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Sargent Centre for Process Systems Engineering

Accelerated Design of Porous Polymers for DAC via Bayesian Optimization

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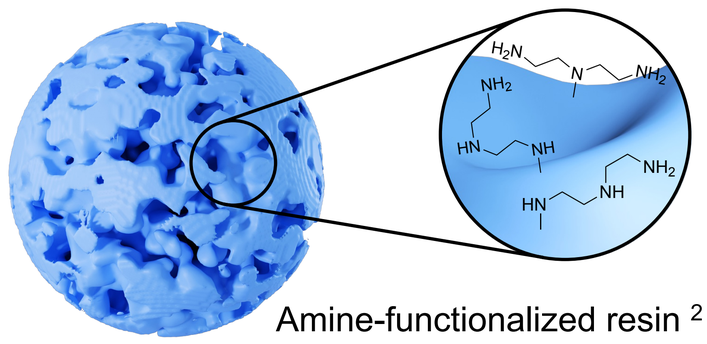
Motivation

- Scale-up of DAC is hindered by **high process cost**
- The current adsorbent **benchmark is unlikely optimal** for DAC
- **Adsorbent design** can increase process efficiency
- Optimization of CO_2 uptake **equilibrium** and **kinetics** is needed [1]
- **Bayesian optimisation** can find the best material **efficiently**

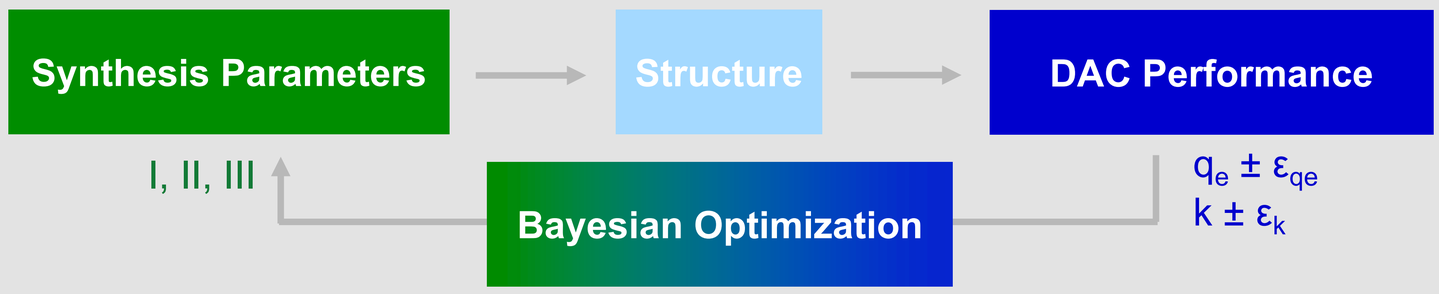
Objectives

1. **Optimize** the **pore structure** for **CO_2** equilibrium **uptake** and **kinetics (at 400 ppm)** in amine-functionalized polymeric resins
2. Develop a **model** to link **structure and performance**



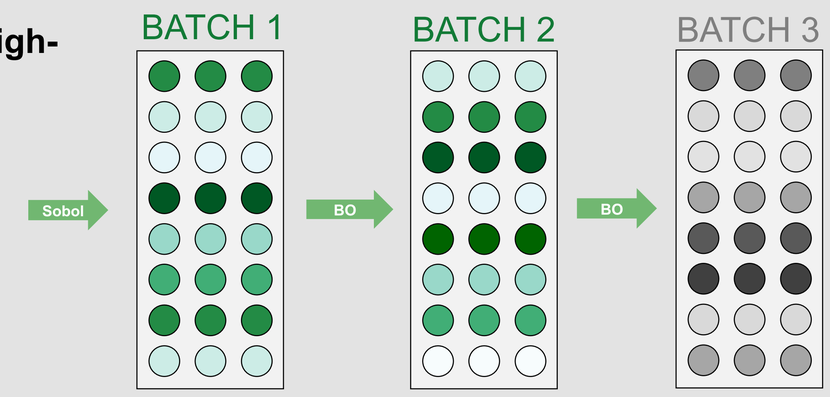
Amine-functionalized resin [2]

Approach – Automated high-throughput synthesis & testing + Bayesian optimization



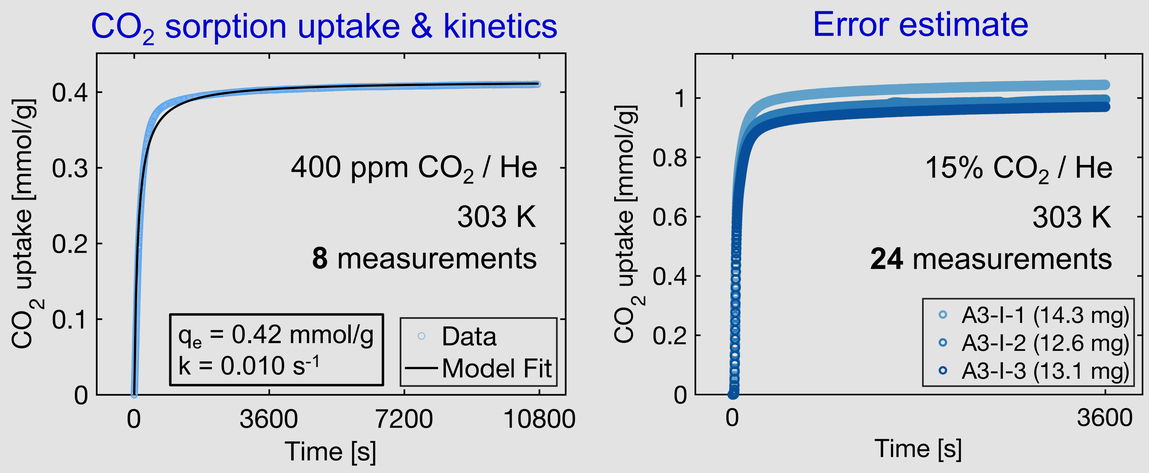
Synthesis ATLAS

- Automated **high-throughput** synthesis
- **24 resins in parallel** per batch (3 repeats, 8 conditions)



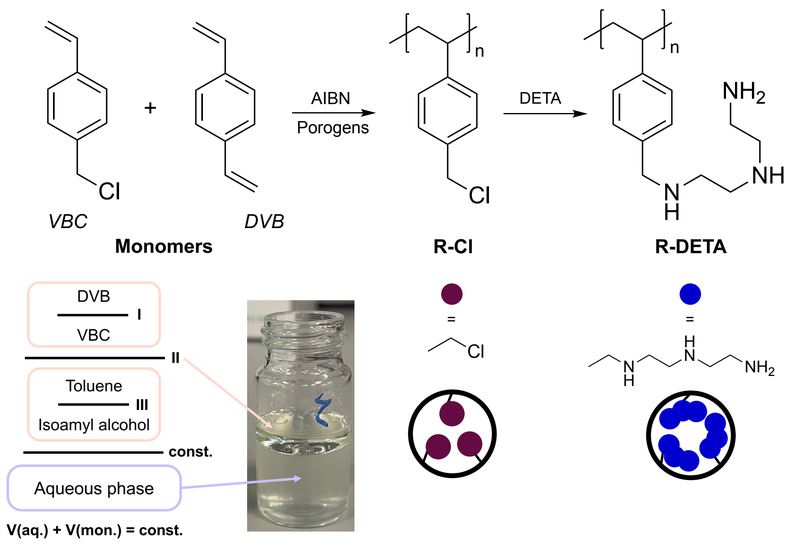
Synthesis variables		
	DVB molar fraction (I)	∈ [0, 1]
	Porogen volume fraction (II)	∈ [0.1, 0.9]
	Toluene volume fraction (III)	∈ [0, 1]

Performance testing
(Thermogravimetric analyzer w/ autosampler)

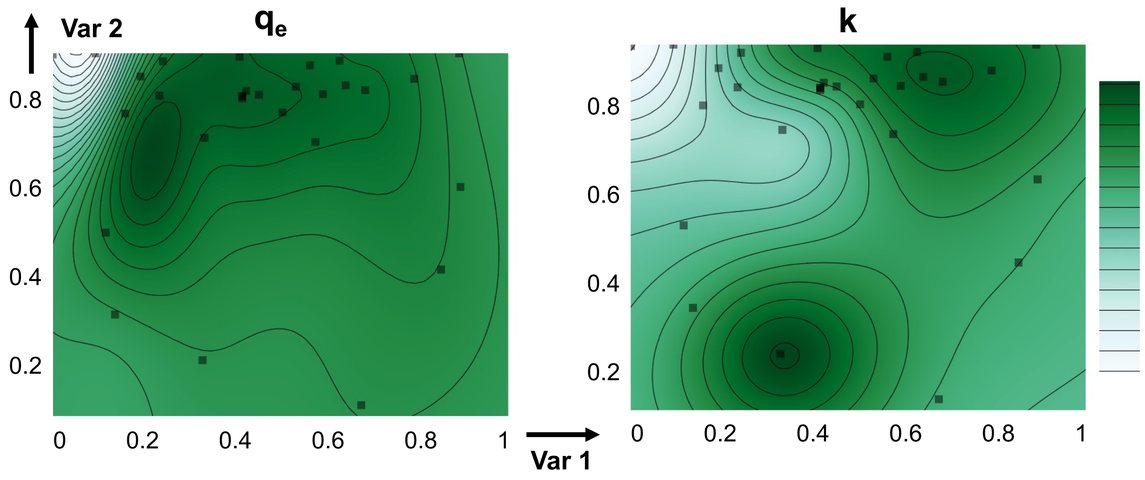


Objectives	q_e (equilibrium CO_2 uptake at 400 ppm)
	k (kinetic constant)

Adsorbent synthesis



Bayesian optimization – GP Model



Var 1: DVB molar fraction (I)

Var 2: Porogen volume fraction (II)

Surrogate Model | Gaussian Process

Acquisition Function | Noisy Expected Improvement (qNEI)

Kernel | Matérn 5/2

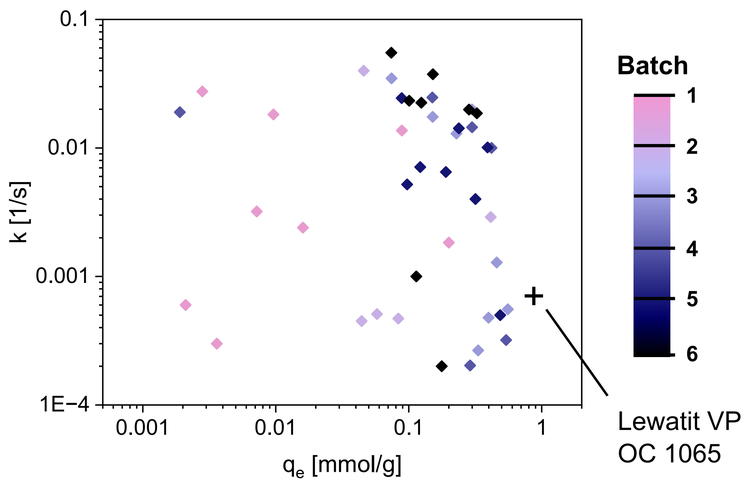
Measurement Noise | Heteroscedastic

Parameter Space Dimensionality | 3

Parallelization | 8 Conditions

Results

- A **near-linear Pareto front** between q_e & k
- A promising material has **q_e = 0.42 mmol/g** & **k = 0.010 s^{-1}** (400 ppm CO_2, 303 K)
- The benchmark adsorbent has **q_e = 0.90 mmol/g** & **k = 0.0070 s^{-1}** (400 ppm CO_2, 303 K)



Conclusions

- Exploration of parameter space of DVB-VBC crosslinked resins via **Bayesian optimization**
- Synthesis and CO_2 adsorption quantification of **140 polymer samples**
- Promising candidates show **significantly faster CO_2 adsorption** than the benchmark Lewatit VP OC 1065

Imperial College London

[1] Young, J. et al. Process-informed adsorbent design for direct air capture. Chem. Eng. J. 456, 141035 (2023).
[2] Ahn, J.-H. et al. Microporosity and surface area control in hyper-cross-linked resins. *Macromolecules* **39**, 627–632 (2005).

Acknowledgements
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