Modelling of Pressure Swing Adsorption Systems at High Pressure Using Fixed Beds for Pre-Combustion Carbon Dioxide Capture

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Introduction

- Pre-combustion carbon capture from Integrated Gasification Combined Cycle (IGCC) coal fired power stations could have a significant impact on reducing carbon dioxide emissions. Current pre-combustion capture uses liquid amines with an efficiency loss of around 7% [1]
- Solid adsorbents in pressure swing adsorption (PSA) process will offer advantages in cost and flexibility at the high pressures used in pre-combustion capture
- A model has been developed in gPROMS and validated to test the optimal design of a PSA process at high pressure
- Project funded by the EPSRC in collaboration with University of Nottingham, University of Warwick, UCL, Tsinghua University and Chinese Institute of Coal Chemistry

Experimental

- Experiment used to validate model
- N_2 and CO_2 passed over a packed bed of Activated Carbon (AC) adsorbent.
- CO_2 mole fractions of 0.1, 0.2, 0.3, 0.4 and 0.5 used
- Pressure – 25 bar; Temperature – 25°C; Flowrate – 200 Nml/min

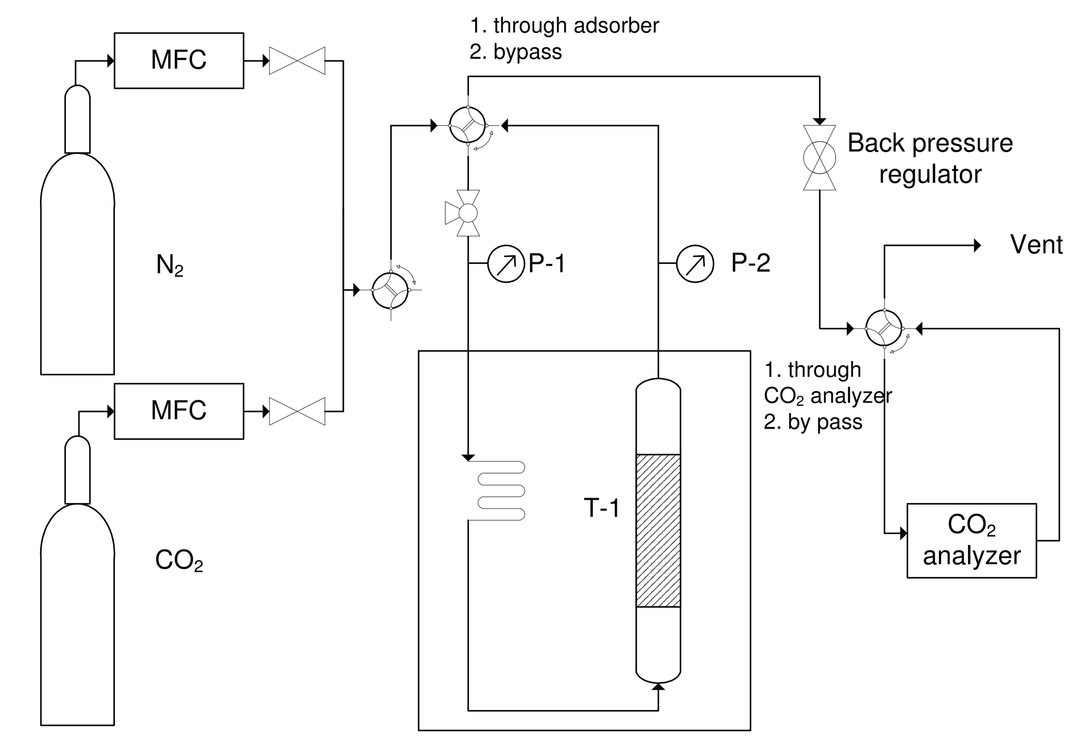
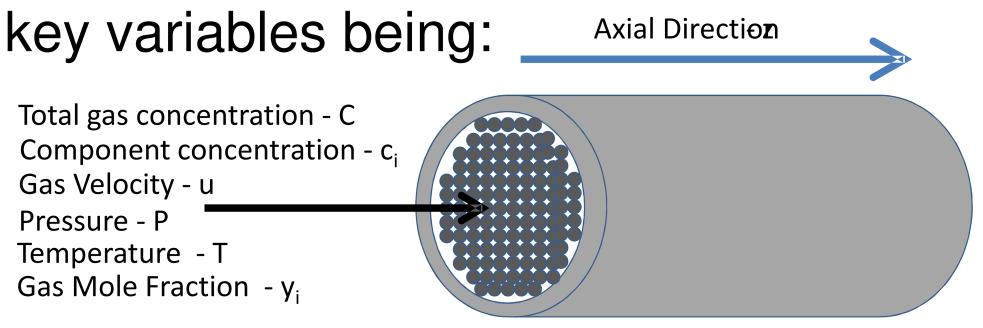


Figure 1: Experimental configuration to produce breakthrough curves using a fixed bed

Model

Key Model equations:

- Reactor modelled as fixed bed reactor with the key variables being:



- Axial Dispersed Plug Flow Model:

$$\frac{\partial C}{\partial t} + D_{ax}\frac{\partial^2 C}{\partial z^2} + \frac{\partial (Cu)}{\partial z} + \frac{(1-\varepsilon)}{\varepsilon}\sum_{i=1}^{n}\frac{\partial q_i}{\partial t} = 0$$

$$\frac{\partial c_i}{\partial t} - D_{ax}\frac{\partial^2 c_i}{\partial z^2} + \frac{\partial (uc_i)}{\partial z} + \frac{(1-\varepsilon)}{\varepsilon}\frac{\partial q_i}{\partial t} = 0$$

- Langmuir-Freundlich Isotherm

$$q_i^* = \frac{q_{s,i}B_i(Py_i)^{n_i}}{\left(1+\sum_{i=1}^{k}B_i(Py_i)^{n_i}\right)}$$

- Linear Driving Force Model

$$\frac{dq_i}{dt} = k_i(q_i^* - q_i)$$

Breakthrough Curves

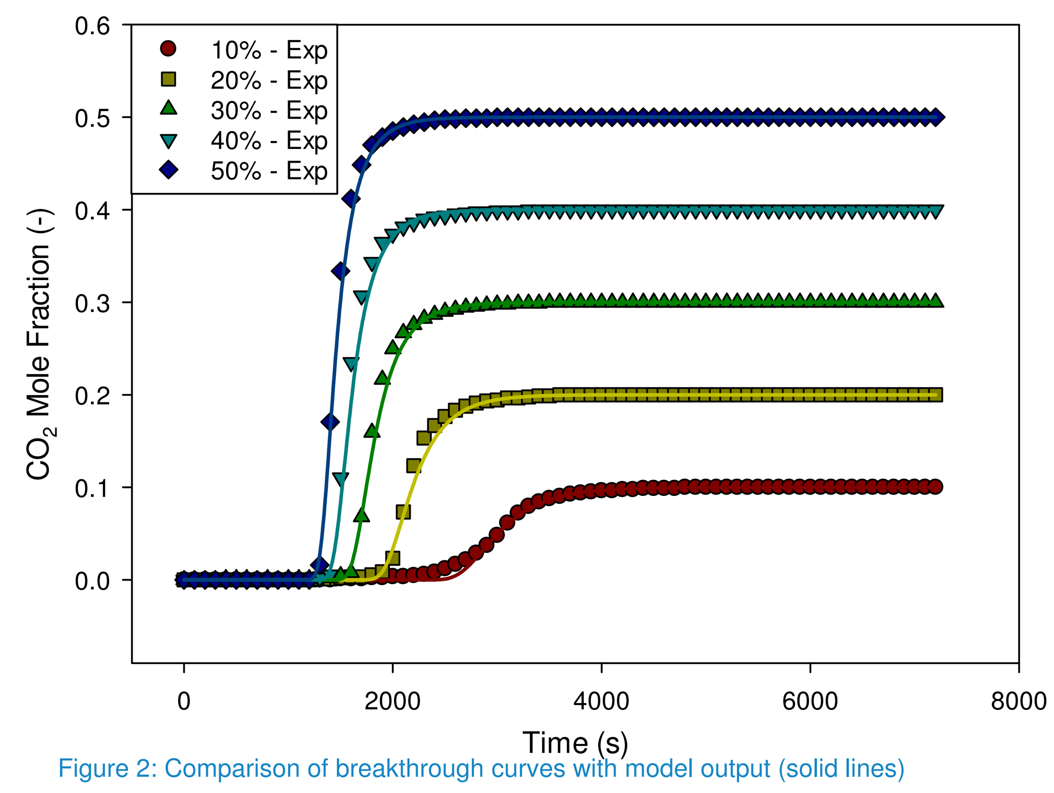


Figure 2: Comparison of breakthrough curves with model output (solid lines)

- All parameter values come from system properties or correlations
- Energy balance gives fit to a-symmetric breakthrough curve
- Strong agreement gives confidence in developing to PSA model

PSA Cycle Set-up

- 4-step cycle used to produce a light and heavy product stream
- Simulated as one bed to reduce computational time
- Cycle run until outlet concentration is 5% of inlet concentration
- Feedback loops used to give constant blowdown flowrate and to control pressurisation
- 4-bed process implemented

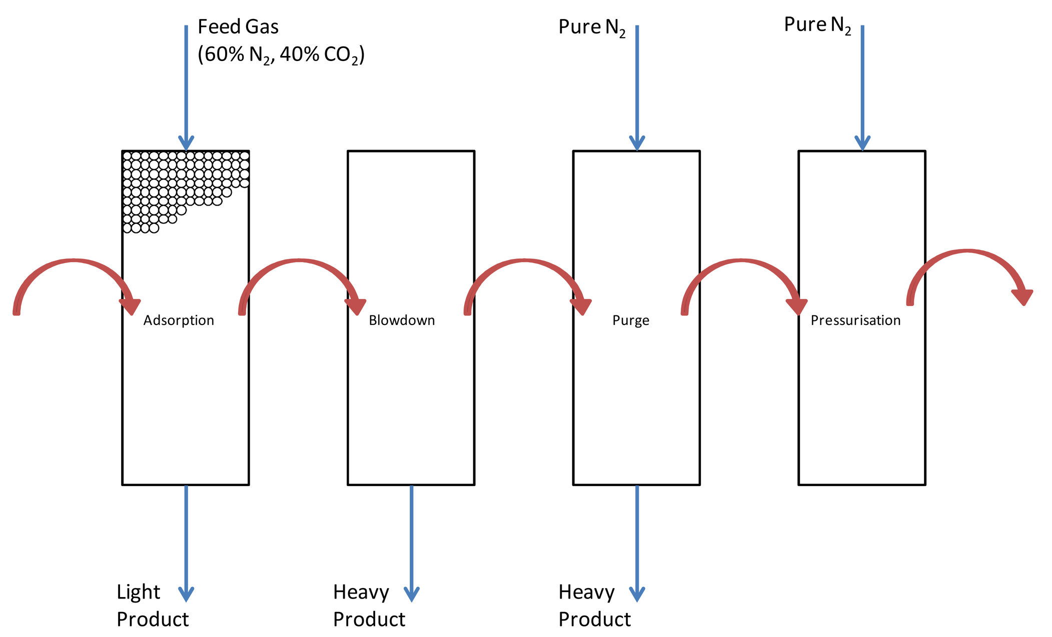


Figure 4: Typical 4-step PSA cycle with recovery of all streams to give light and heavy products

Cycle Output

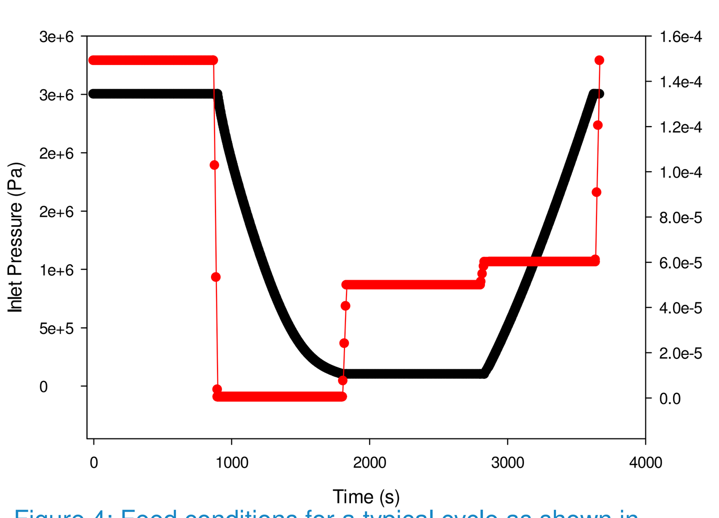


Figure 4: Feed conditions for a typical cycle as shown in figure 3

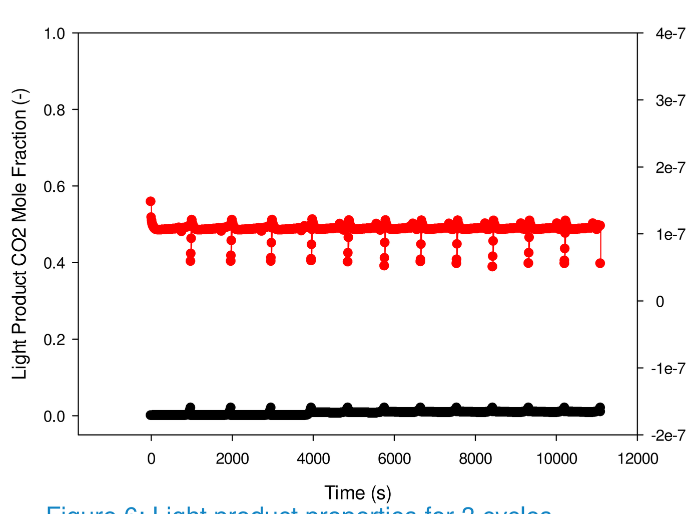


Figure 6: Light product properties for 3 cycles

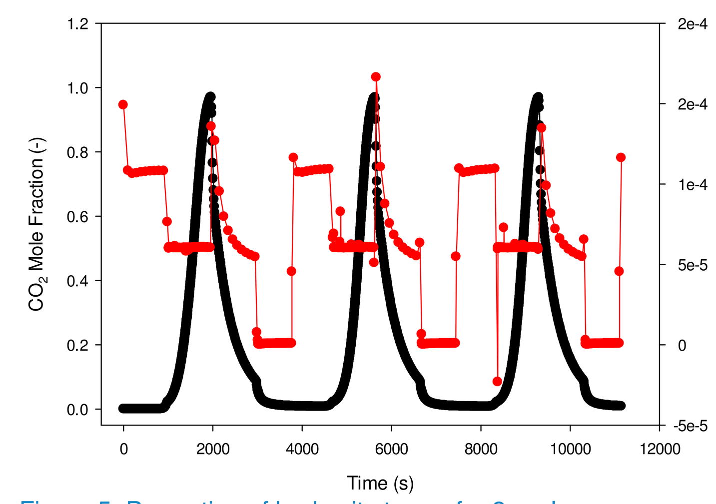


Figure 5: Properties of bed exit stream for 3 cycles

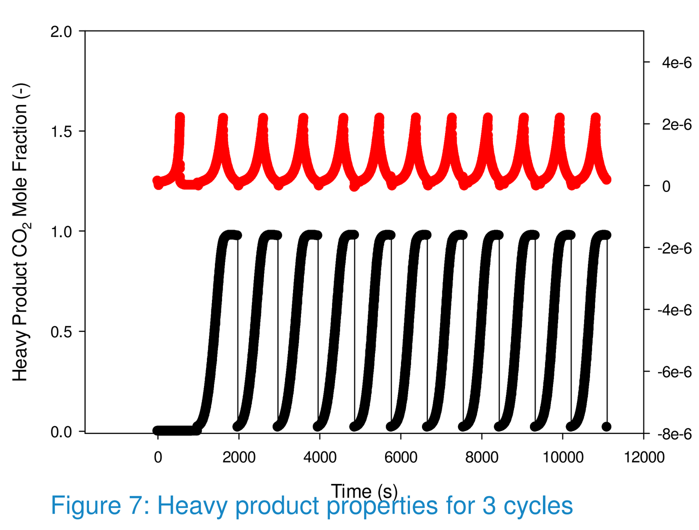


Figure 7: Heavy product properties for 3 cycles

- Control of pressurisation and blowdown gives equal step sizes.
- Depressurisation shape results from a release of gas from AC at lower pressures
- Cyclic steady state is achieved rapidly due to purge with light product
- High purity light product stream can be produced with a steady flowrate by use of 4-beds operating in series
- Purity of heavy product stream greatly reduced and recovery increased by collecting entire blowdown and purge stream

Conclusion

- Model able to replicate breakthrough curves with high degree of accuracy
- 4-step process cable to producing a pure and constant light product stream when used with a 4-bed system
- Constant molar flowrate for heavy product achieved
- Light product recovery greatly reduced by using as a purge and pressurisation gas
- Heavy product purity very low as entire blowdown stream is collected
- Additional pressure equalisation steps required to maximise the purity and recovery of both the heavy and light products

Future Work

- Implement pressure equalisation steps to increase purity of CO2 and recovery of N2
- Optimise blowdown, purge and pressurisation conditions to maximise recovery and purity of both products
- Scale system up to operate at flowrates similar to those of an IGCC power plant
- Connect capture model with IGCC power plant model to find effect of capture rate on efficiency

1. Chiesa, P., et al., *Co-production of hydrogen, electricity and CO2 from coal with commercially ready technology. Part A: Performance and emissions.* International Journal of Hydrogen Energy, 2005. **30**: p. 747-767.

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