Solids-based cycles for carbon capture (WP AC3 Detailed Models)

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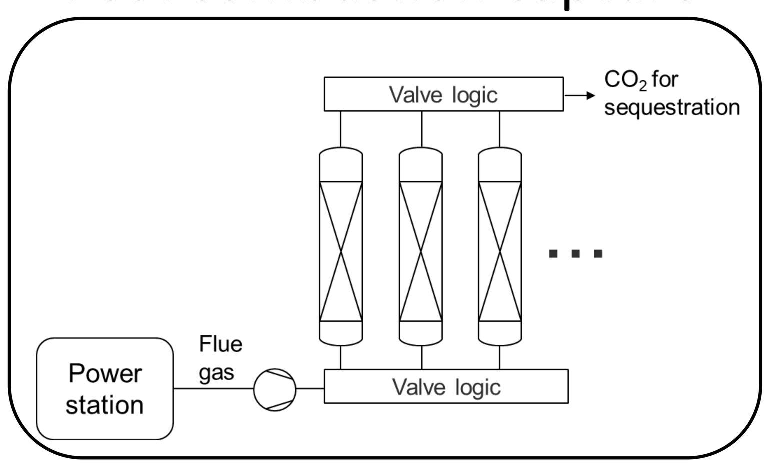
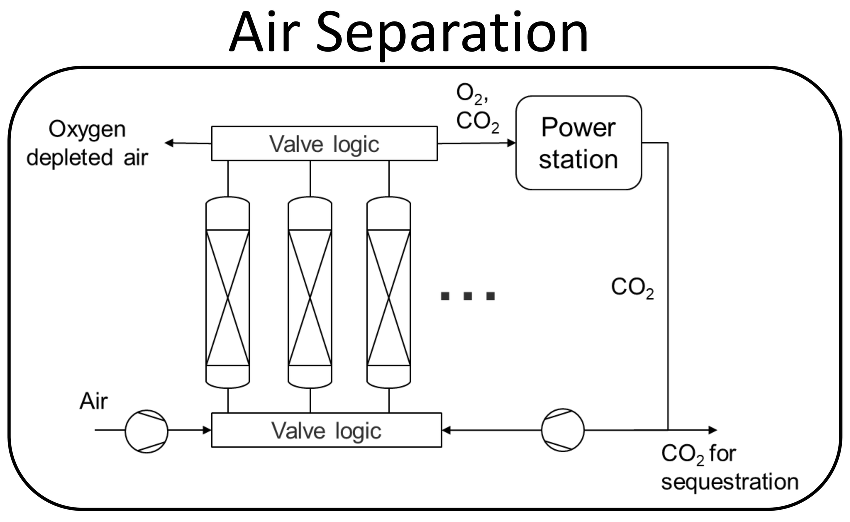
Project overview

- A number of different options are available for carbon capture with solids-based cycles.
- The focus here is on fixed bed processes. They offer an interesting and industrially relevant alternative to continuous fluidised beds. Furthermore pressure swing is possible.

Post combustion capture



Air Separation



Key objectives:

- Utilise advanced modelling environments to develop detailed steady-state and dynamic models of advanced solids-based cycles for carbon capture.
- Models will use experimental results or hypothetical material properties, *e.g.* isotherms, as inputs.
- Strategies will be developed to enable fair comparisons to be made between different capture options.
- The models or their outputs will be used to generate reduced-order-models for use in system level models.

Research highlights

Regardless of the system, or solid material, the underlying equations and rate expressions are the same:

Gas balances: $$\epsilon \frac{\partial c_i}{\partial t} = -\frac{\partial}{\partial z}\left(\rho u \epsilon y_i - D_{ax} C_t \frac{\partial y_i}{\partial z}\right) + r$$

Solid balance: $$(1-\epsilon)\frac{\partial q_i}{\partial t} = -r$$

Momentum balance: $$\frac{\partial P}{\partial z} = -k_f u$$

Energy balance: $$\frac{\partial U}{\partial t} = \ldots$$

Rate expression: $$r = k(P_i - P^*(q,T))$$

Rate expression is a relaxation of the equilibrium.

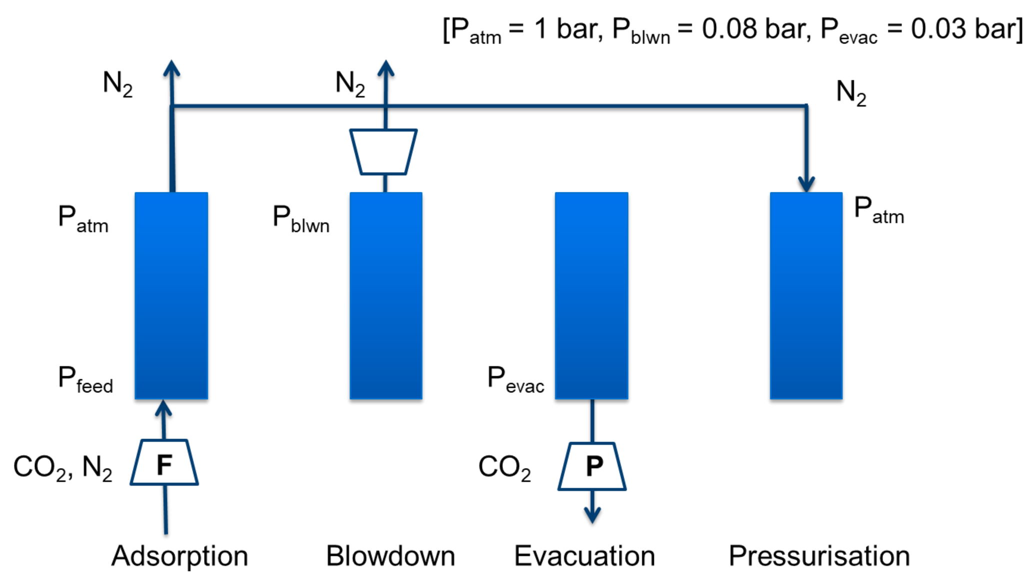
- k is a rate constant or a mass transfer coefficient
- $P*(q,T)$ is the equilibrium partial pressure exerted by a solid at conversion or loading, q.
- For physical sorbents or reactants showing non-stoichiometry, *e.g.* perovskites, $P*$ is a continuous function of q.
- For reacting systems, *e.g.* oxidation of copper (I) oxide, $P*$ is not a function of q except at the discontinuity at the phase transition.

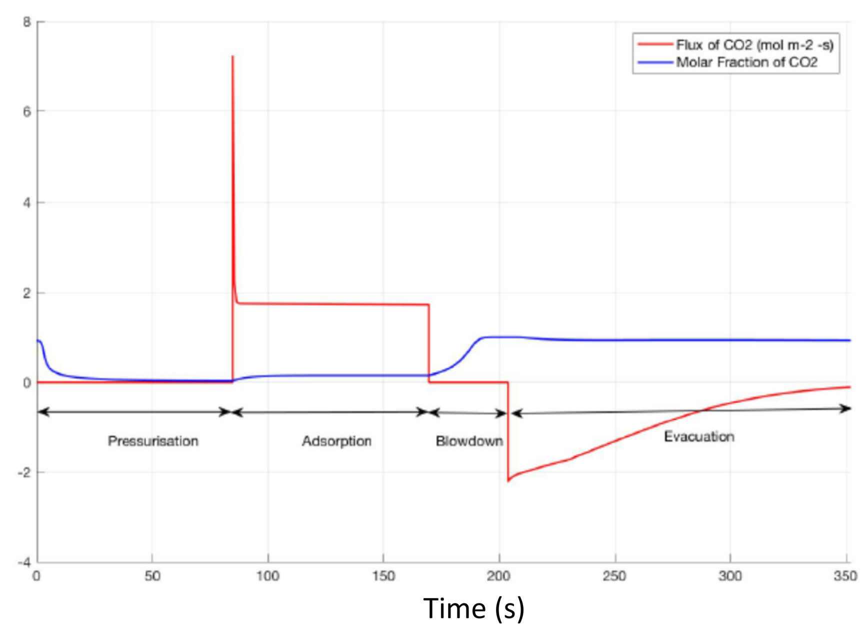
ϵ – voidage, c – concentration, u – velocity, ρ – density, y – mole fraction, z – axial distance, t – time, P - pressure

Emerging findings

Post combustion capture using a vacuum swing adsorption process

- 4-step cycle with Zeolite-X able to achieve > 90% purity and recovery of CO_2 from a typical flue gas emerging from a CCGT power plant (~4% CO_2 in N_2).





- By adjusting the step timings and, or the pressures, the cycle can operate dynamically with a power plant, while maintaining the required purity and recovery.

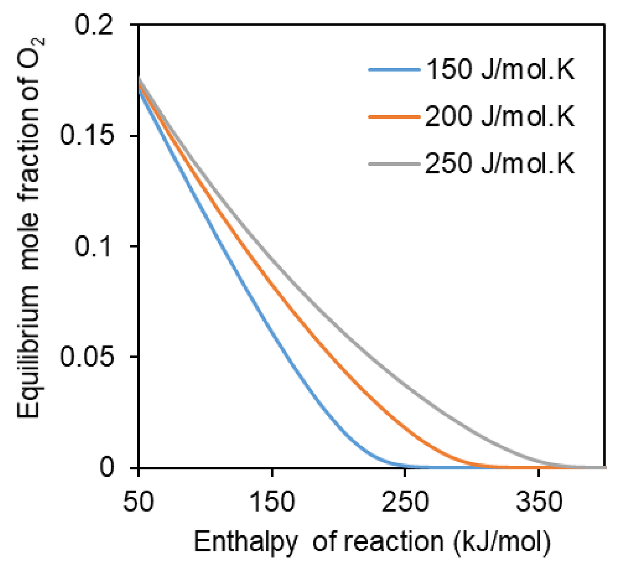
Air separation using a chemical looping approach

- Cycle consists of a reduction followed by an oxidation.
- The following material is ideally suited for operation in continuous, fluidized bed systems [1]:

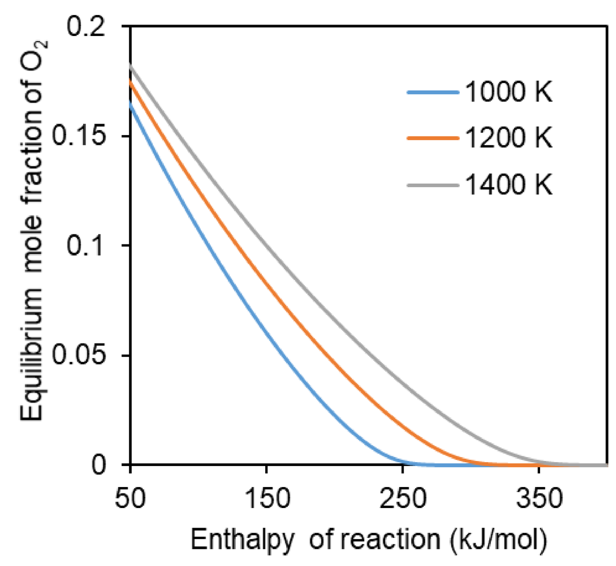
$$\mathrm{CuMn_2O_4} \leftrightarrow \mathrm{CuMnO_2} + \frac{1}{3}\mathrm{Mn_3O_4} + \frac{1}{3}\mathrm{O_2}$$

- In a fixed bed system a significant challenge is achieving a sufficiently high mole fraction of oxygen during reduction.
- The aforementioned material is not suitable – it is necessary to use materials with a lower enthalpy of reaction. Higher inlet temperatures and entropies of reaction are also desirable.

Entropy of reaction



Inlet temperature



Next steps

- VSA: (1) Complete a scenario analysis to determine the optimal design and operation of a VSA system for power plants at different points in the merit order, (2) Conduct a material screen.
- CLAS: (1) Explore combination of pressure and temperature swing as an option to increase mole fraction of oxygen, (2) Explore heat integration configurations with a power plant.

[1] Görke *et al.* (2018). Exploration of the material property space for chemical looping air separation applied to carbon capture and storage. Applied Energy, 212, 478–488.

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