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

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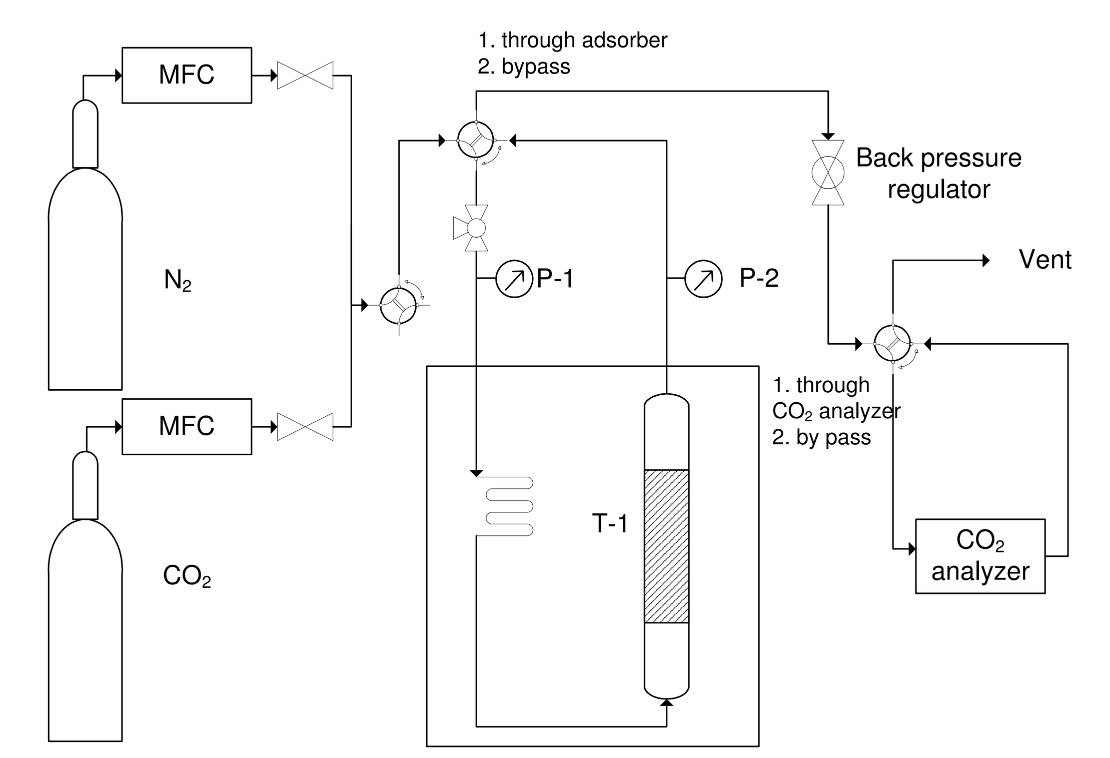
Introduction

- 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 is being developed to test the viability of a PSA system using Activated Carbon for carbon capture in an IGCC coal fired power plant
- Work to date looks at simulating adsorption breakthrough curves for the separation of a CO_2/N_2 mixture
- 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 adsorbent.
- CO_2 mole fractions of 0.05, 0.1, 0.15 and 0.2 used for parameter estimation
- Partially filled beds giving various bed lengths used to test estimated parameters

Conditions	
Bed Pressure (bar)	25
Bed Temperature (°C)	25
Flowrate (Nml/min)	200

Parameter Estimation

- Parameter values taken from gas properties, literature or independent experiment where possible.
- Remaining tuning parameters are the nitrogen Langmuir-Freundlich constant (B_{N2}) and the nitogen exponent (n_{n2})
- Prediction of constants for all experimental runs gives good agreement (Figure 1)
- Excellent agreement seen if value predicted for each run
- Predicted B_{N2} show strong empirical relationship to carbon dioxide mole fraction (y_{CO2})and n_{n2}, where D,E and c are constants:

$$B_{N2} = (Dy_{CO2} + E).exp(c.n_{N2})$$

Results

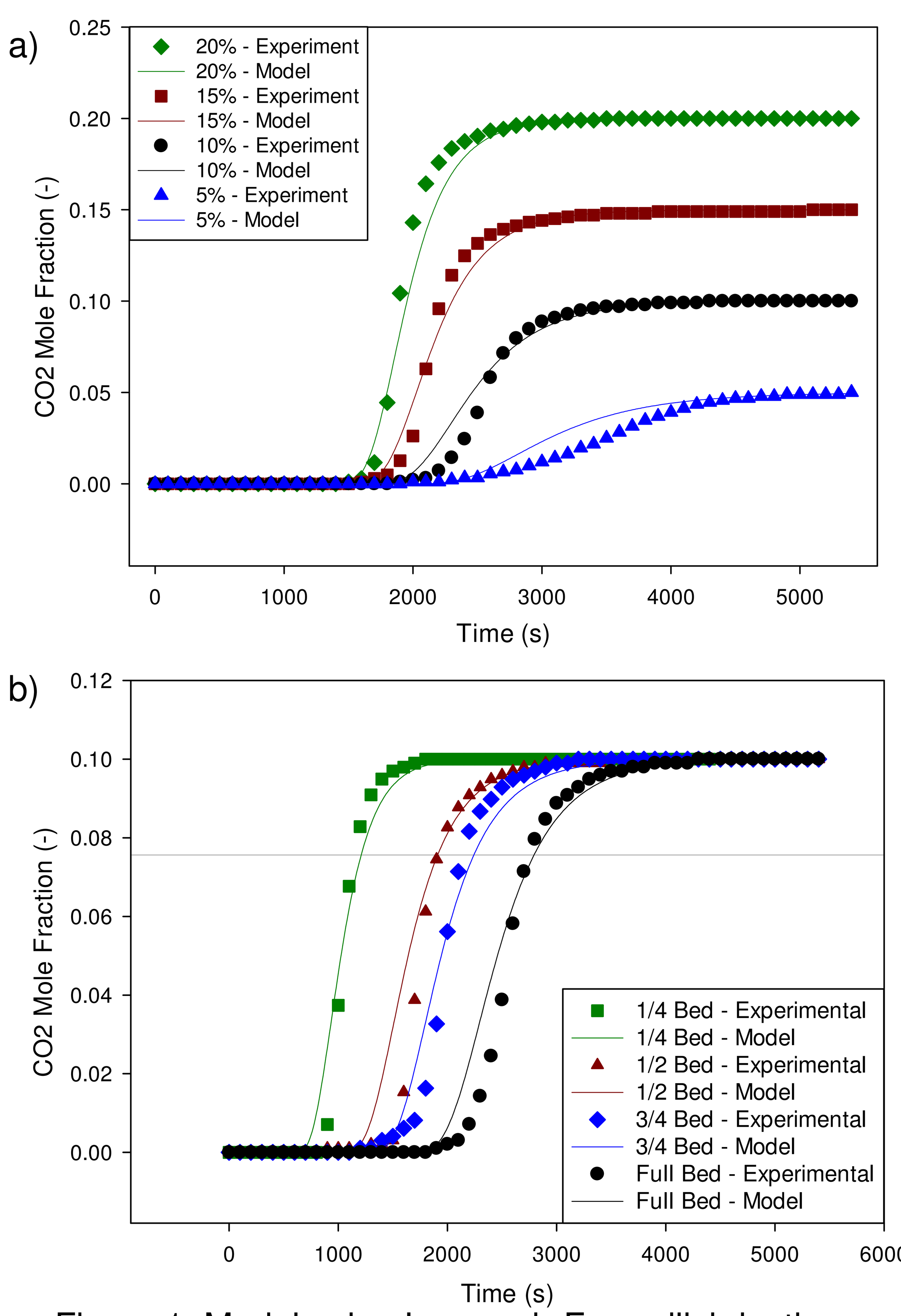


Figure 1: Model using Langmuir-Freundlich isotherm

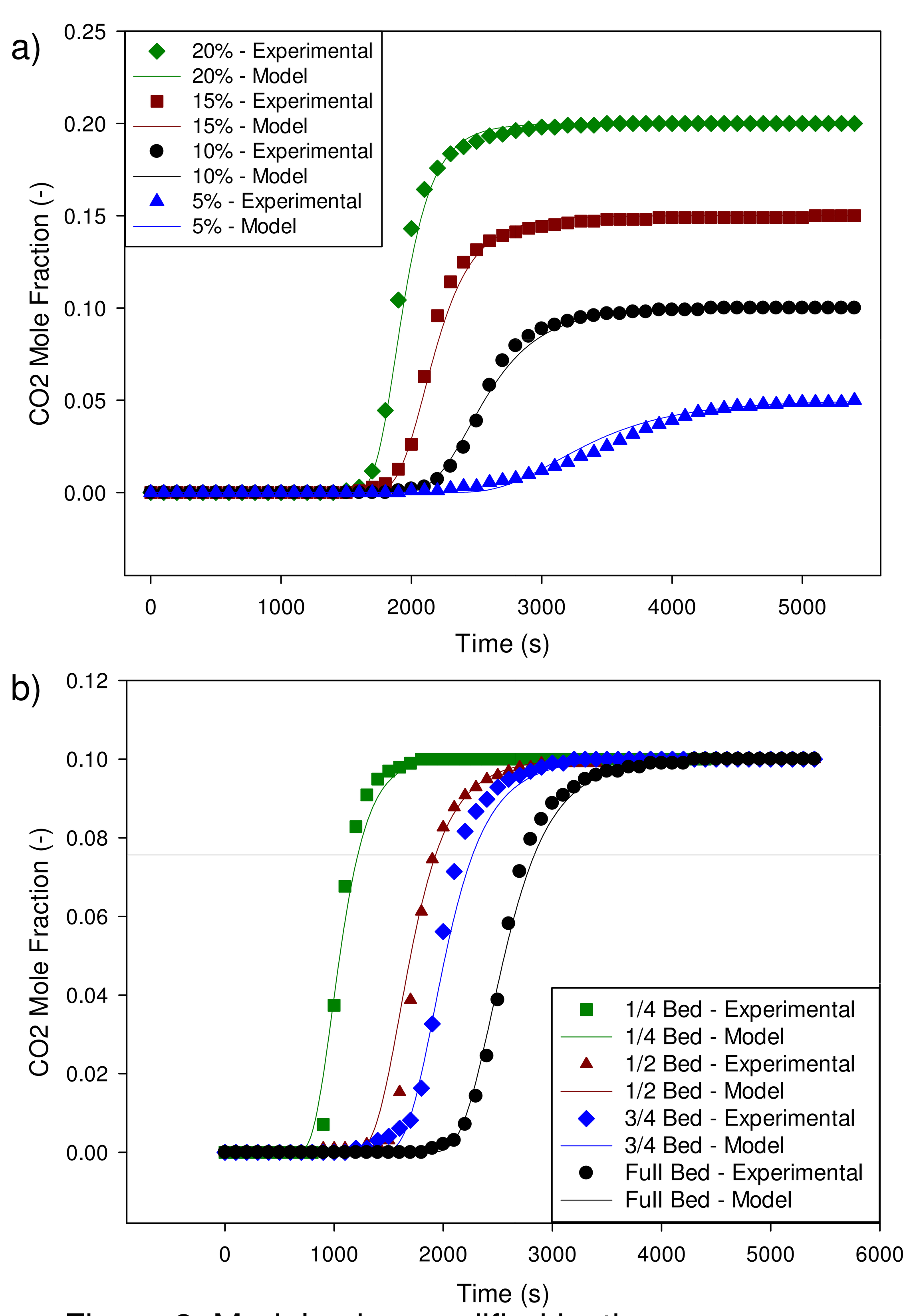
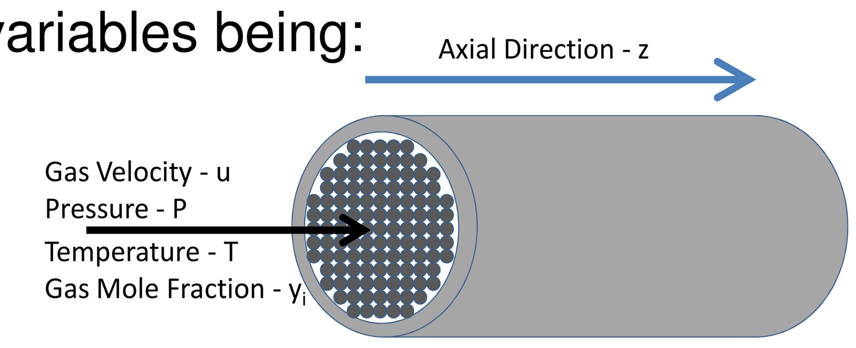


Figure 2: Model using modified isotherm

Model

Key Model equations:

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



- Axial Dispersed Plug Flow Model:

$$\frac{\partial (Py_i)}{\partial t} - D_{disp}\frac{\partial^2 (Py_i)}{\partial z^2} + \frac{\partial (uPy_i)}{\partial z} + \frac{(1-\varepsilon)}{\varepsilon}RT\frac{\partial q_i}{\partial t} = 0$$

$$\frac{\partial P}{\partial t} - D_{disp}\frac{\partial^2 P}{\partial z^2} + \frac{\partial (uP)}{\partial z} + \frac{(1-\varepsilon)}{\varepsilon}RT\frac{\partial q_i}{\partial t} = 0$$

- 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

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

Conclusion

- Parameter estimation is applied to the model successfully to match the results for various feed mole fractions of carbon dioxide
- These parameters were validated against results for various bed lengths
- A relationship was found for predicted B_{N2} values based on n_{n2} and y_{CO2}
- The empirical modified isotherm showed improved agreement for all results (Figure 2)

Future Work

- The model will be taken forward for development into a full pressure swing adsorption (PSA) model.
- The model will consist of the basic steps of adsorption, purge, blowdown and pressurisation steps. [2]
- Model will predict CO_2 purity, CO_2 recovery and the efficiency.
- The experimental set up will need to be altered to match PSA cycles used in industry.
- The model will then be integrated with an IGCC power plant model to look at the overall effect of CO_2 capture by this process

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.
2. Kikkinides, E.S., Yang, R.T., Cho, S.H., 1993. *Concentration and recovery of carbon dioxide from flue gas by pressure swing adsorption.* Industrial & Engineering Chemistry Research 32, 2714-2720.

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