Surrogate-based Multi-objective Optimisation for the Design of Pressure Swing Adsorption Systems

Joakim Beck[a], Daniel Friedrich[b], Stefano Brandani[b], Eric S Fraga[a]
[a]Centre for Process Systems Engineering, University College London
[b]SCCS, School of Engineering, University of Edinburgh
S.Brandani@ed.ac.uk, E.Fraga@ucl.ac.uk

Overview of PSA design challenges and the example system

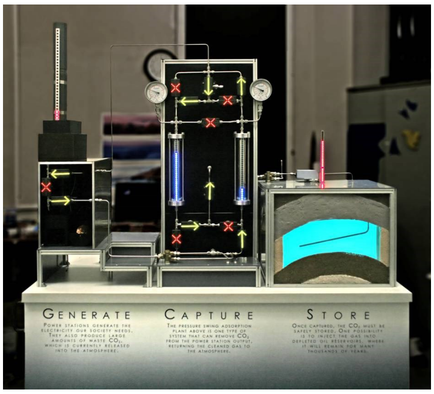


Figure 1. Carbon Capture and Storage interactive (CCSi)

Aim

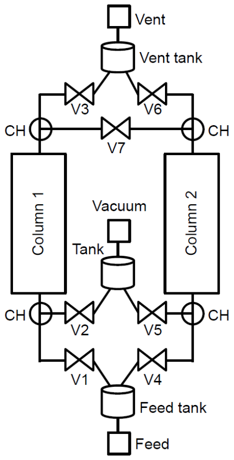
To design an efficient CO_2 separation process for carbon capture and storage.

Challenges

- The performance of Pressure Swing Adsorption processes depends on a large number of parameters
- Numerical simulations coupled to optimisation routines are required for the design of efficient systems

Example system

- 2-bed Skarstrom cycle with one-sided pressure equalisation
- Separation of CO_2 from post-combustion flue gas with silicalite HiSIV-3000
- Simulations are performed with in-house adsorption cycle simulator[1]



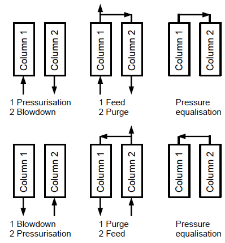
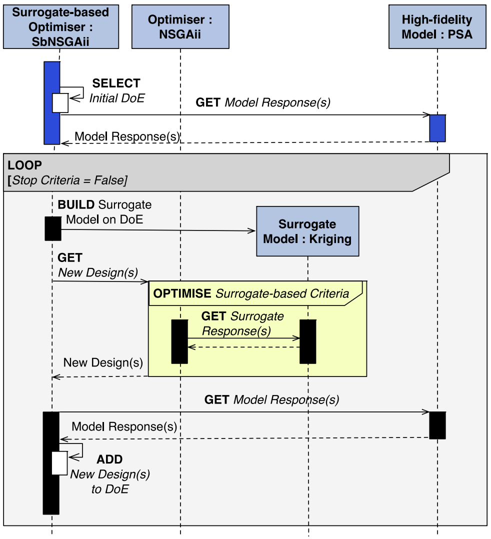


Figure 2. (Left) Schematic showing the capture unit of the CCSi and (top) steps of the Skarstrom cycle with one-sided pressure equalisation.

Surrogate based multi-objective optimisation



Idea

Perform the optimisation on a surrogate model[2] of the high-fidelity model[1]

Procedure

1. Choose an initial Design of Experiment (DoE) and simulate the response of the high-fidelity model for this DoE
2. Build a surrogate model, for each of the objectives, on the high-fidelity model responses obtained so far
3. Use an optimisation routine with the current surrogate model to find the optimal design. For multiple objectives this is the design predicted to yield the largest improvement to the Pareto front of the high-fidelity simulations obtained
4. Simulate the response of the new design with the high-fidelity model
5. If the stop criteria are not met, repeat steps 2-4

Figure 3. Schematic of the surrogate based optimisation routine

Parameters and objectives

Table 1. Optimisation parameters

Parameter	Range	Unit
Purge-to-feed ratio	0-1	-
Feed/purge time	10-200	s
Feed flow rate	0.0005-0.008	mol s^{-1}
Vacuum pressure	0.02-0.4	bar
Feed pressure	0.3-1.0	-
Feed temperature	290-340	K

Objectives

- Purity: percentage of CO_2 in the stream leaving the system at the vacuum outlet
- Recovery: percentage of CO_2 feed into the system which is recovered at the vacuum outlet
- Molar energy consumption: energy required to recover one mole of CO_2 at the vacuum outlet

Optimisation results and comparison to conventional optimisation routines

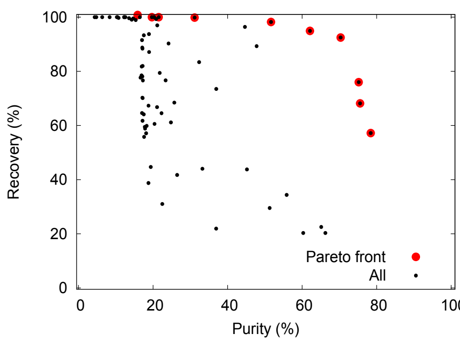


Figure 4. Trade-off of purity and recovery. Here the surrogate-based optimisation required 15 evaluations of the high-fidelity model (above the 64 initial design points)

Optimisation results

- Conventional and surrogate-based optimisation are performed with multi-objective genetic algorithm NSGAii
- Both start off with the same initial design (size of 64) generated by maximin Latin Hypercube Sampling

Conclusion

- Surrogate-based optimisation with the same underlying optimisation routine reaches a more attractive Pareto front with less than 25% of the high-fidelity model simulations
- The design with 90% recovery and 70% purity compares favourable to previous optimisation studies
- The surrogate-based optimisation enables the optimisation of complex PSA processes

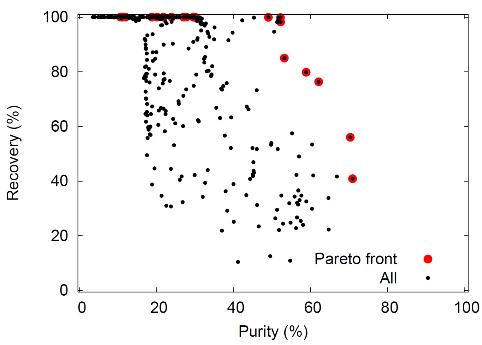


Figure 5. Comparison with a conventional optimisation routine (NSGAii) that used 319 points above the initial design

Acknowledgements

Financial support from the Engineering and Physical Sciences Research Council, grants EP/G02037X/1 and EP/G062129/1, is gratefully acknowledged.

References

1. Friedrich, Ferrari, Brandani: Efficient Simulation and Acceleration of Convergence for a Dual Piston Pressure Swing Adsorption System, Industrial & Engineering Chemistry Research, 2013.
2. Beck, Friedrich, Brandani, Guillas, Fraga: Surrogate based Optimisation for Design of Pressure Swing Adsorption Systems, Proceedings of the 22nd European Symposium on Computer Aided Process Engineering, 2012.