Imperial College London

Adsorbent screening for CO_2/N_2 separations using TSA

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UKCCSRC Autumn Web Series, 15/10/2020

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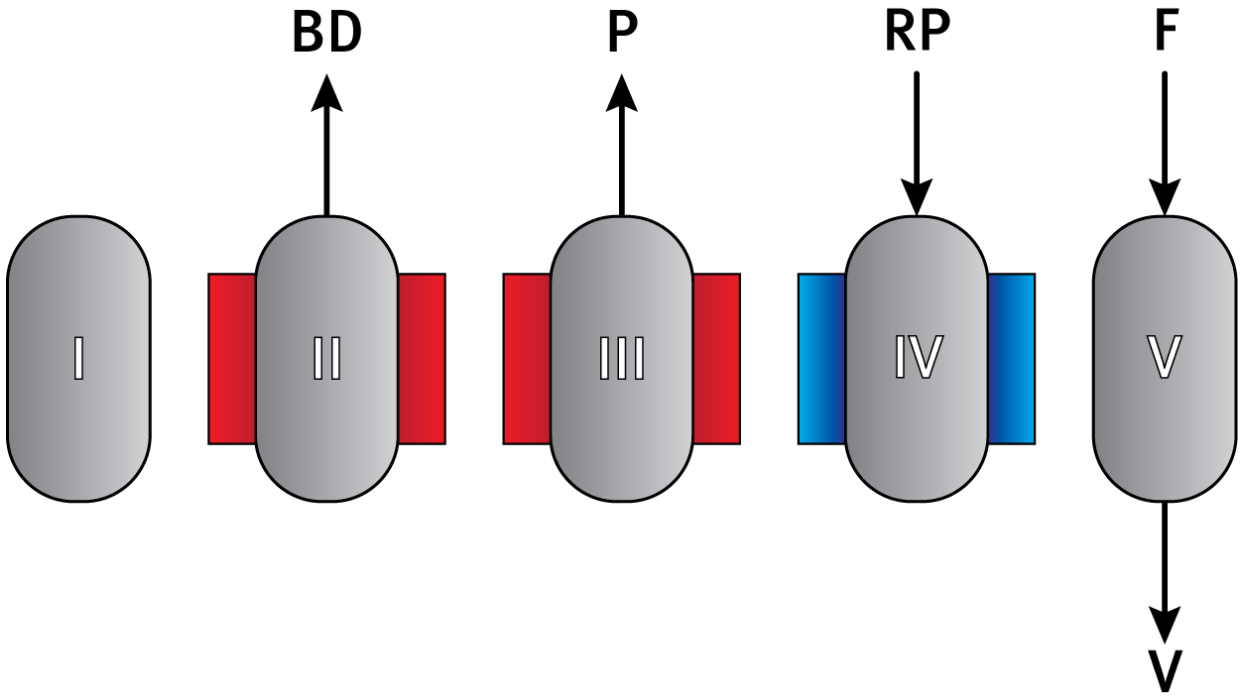
Introduction

- Significant focus on materials for CO_2 capture
- Little focus on cyclic performance
- Adsorbent screening tool
- Follow on from previous work on PVSA
  - Danaci *et al.*, *Mol. Syst. Des. Eng.*, 2020, 5, 212

- How do MOFs compare for large-scale post-combustion CO_2 capture?
- Where are improvements necessary to increase accessibility and reduce costs?

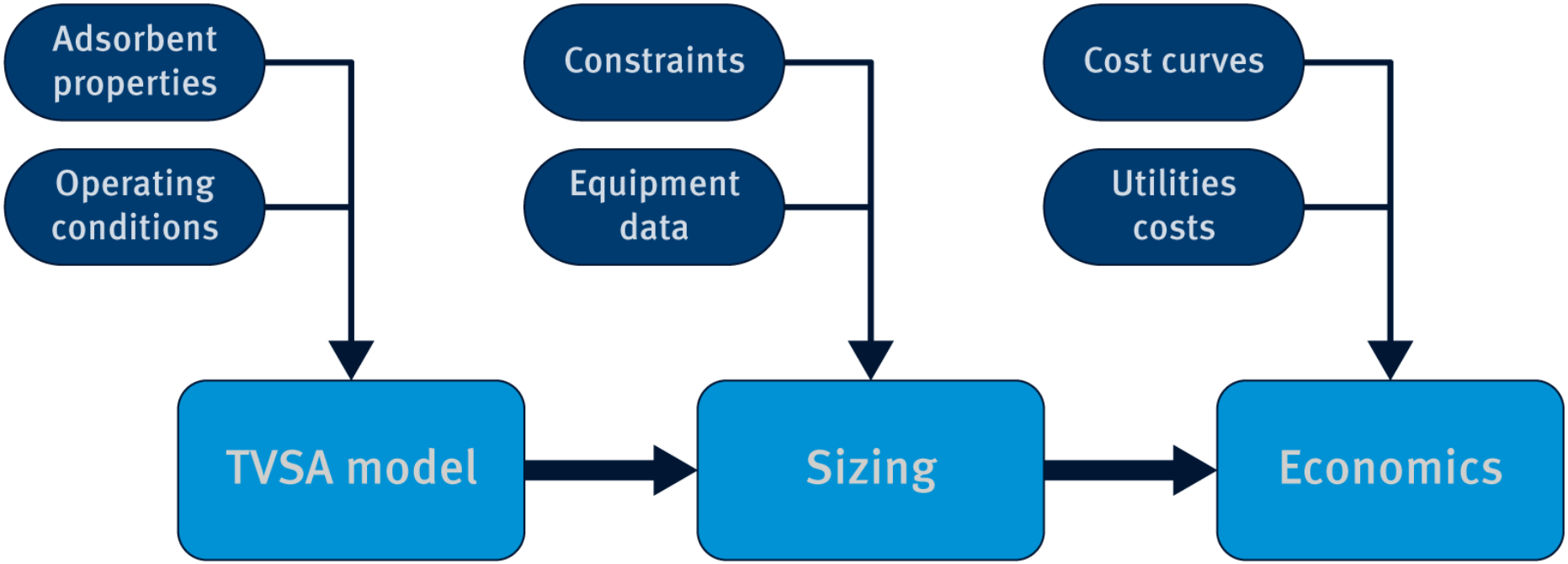
TVSA model



- BD – Blowdown
- P – CO_2 product
- RP – Re-pressurisation
- F – feed
- V – vent / N_2 product

- Equilibrium model
- Well mixed

Adsorbent screening tool



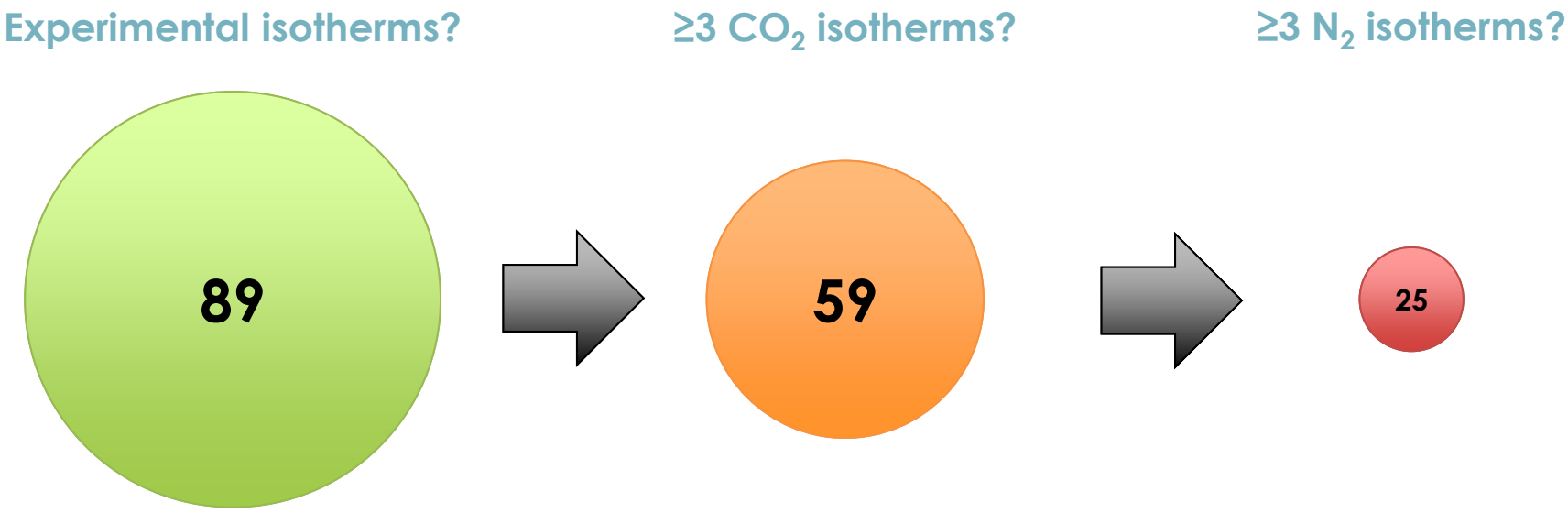
Model limitations and benefits

- Adsorption kinetics are not considered
  - Unsuitable for rigorous process design
  - Adsorbent performance generally overestimated

- Rapid evaluation (<5 seconds)
- Representative of cyclic performance
- Can be coupled with process economics
- Screening accounting for process design aspects and economics

Input data limitations

- Insufficient isotherm data in published literature
- Lack of adsorbent heat capacity data
- Help facilitate process evaluation!



Energy consumption

- Mechanical energy input
  - Feed gas blower
  - Vacuum pump
- Thermal energy input
- Are all joules equal?

$$E_W^{eq} = \eta_{isen}\left(1 - \frac{T_L}{T_H}\right)Q_H + W_S$$

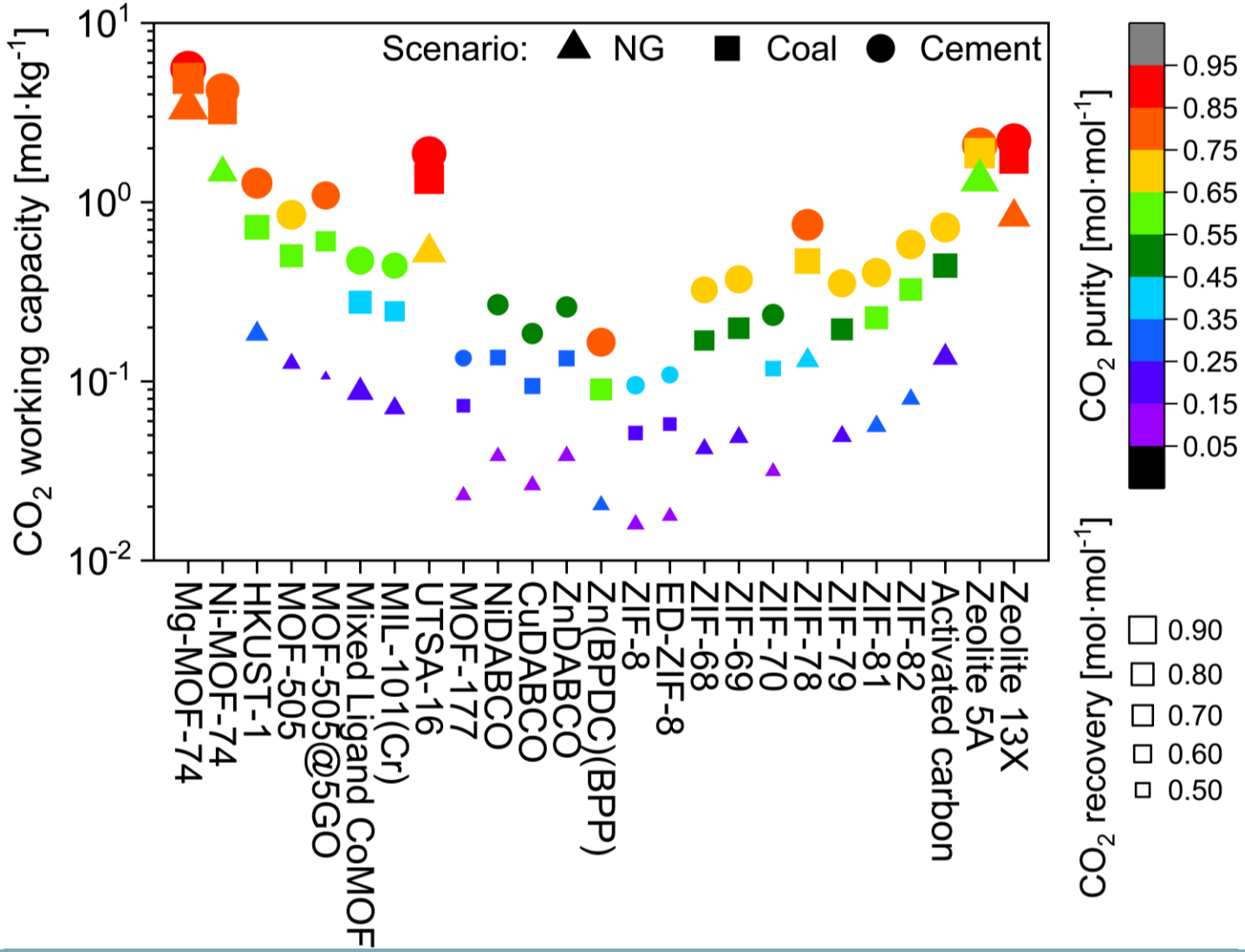
$$E_Q^{eq} = Q_H + \frac{W_S}{\eta}$$

Scenarios investigated

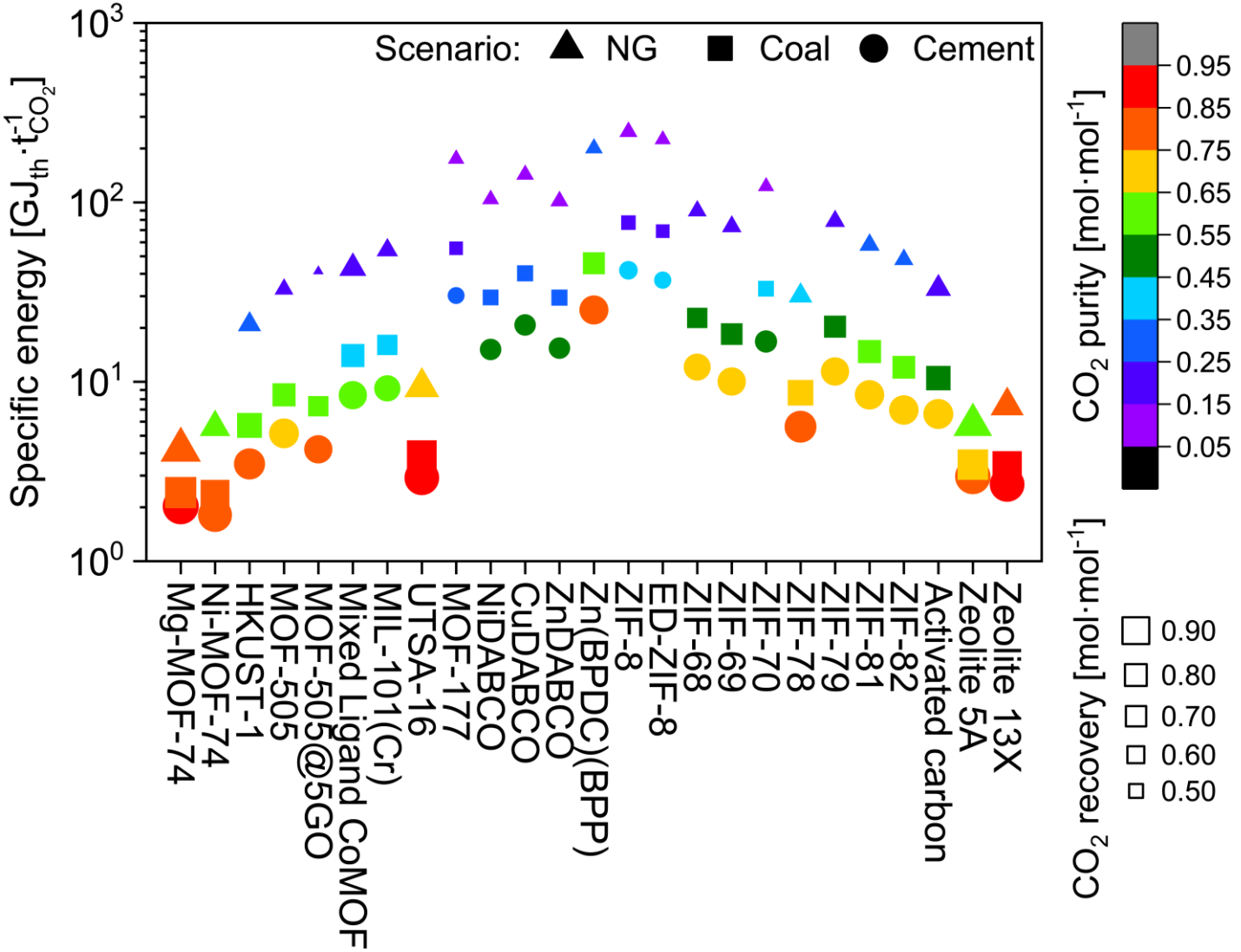
- CO_2/N_2 mixtures only
  - Natural gas fired power – 4.38%$_{mol}$ CO_2
  - Coal fired power – 12.5%$_{mol}$ CO_2
  - Cement plant – 21.0%$_{mol}$ CO_2

- Fixed operating conditions
  - Desorption at 200 °C, no blowdown – TSA only
- Variable operating conditions
  - TVSA investigated

Adsorbent screening – fixed conditions



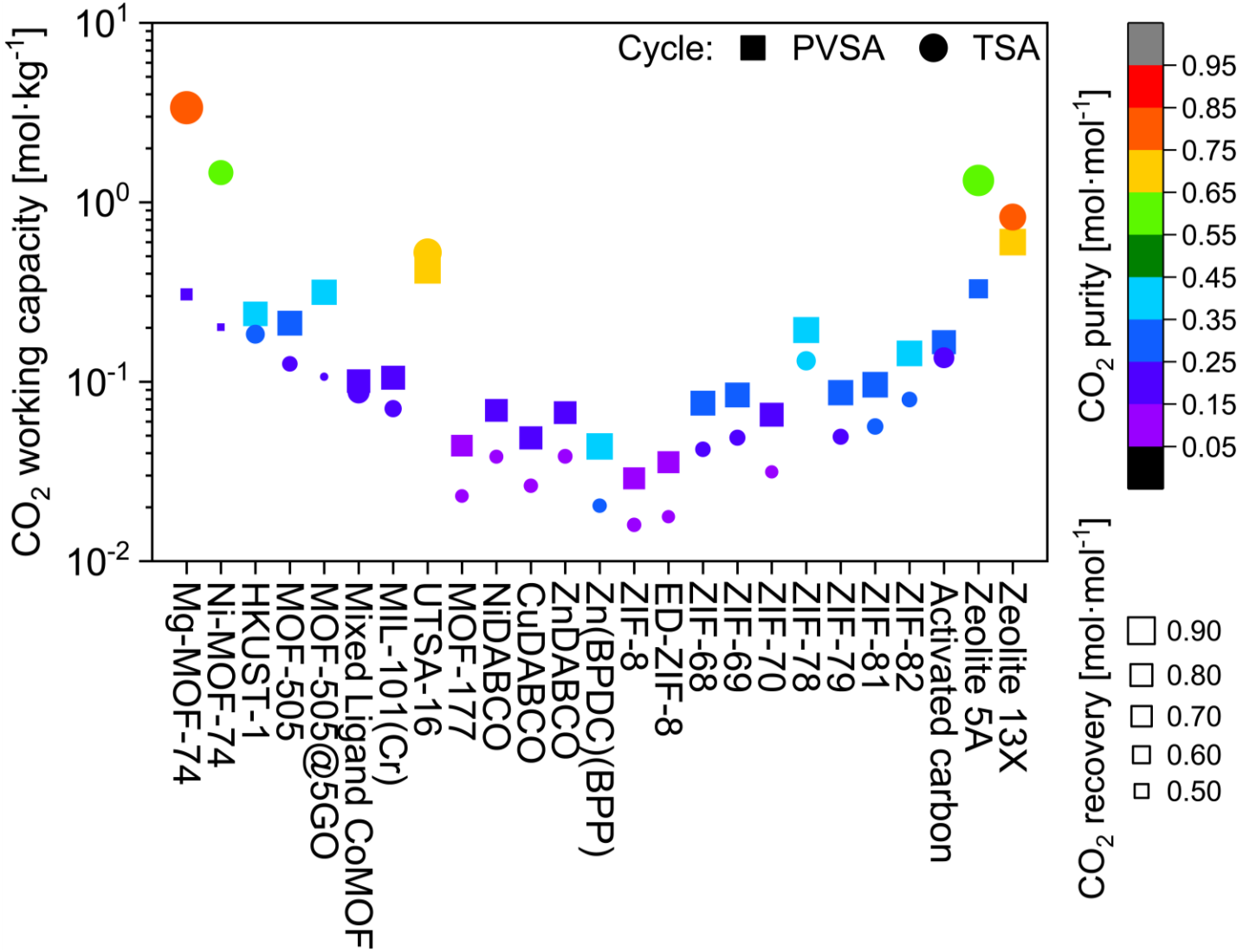
Adsorbent screening – fixed conditions



Comparing TSA and PVSA

- Fixed operating conditions for both
  - For TSA: T_{des} = 200 °C
  - For PVSA: P_{des} = 0.01bar_a
  - Not really a fair comparison
- Highlights importance of combined adsorbent-process selection

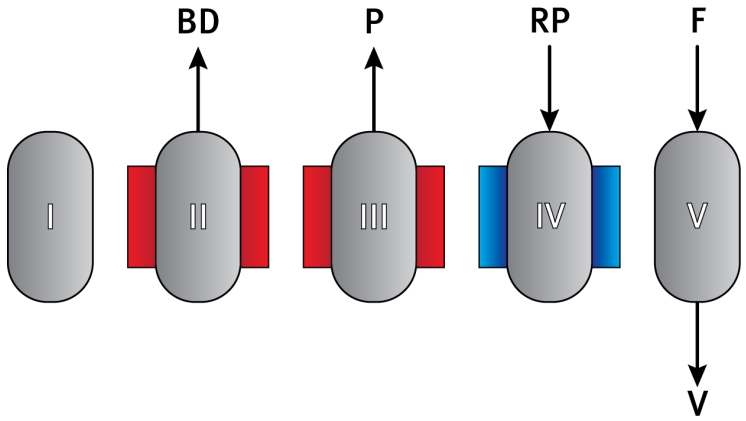
Comparison to PVSA



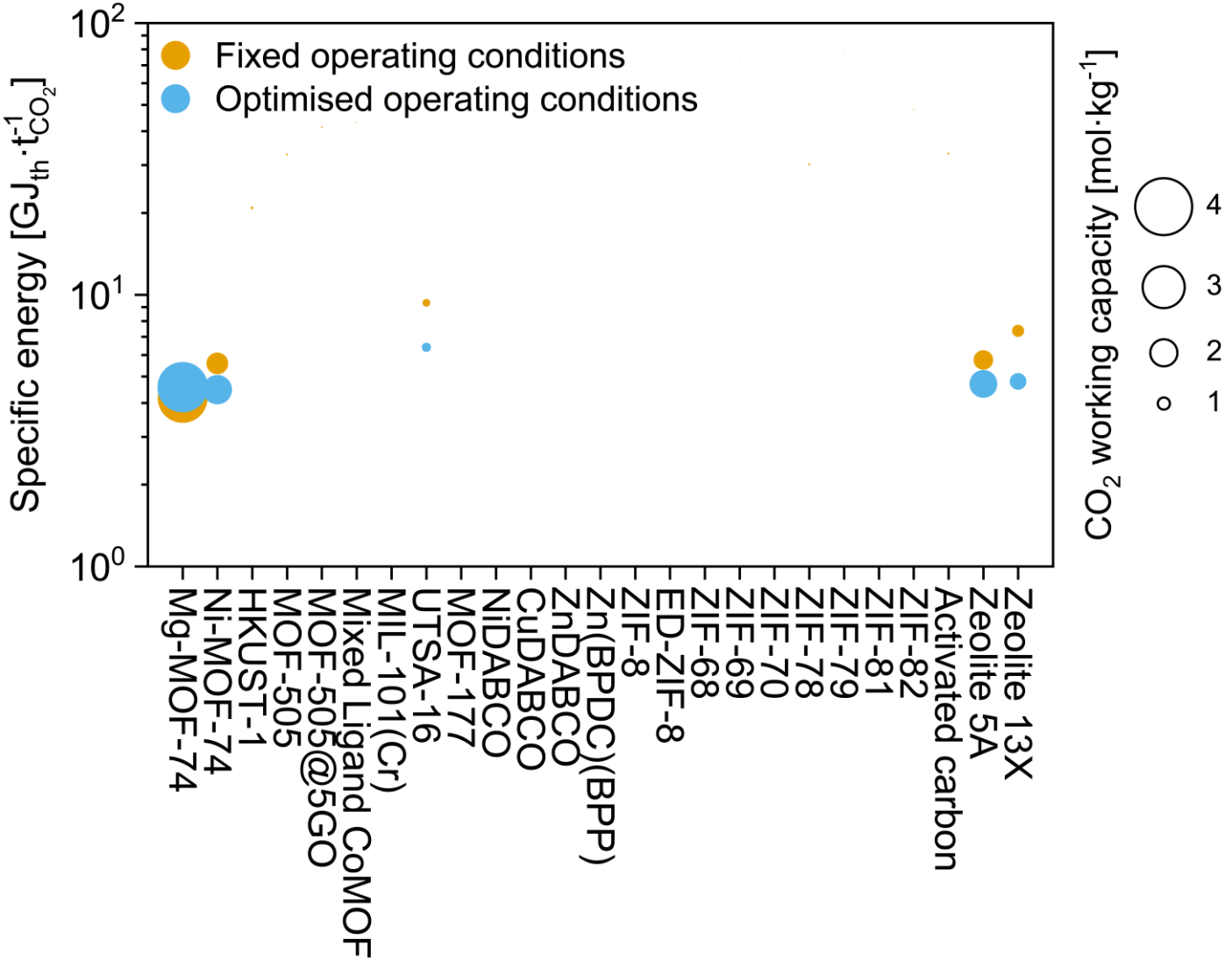
Target purity and recovery

- Optimise operating conditions
  - Desorption temperature & pressure, blowdown – TVSA
  - Target 95%$_{mol}$ purity, and 90% recovery
  - Minimise energy consumption

- Variable range:
  - T_{des}: 80 °C to 250 °C
  - P_{des}: 0.01 bar_a to P_{ads} (1.50 bar_a)
  - Blowdown: 0 to 95%



Optimised operating conditions – NG

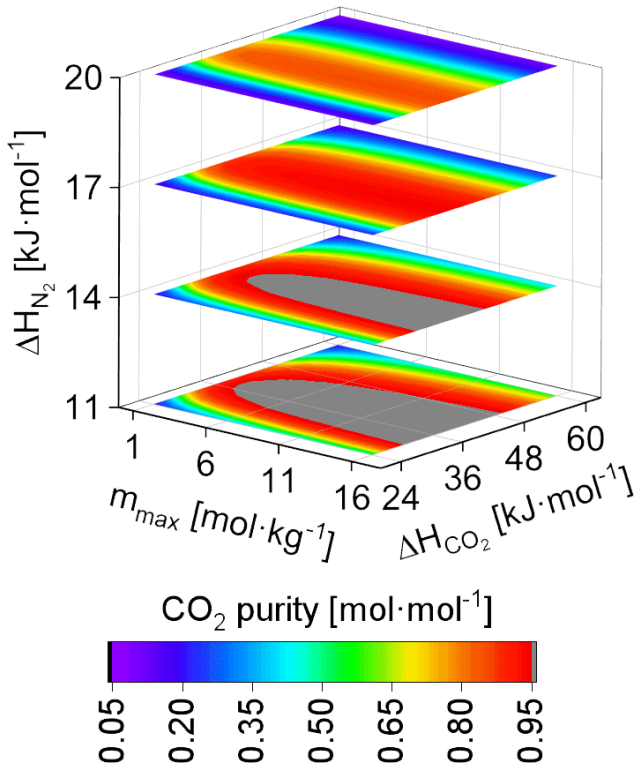


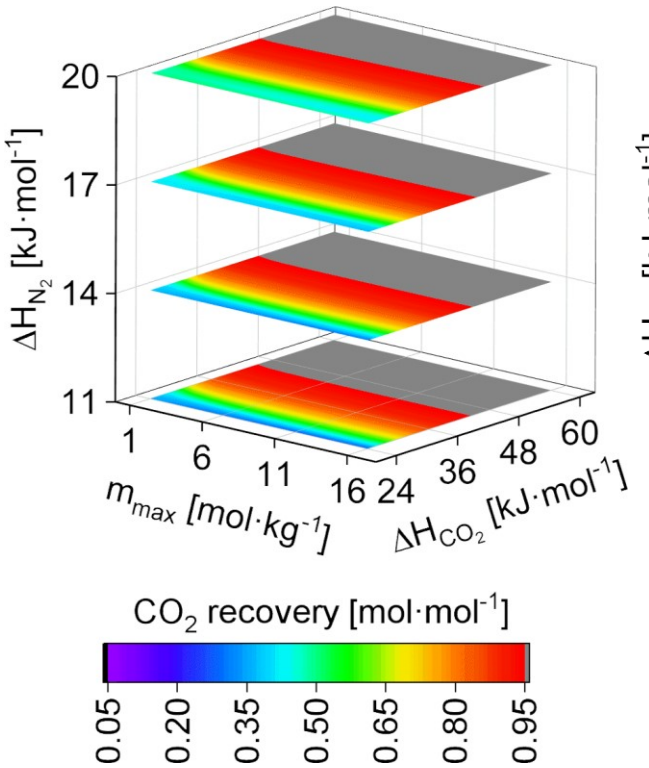
‘Ideal adsorbent’

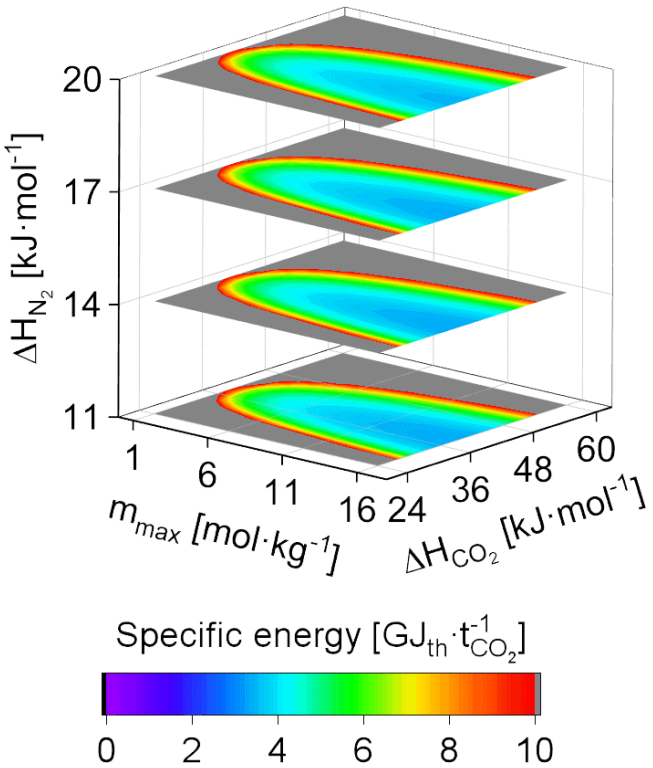
- Which isotherm properties are best?
  - Related to adsorbent properties
- Operating conditions are fixed

$$n_i = m_{\max} \frac{b_0 \exp\left(\frac{\Delta H_i}{RT}\right) P}{1 + b_0 \exp\left(\frac{\Delta H_i}{RT}\right) P}$$

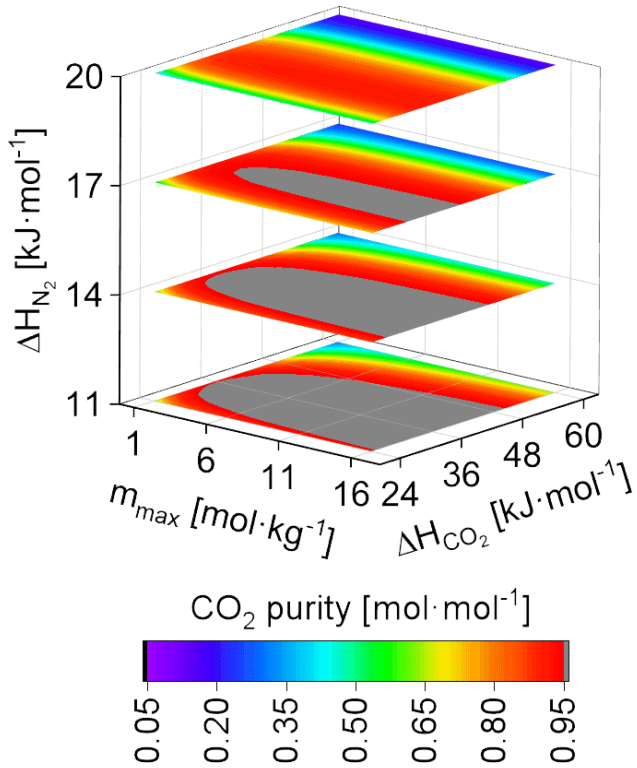
Natural gas scenario

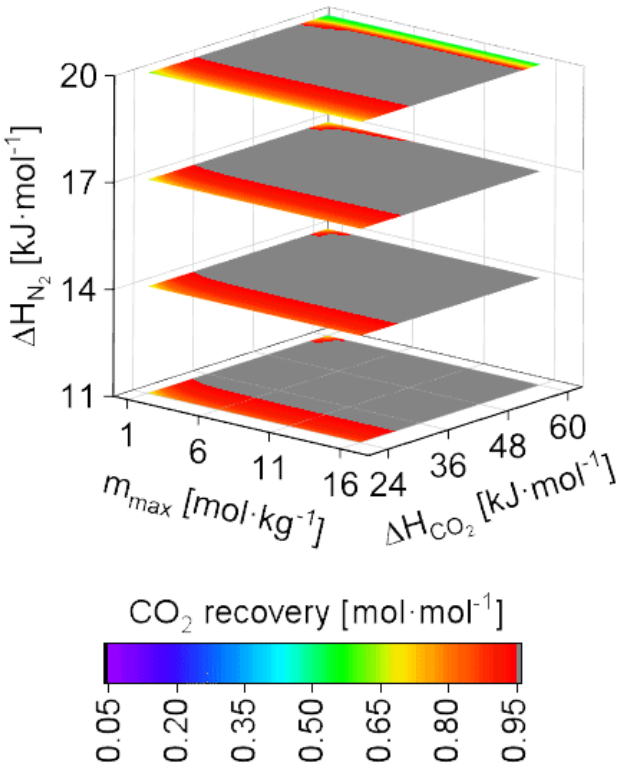


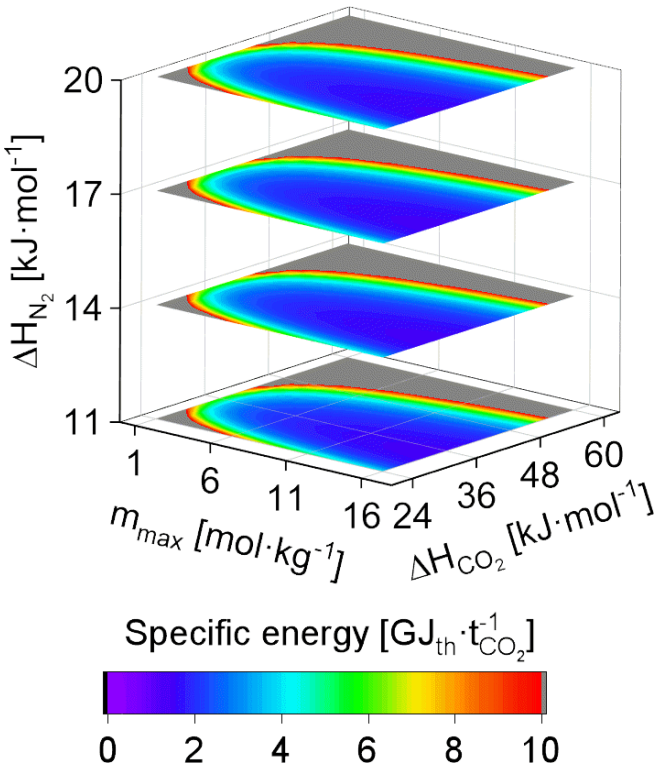




Cement scenario

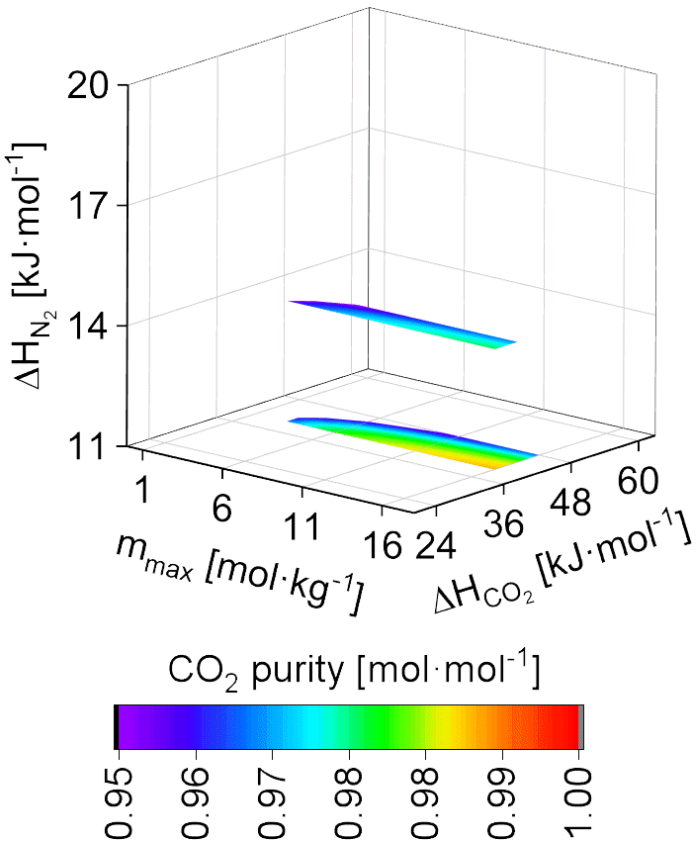




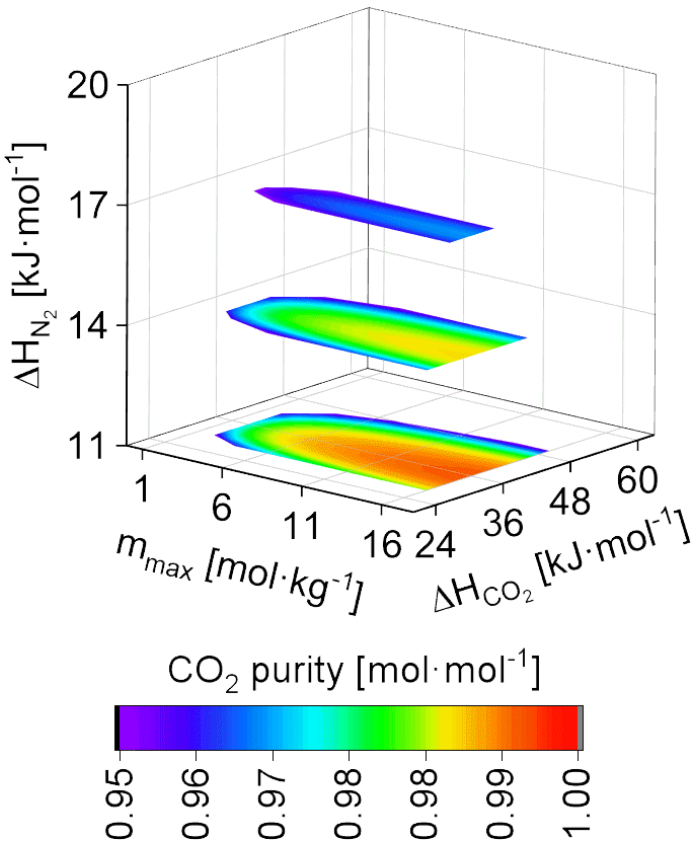


Zones that achieve 95/90 target

Natural gas scenario



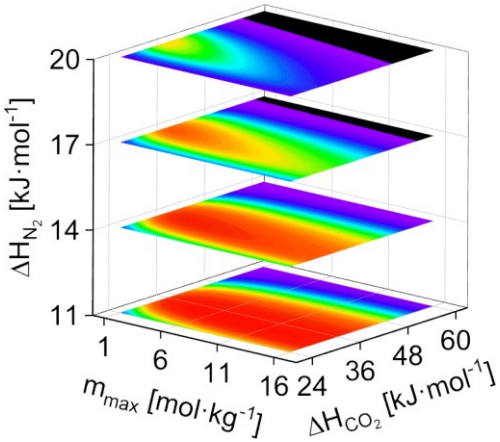
Cement scenario

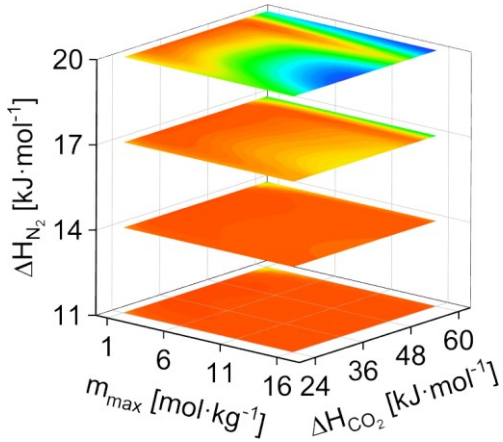


Comparison to PVSA – NG

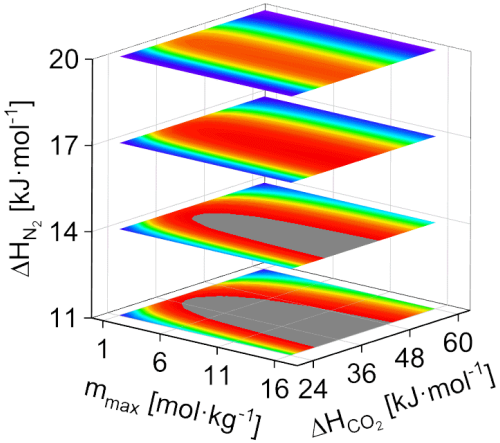
Purity | **Recovery**

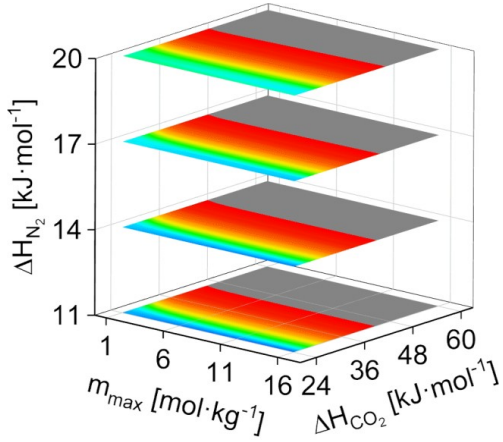
PVSA

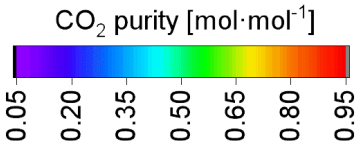


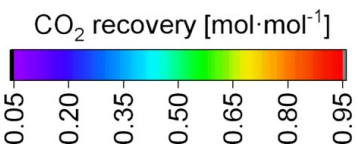


TSA









Process economics

- Currently in progress
- Indirect heat transfer
- Coupled design of adsorber & heat exchanger

- Major limitation for TSA is cooling time
  - Heat transfer in bed very poor
- Although WC can be high, productivity is very low
  - Non packed-bed processes could help

Conclusions and future work

- 22 MOFs and 3 reference adsorbents evaluated
- Promising results in terms of CO_2 purity and recovery
- Need to evaluate process economics before making further conclusions

- Finalise process economics
- Rapid cycles, and non-packed bed processes
- Impact of gas impurities and costs of pre-treatment

Acknowledgments

Petit group

Mac Dowell group

We are grateful to the EPSRC for providing the funding to undertake this research via the UK Carbon Capture and Storage Research Centre (UKCCSRC, grant EP/P026214/1).

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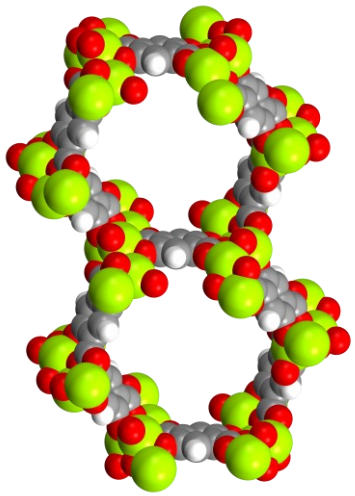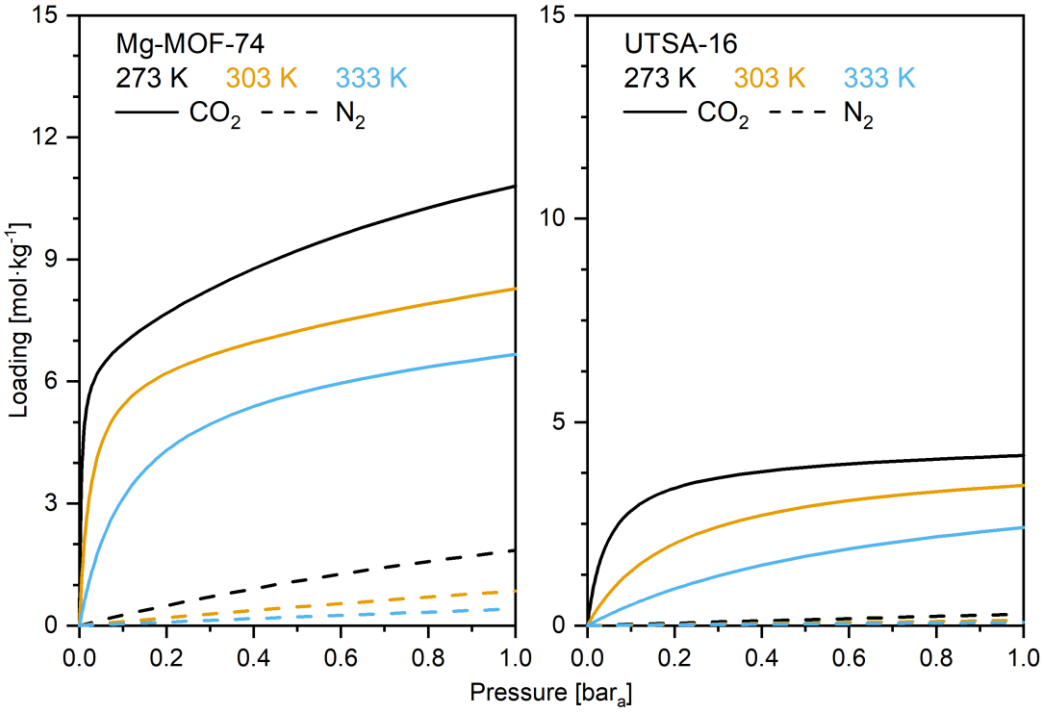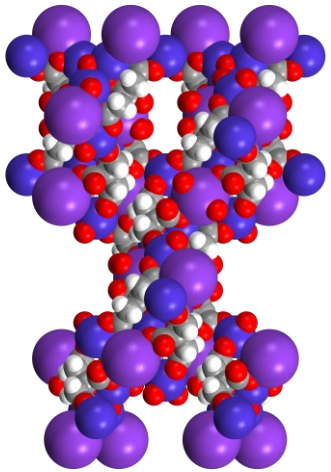
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