A Holistic Approach to Direct-Air Capture

Discovery novel materials (metal-organic frameworks) for DAC

Duncan McMillan dm4053@hw.ac.uk
Susana Garcia, Mijndert van der Spek
Research Centre for Carbon Solutions (RCCS), Heriot-Watt University

Green Industrial Futures
Centre for Doctoral Training

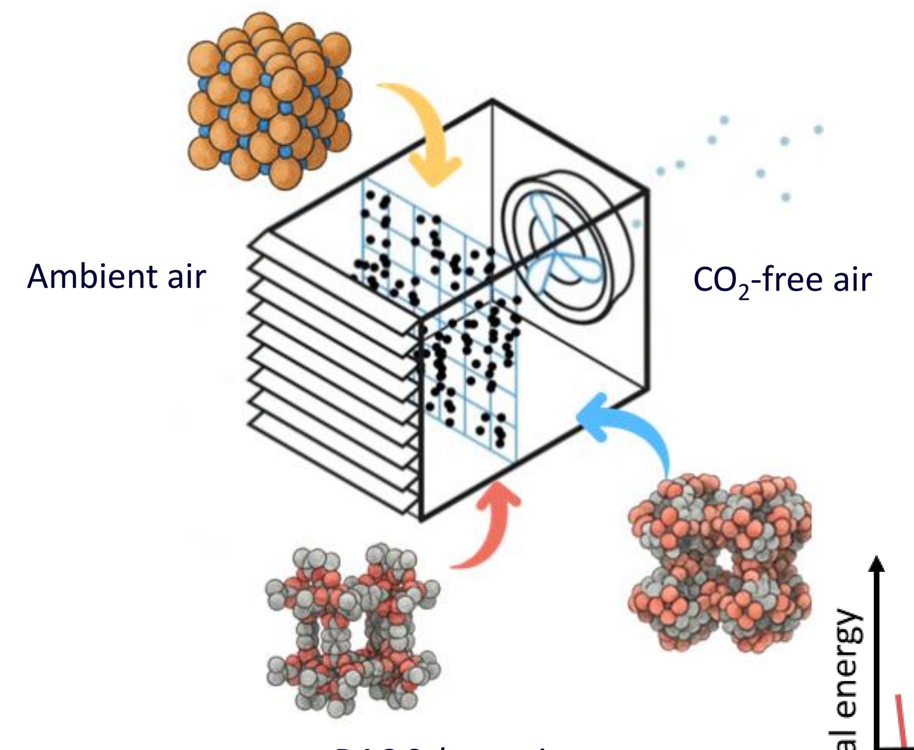
HERIOT WATT UNIVERSITY

RCCS

1 The Challenge

DAC today

- Scalable ✓
- Durable ✓
- Low land use ✓
- Affordable ✗



DAC Schematic

DAC is currently high-cost. Even optimistic estimates place long-run costs at \$100–170/tCO_2, with significant uncertainty around whether sub-\$100/tCO_2 is achievable[1].

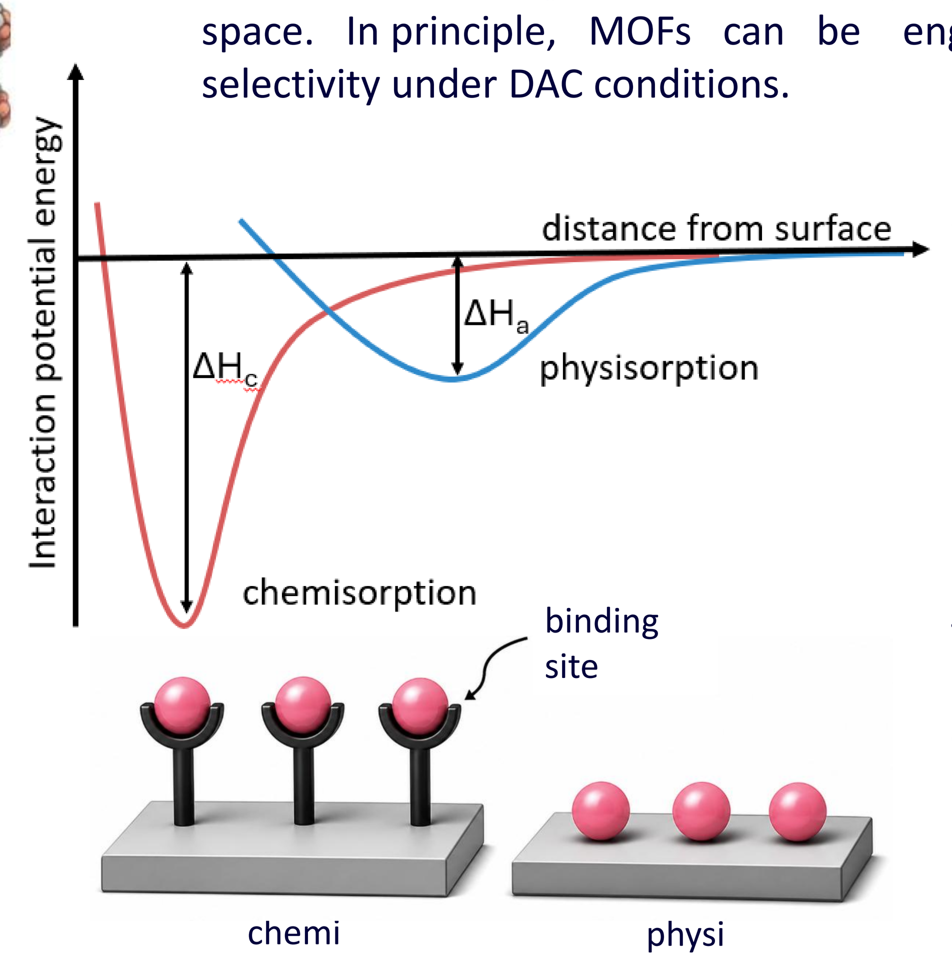
AR6 scenarios project DAC deployment of 0.5–5 GtCO_2/yr by 2050[2].

At \$100/tCO_2, this corresponds to \$50–500 billion per year, equivalent to 70–700 GW of solar capacity (3–30% of current global capacity). DAC viability therefore hinges on whether material and process-level performance can meet these cost and energy targets.

2 State of the Art

DAC companies today use either liquid sorbents or solid chemisorbents.
Physisorbents offer a potential advantage due to lower heats of adsorption (~25–40 kJ/mol vs ~75–95 kJ/mol for chemisorbents), enabling lower regeneration energy and potentially improved cycle efficiency.

MOFs are promising candidates as they offer highly tunable pore environments and a large design space. In principle, MOFs can be engineered to optimise CO_2 affinity, kinetics, and selectivity under DAC conditions.



Chemisorption vs Physisorption

For MOFs to be viable for DAC, they must simultaneously achieve:

- high CO_2 working capacity at low partial pressure.
- strong selectivity over H_2O.
- stability under humid, oxidative cycling.
- low-cost, scalable synthesis.
- fast adsorption/desorption kinetics.

The central research challenge is therefore not identifying high-performing materials in isolation but whether any material class can meet these requirements under realistic process conditions, at a competitive levelized cost.

3 Aim & Objectives

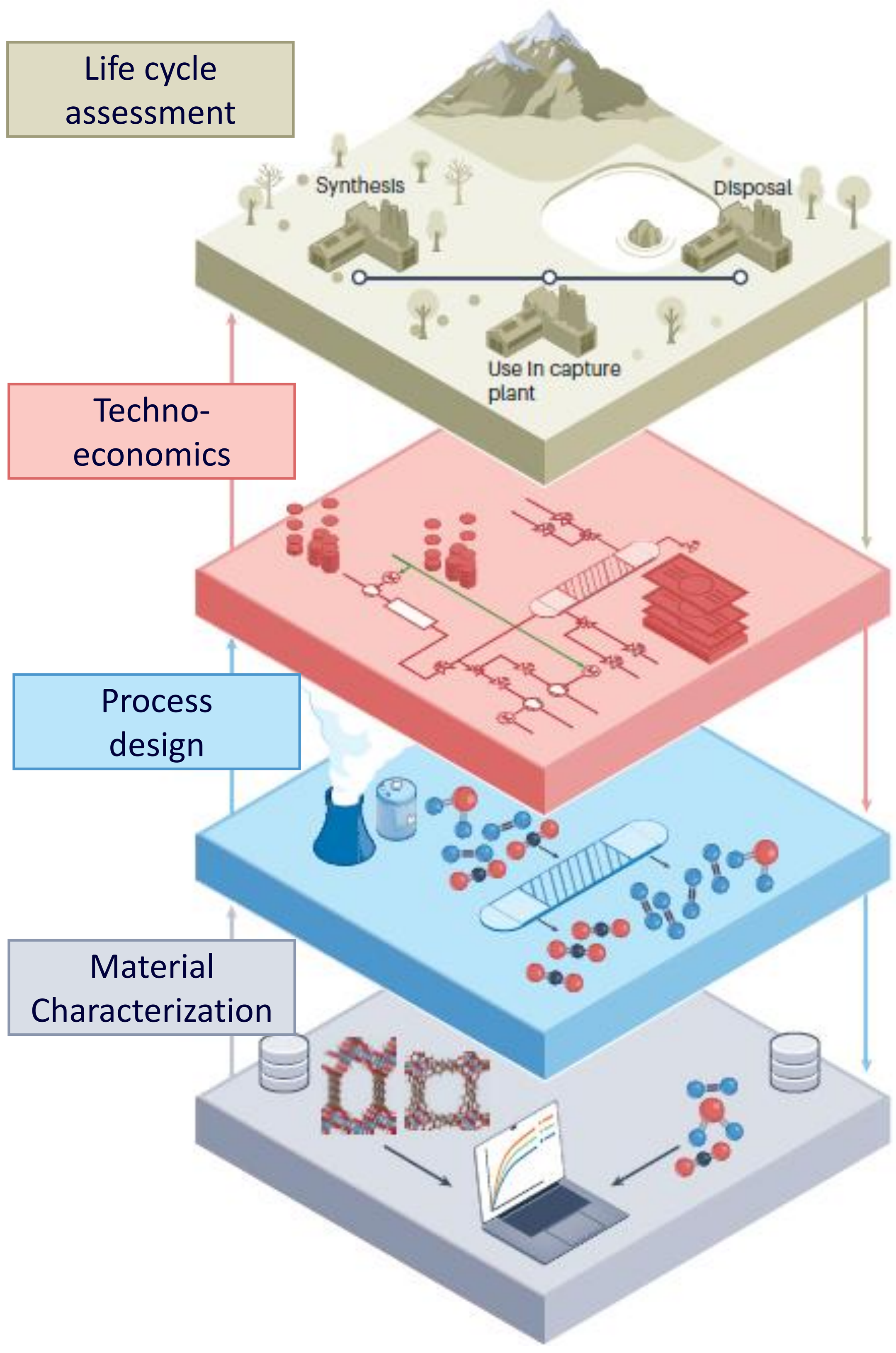
Aim: Determine whether adsorption-based DAC can achieve cost-competitive performance under realistic constraints.

Objectives:

- Link material properties to DAC cost floors.
- Quantify the impact of geometry and cycle design.
- Evaluate the role of process flexibility.
- Assess changes in material rankings under realistic conditions.
- Evaluate DAC deployment in cost-optimal energy systems under realistic cost assumptions.

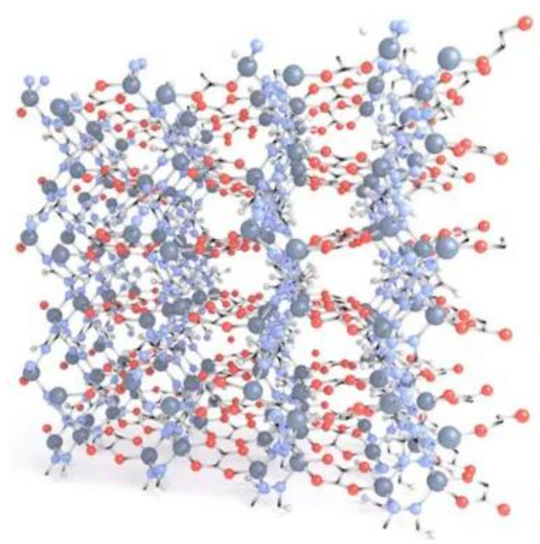
To address these objectives, the PrISMa platform links material properties to process-level performance and system-level cost, enabling physically grounded evaluation under realistic constraints.

They requires moving beyond equilibrium-based material screening to evaluate system design. The final objective requires a PrISMa / PyPSA integration, minimizing the cost of net zero infrastructure over a network (PyPSA-Europe) using PrISMa performance metrics.



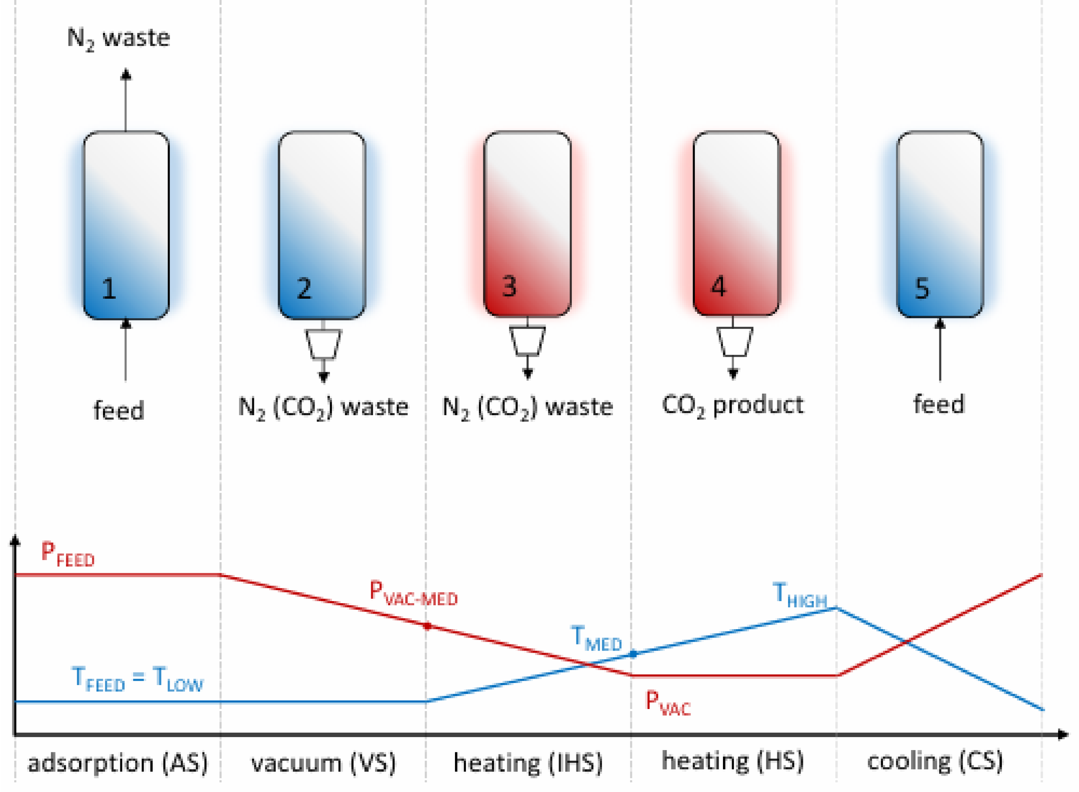
PrISMa Platform[3]

please ask about me...



CALF-20: One of the few MOFs to perform well in humid conditions

Climate solutions do not exist in the lab, they exist at industrial scale, and as such the industrial process needs to be modelled to assess performance and cost.



PrISMa Platform TVSA Cycle

References
[1] Young J, McQueen N, Charalambous C ...
The cost of direct air capture and storage can be reduced via strategic deployment but is unlikely to fall below stated cost targets
One Earth, 2023; 6, 899-917
[2] IPCC, 2023: Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team, H. Lee and J. Romero (eds.)]. IPCC, Geneva, Switzerland, pp. 35-115, doi: 10.59327/IPCC/AR6-9789291691647.
[3] Charalambous, C., Moubarak, E., Schilling, J. et al. A holistic platform for accelerating sorbent-based carbon capture. Nature 632, 89–94 (2024). https://doi.org/10.1038/s41586-024-07683-8

4 Results

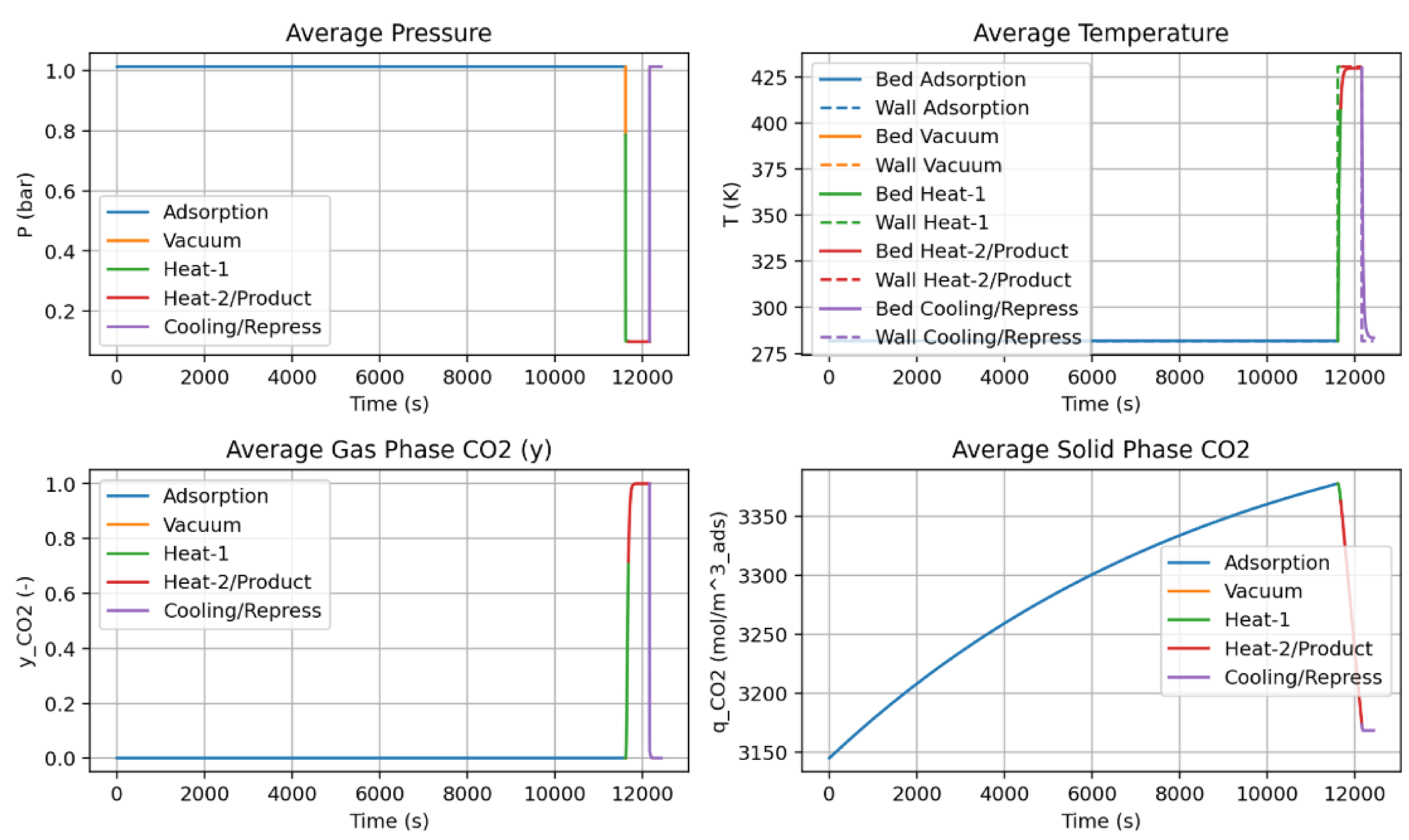
We developed pyAdsCycle*, a flexible and rigorous open-source framework for simulating cyclic adsorption processes, addressing the lack of reproducible and extensible modelling tools in the field.

Impact:

- Provides a shared foundation for material and process evaluation.
- Enables reproducible and comparable adsorption cycle modelling.
- Establishes a standardised framework for extending adsorption research.

open source

*(python Adsorption Cycle)



pyAdsCycle 1D simulation of LAGNAK under DAC conditions

We integrated the pyAdsCycle 1D model within the PrISMa framework, enabling spatially and temporally resolved simulation of DAC processes beyond equilibrium (0D) screening.

New capability:

- Quantify transport-limited performance under DAC conditions.
- Evaluate the impact of bed geometry and cycle timing on productivity and energy use.
- Assess the role and optimisation of air pre-treatment (desiccation).

A challenge is resolving these dynamics across large material spaces introduces significant computational cost, motivating efficient model implementations.

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