IMPERIAL

Sargent Centre for Process Systems Engineering

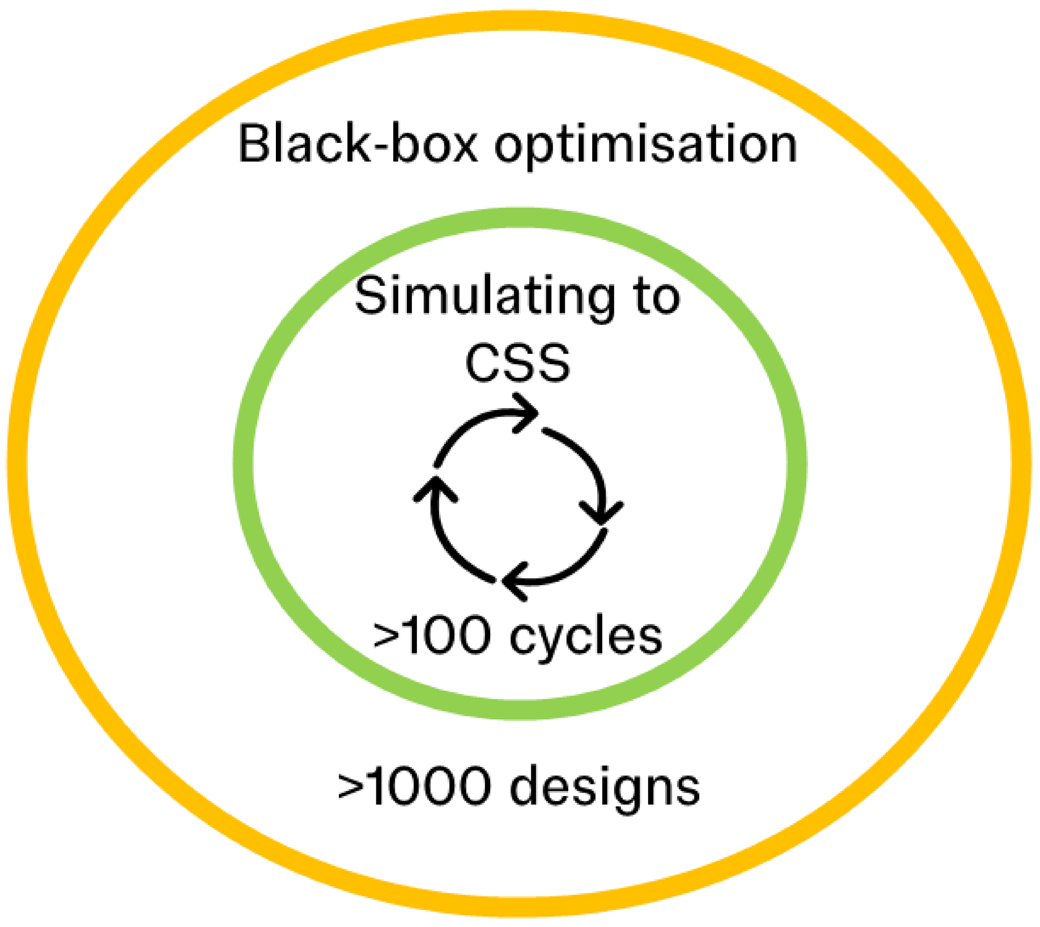
Accelerating Simulation and Optimisation of Adsorption Processes with Differentiable Programming

Alex Glover[1,2], Maria M. Papathanasiou[1,2], Ronny Pini[1,2]

1. Department of Chemical Engineering, Imperial College London
2. The Sargent Centre for Process Systems Engineering, Imperial College London

Background

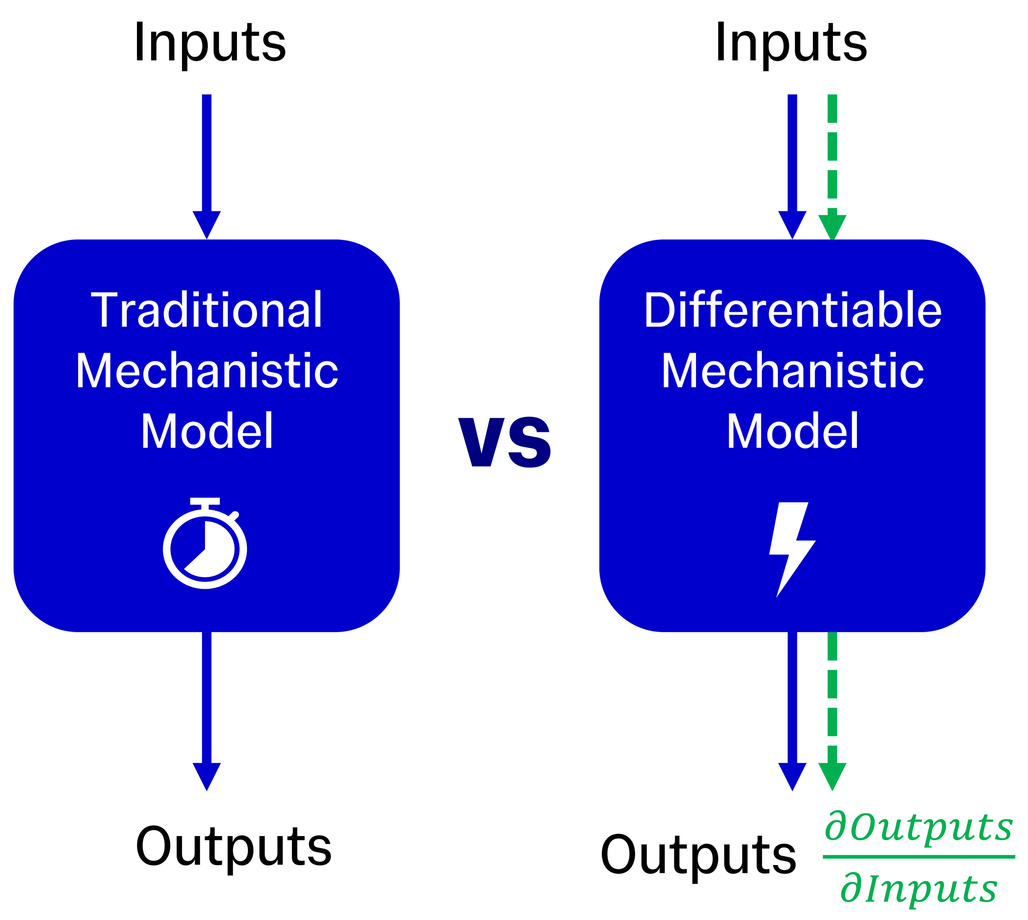
- Cyclic adsorption processes are typically **designed at cyclic steady state** (CSS)



- Requires solving **~100 DAEs, ~10^6 times**
- Optimisation studies **require hundreds or thousands of CPU hours**[1,2].
- **Differentiable programming** offers **faster simulations** and **gradient-based methods**

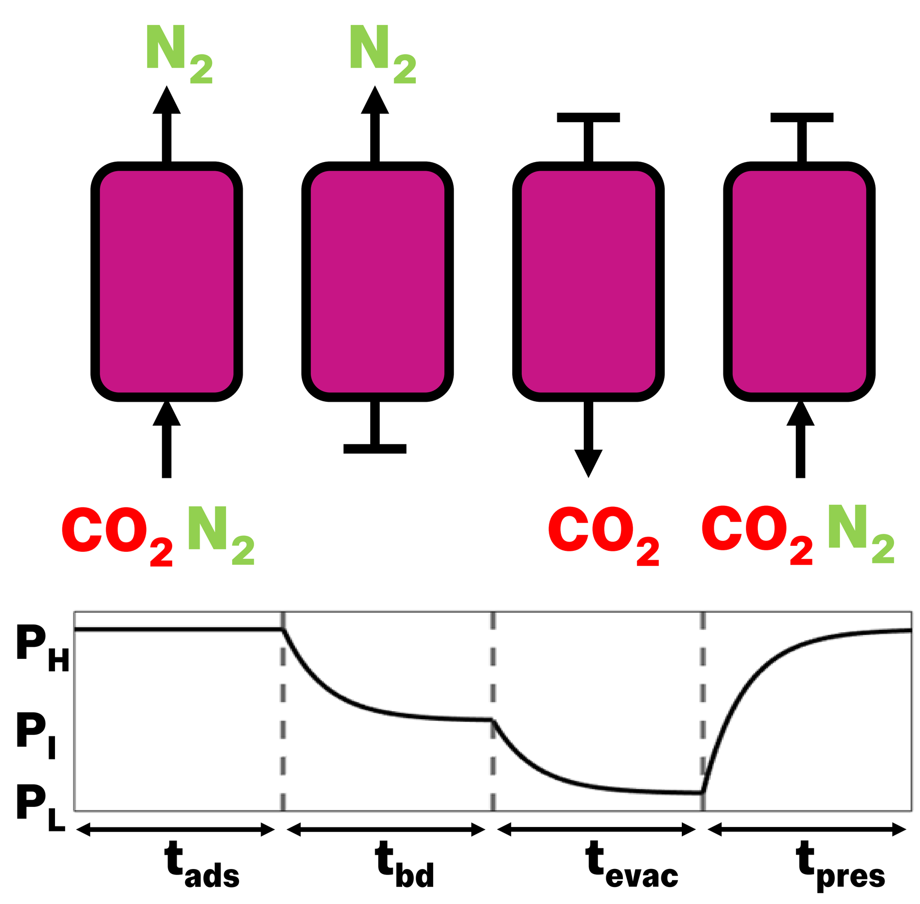
Differentiable Programming

- **Accelerated simulations** using JIT compilation
- **Efficient and accurate gradients** for solution of PDEs and sensitivity equations
- **End-to-end differentiability** – Obtain gradients for model output with respect to inputs

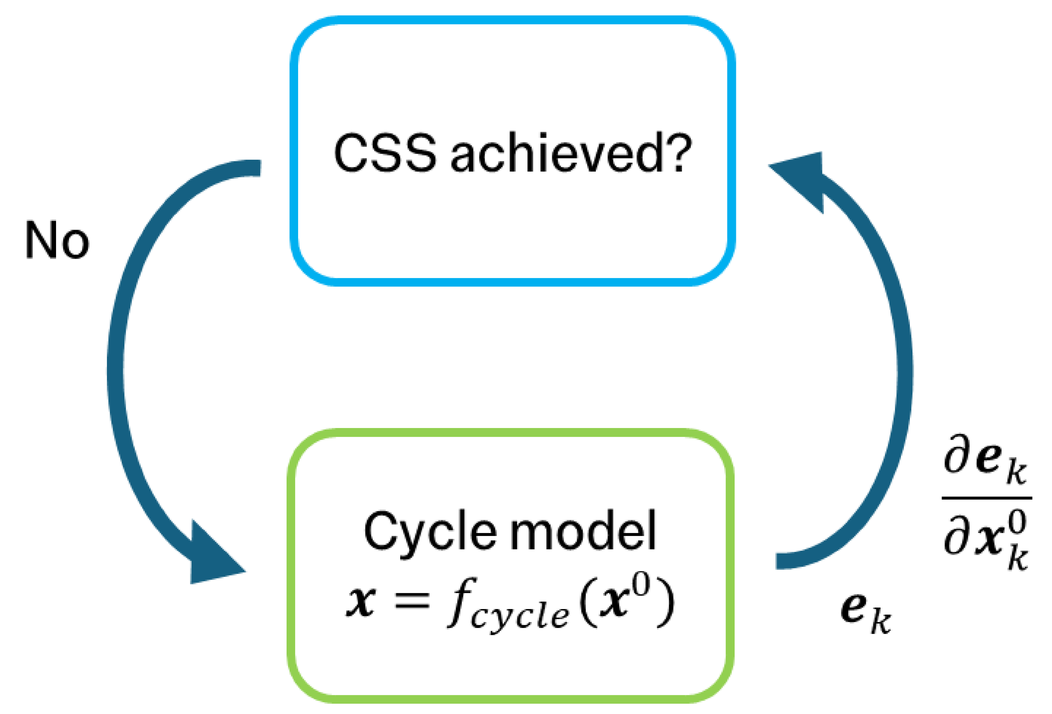


Carbon Capture Case Study

- Mechanistic model described by mass and energy balances
- Aim: **6 parameter design optimisation**:
  - Feed velocity
  - Step time: adsorption, blowdown, evacuation
  - Pressure set points: high and intermediate



Direct Determination of CSS

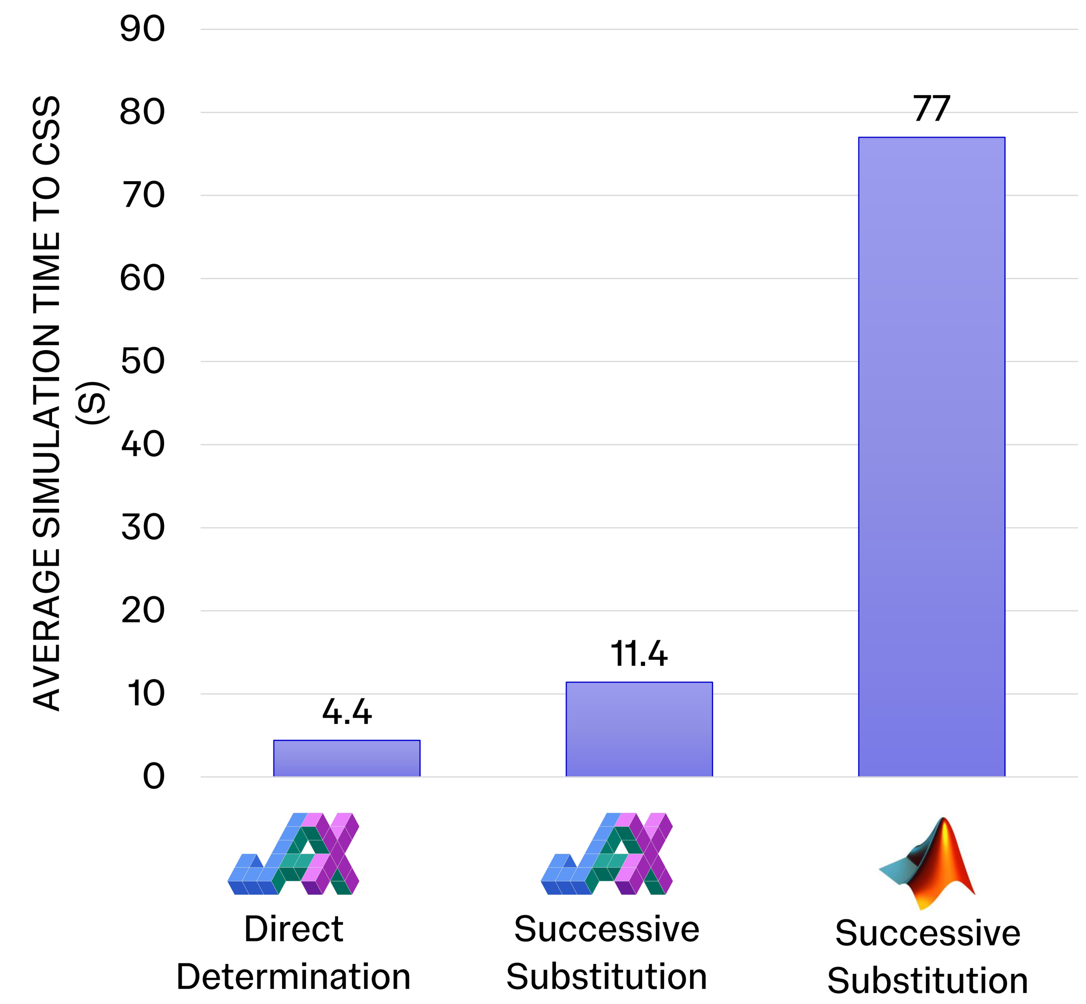


$$x_{k+1}^0 = x_k - \frac{\partial e_k}{\partial x_k^0}^{-1} e_k$$

- **Error** e_k: difference between start and end of cycle states
- **Gradients:** error with respect to the initial state
- **Newton iteration** for next initial state guess[3]

- **4096** different designs compared
  - **Successive substitution: 145 cycles** to reach CSS on average
  - **Direct determination: 6 Newton iterations** to reach CSS on average

- Differentiable model ➔ nearly **20x faster**



Gradient-Based Optimisation

- **Sensitivities** of **KPIs** at CSS
- Gradient-based **constrained multi-objective optimisation**

- **Improved pareto front** compared to Sobol sampling and genetic algorithm (NSGA-ii)
- **Fewer model evaluations** required than data driven methods
- **Optimality guarantee**

- Demonstrates the **speed and accuracy** capabilities **of differentiable programming**

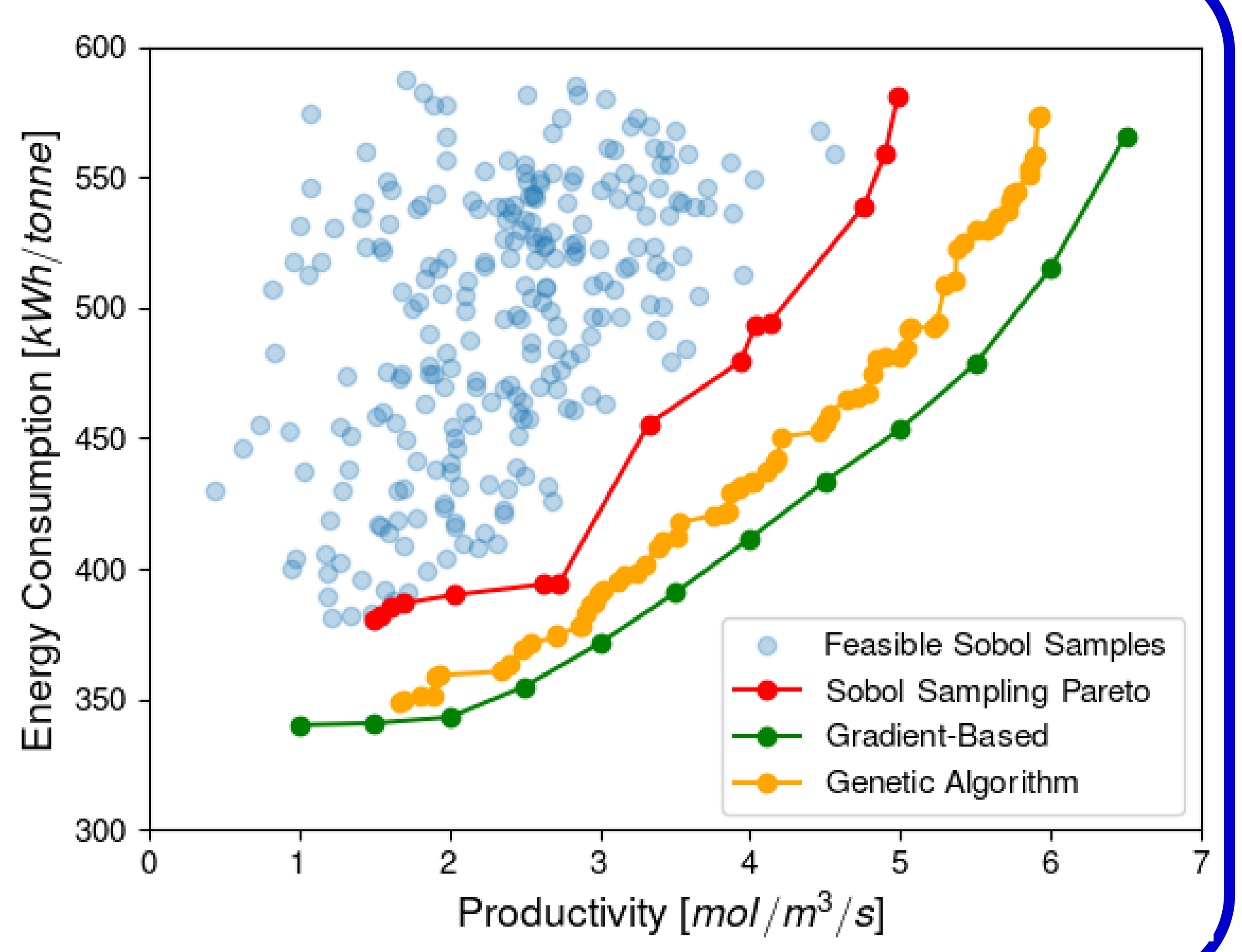
$$\min_{\theta} \text{ Energy Consumption}(\theta)$$

s.t. Productivity ≥ ε

Purity ≥ 95%

Recovery ≥ 90%

$\theta^L \leq \theta \leq \theta^U$



1. Peh, S.B., Farooq, S., Zhao, D., 2022. A metal-organic framework (MOF)-based temperature swing adsorption cycle for postcombustion CO2 capture from wet flue gas. Chemical Engineering Science 250, 117399
2. Ward, A., Pini, R., 2022. Efficient Bayesian Optimization of Industrial-Scale Pressure-Vacuum Swing Adsorption Processes for CO2 Capture. Ind. Eng. Chem. Res. 61, 13650–13668.
3. Croft DT, LeVan MD (1994) Periodic states of adsorption cycles—I. Direct determination and stability. Chemical Engineering Science 49:1821–1829.

Imperial College London

alex.glover20@imperial.ac.uk