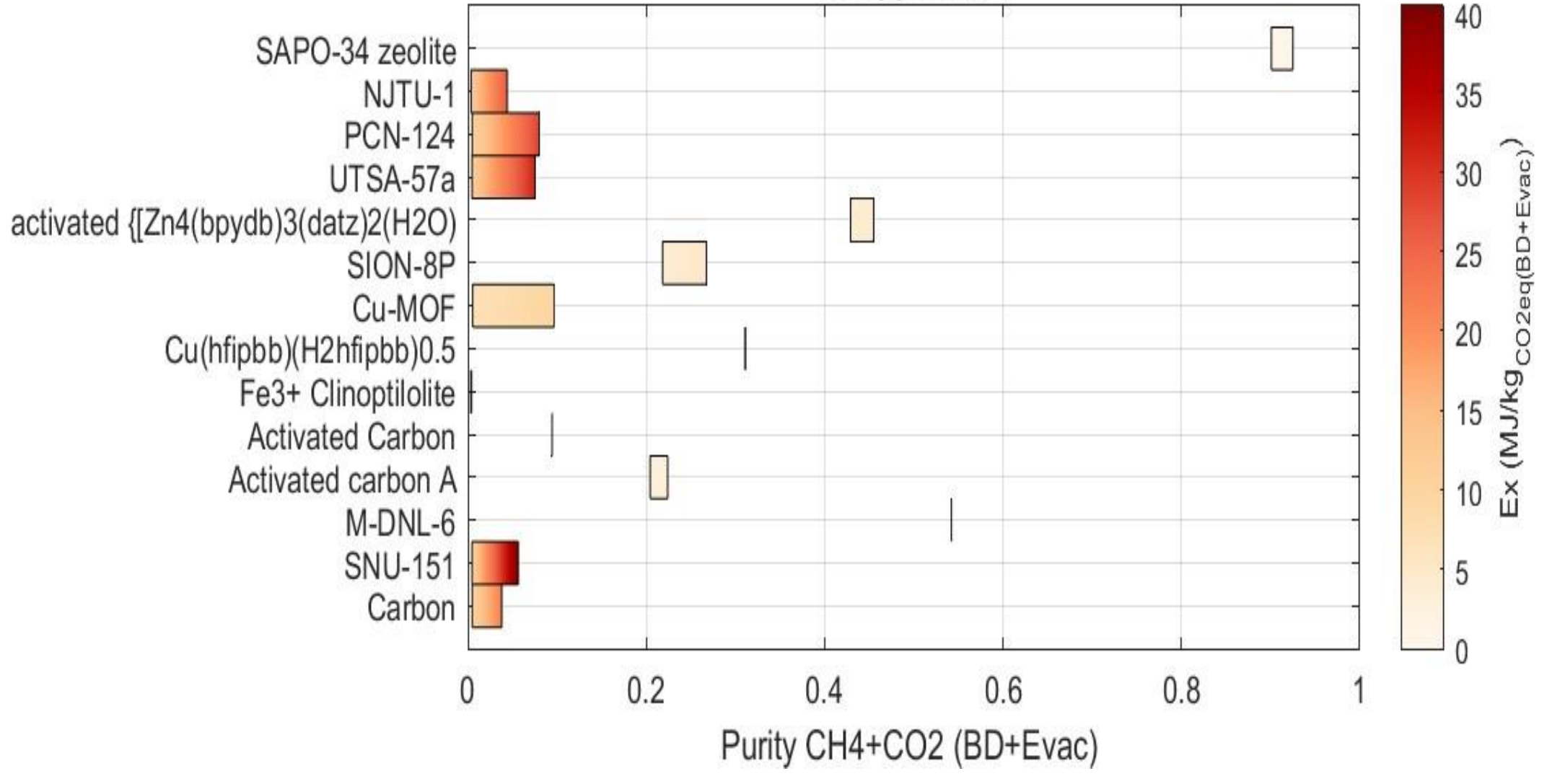
CH_4 Capture

Feed: **100 ppm** CH_4 -1800 ppm CO_2



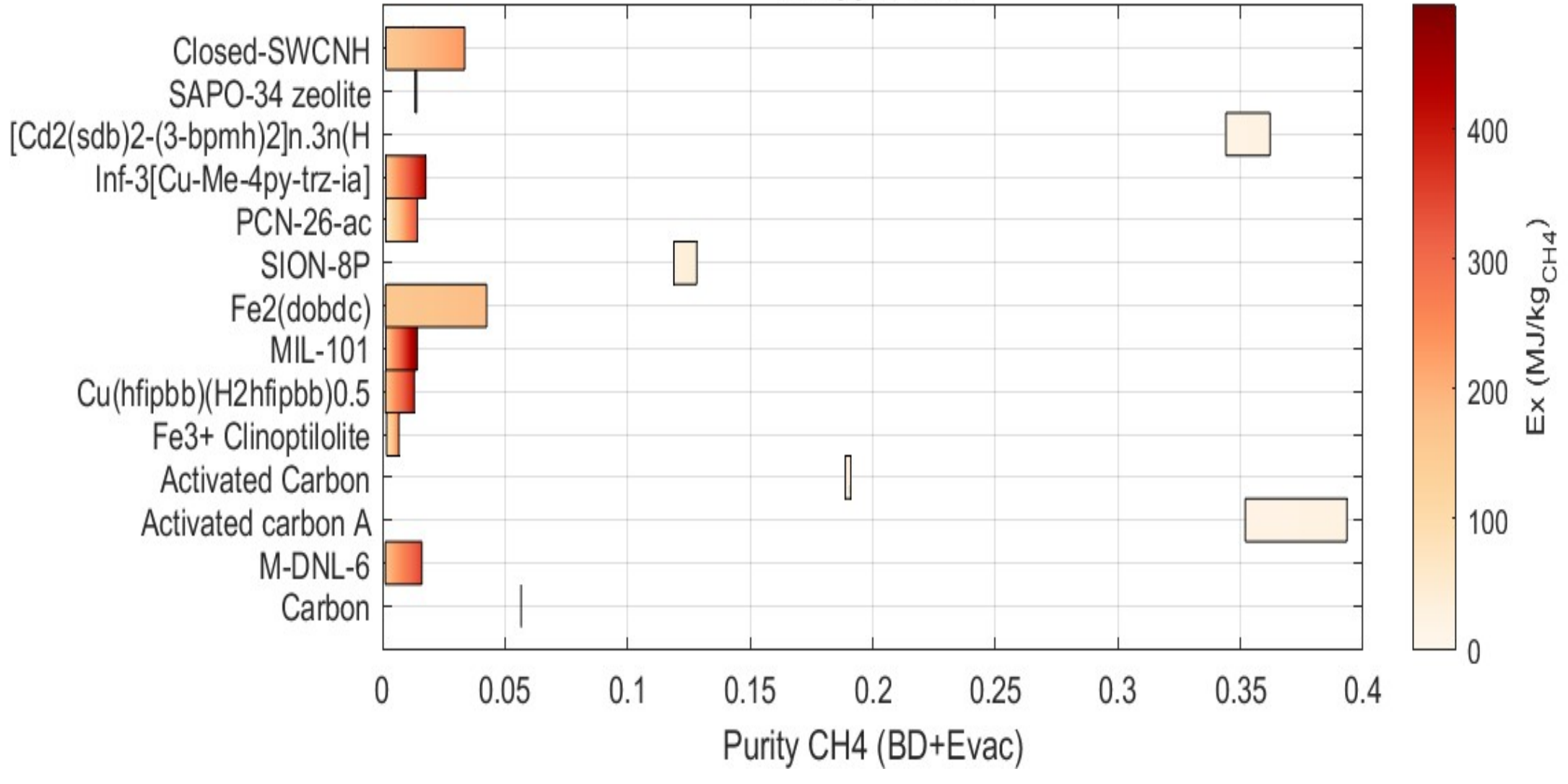
CH_4-CO_2 Co-capture

Feed: 100 ppm CH_4 -1800 ppm CO_2



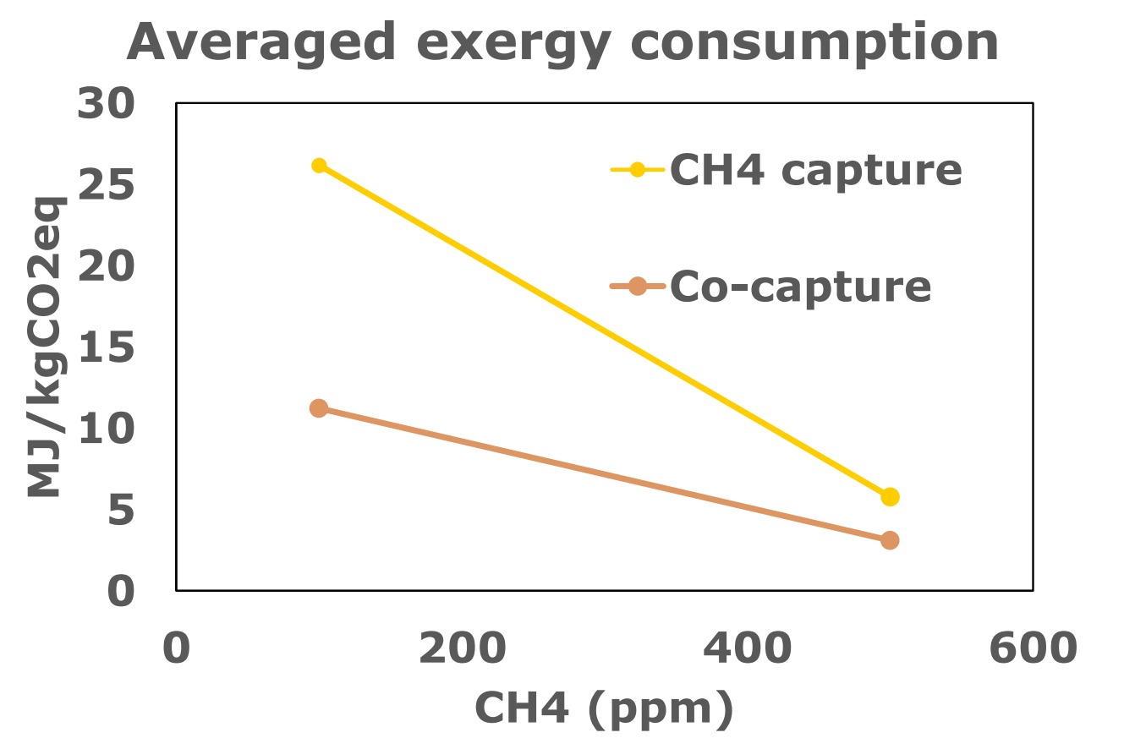
CH_4 Capture

Feed: **500 ppm** CH_4 -1800 ppm CO_2



Conclusions

- Despite the low working capacity for methane adsorption from diluted sources, there are promising materials that are suitable candidates for methane capture.
- Co-capture of CH_4 and CO_2 is an interesting scenario that can lead to lower exergy consumption (MJ/kgCO2eq).
- Concentration of the greenhouse gas plays a key role in exergy consumption of the capture process, with higher concentration being more favourable.
- 0D modelling is an effective tool for screening a large material database, but 1D model simulations are required for final design of the process.



References

1. Alexa Grimm, Matteo Gazzani, *Ind. & Eng. Chem. Res, 61* (37), 2022
2. Global Carbon Project, 2020

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Acknowledgement
This work was carried out as a part of the project "Removing non-CO2 greenhouse gas emissions to support ambitious climate transitions (REPAIR)" (Project number: 101069905) funded by the European Commission via the European Climate, Infrastructure and Environment Executive Agency (CINEA) within the Horizon Europe framework.

REPAIR