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Modelling and optimisation of materials and processes for post-combustion CO_2 capture from flue gas by Pressure Swing Adsorption (PSA) and Vacuum Swing Adsorption (VSA)

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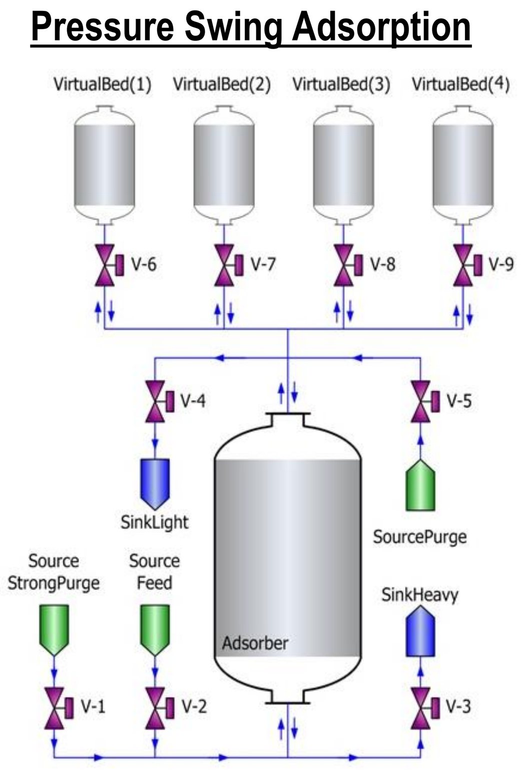
1. Aim Of Research

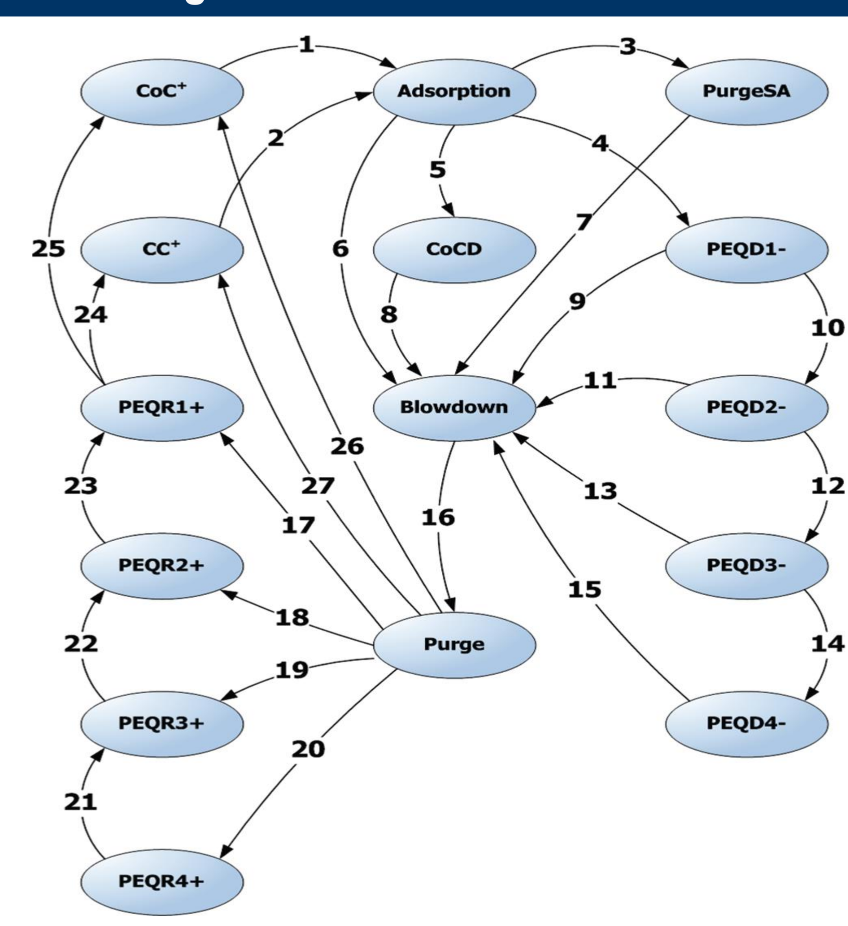
Pressure Swing Adsorption (PSA) and Vacuum Swing Adsorption (VSA) are gas separation processes which have attracted increasing interest because of their low energy requirements as well as low capital investment costs in comparison to the traditional separation processes. A detailed modelling framework of Pressure Swing Adsorption (PSA) for gas separation processes has been developed. The overall concept has been applied in the post-combustion Carbon Dioxide (CO_2) capture from dry flue gas. Detailed adsorption and transport models have been studied for three different adsorbent types. Depending on the general assumptions describing the adsorbent (porous solid) – adsorbate (gas mixture) system one can employ a broad variety of mathematical models and equations to describe the PSA/VSA process. Complex operating procedures are automatically derived and the most efficient ones are selected. The developed framework has been implemented in the gPROMS™ modelling environment.

3. Mathematical Modelling

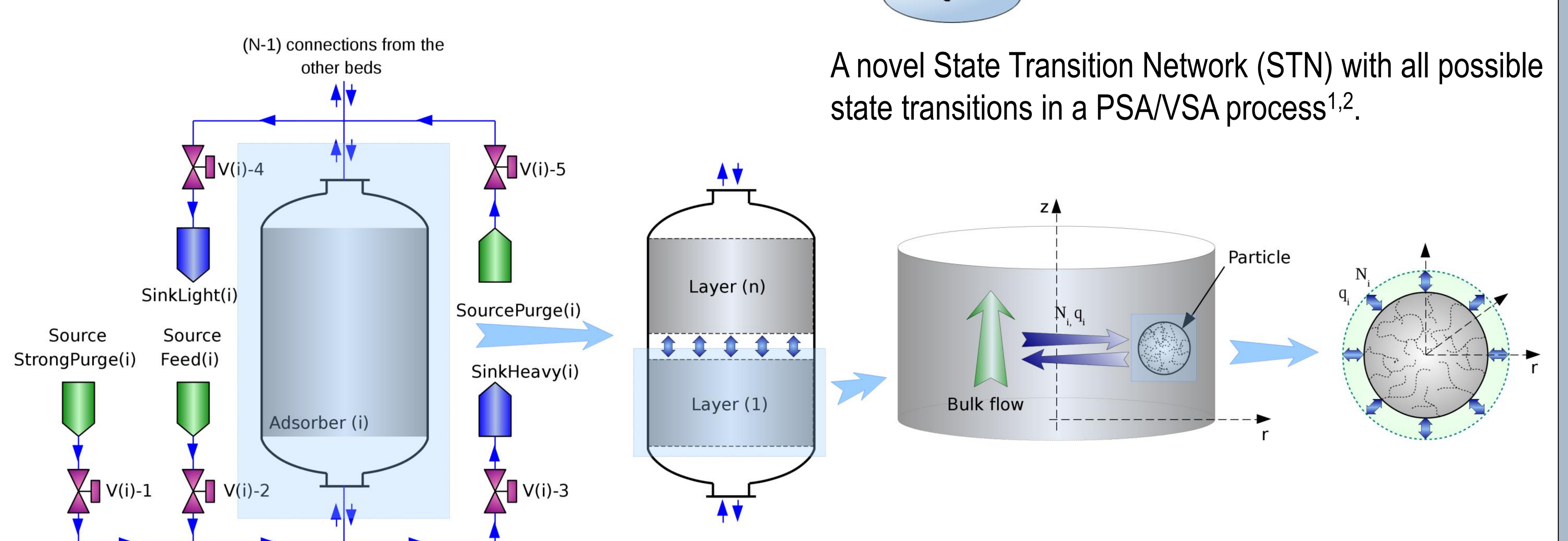
Pressure Swing Adsorption



Hierarchical model decomposition[1,2].



A novel State Transition Network (STN) with all possible state transitions in a PSA/VSA process[1,2].



Main assumptions:
- The flow pattern in the bed is described by the axially dispersed plug flow.
- The adsorbent is represented by uniform micro-porous spheres.
- No concentration, temperature and pressure gradients exist in the radial direction.

a) Mass transfer in particles:
- Local equilibrium (LEQ)
- Linear driving force (LDF)
- Surface diffusion (SD)
- Pore diffusion (PD)

b) Thermal operating modes:
- Isothermal
- Non-isothermal
- Adiabatic

c) Momentum balance:
- Blake Kozeny equation
- Ergun's equation

d) Multicomponent adsorption equilibrium:
- Henry's law
- Extended Langmuir
- Dual site Langmuir
- Ideal Adsorbed Solution Theory (IAS)

e) Thermophysical properties:
- Ideal gas law
- Equation of state

f) Transport properties:
- Constant values
- Correlations

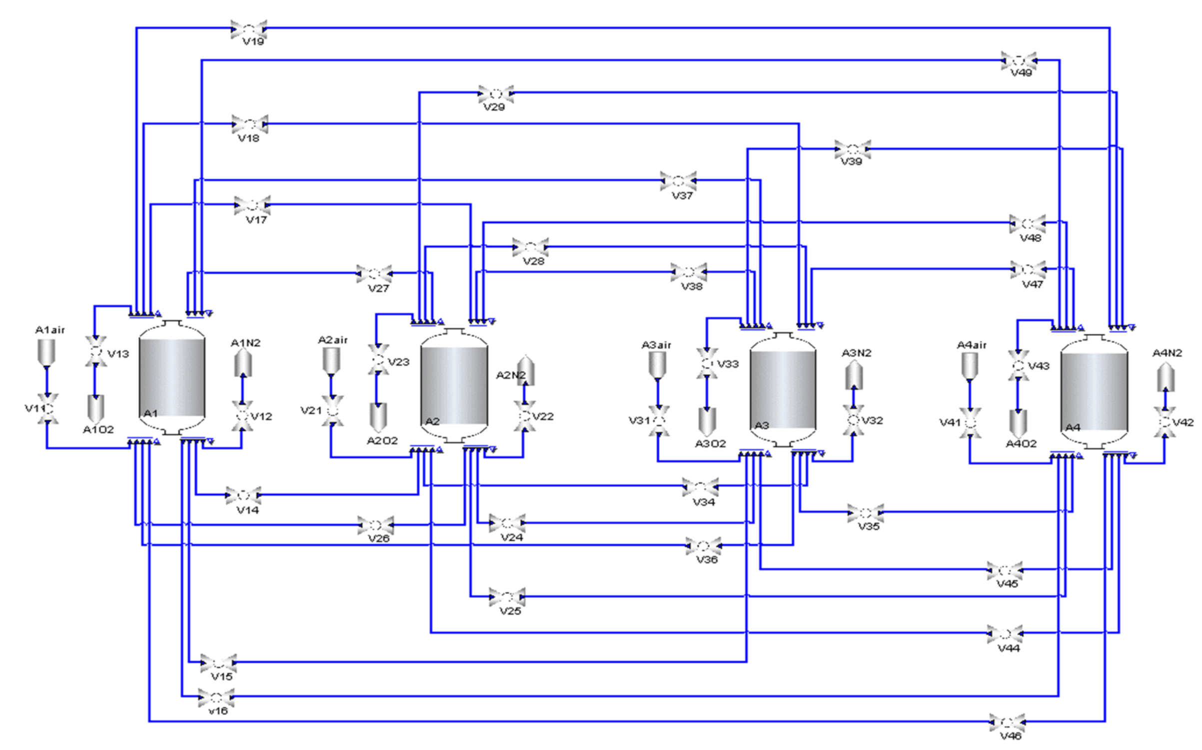
5. Conclusions

- A gPROMS™-based modelling framework for multi-bed PSA/VSA flowsheets.
- Customized gPROMS™ Output Channel Interface for real time plotting and user friendly visualization of key variables in the PSA/VSA plant.
- Formulation of detailed mathematical models at different scales in the adsorbent bed.
- Complex gas-valves control bed interactions.
- Suitable for arbitrary number of beds.
- Implementation of complex operating procedures.
- Incorporation of all feasible bed interconnections.
- Efficient implementations issues.
- Good predictive power (simulation results are in good agreement with literature results).
- Sensitivity analysis illustrates the typical trade-offs between process performance indicators.
- Extension of the modelling framework with other types of adsorbents.

6. Current Work

- Multilayer adsorbent studies.
- Optimisation studies of the PSA/VSA process in order to maximize CO_2 purity, CO_2 recovery and minimize power consumption.
- Modelling of hybrid PSA/VSA and membrane processes.
- Investigation studies of the optimal structural properties of the selected adsorbent based on the equilibrium and mass transfer characteristics determined by process optimisation studies.
- Synergies between material design and process design are systematically explored.

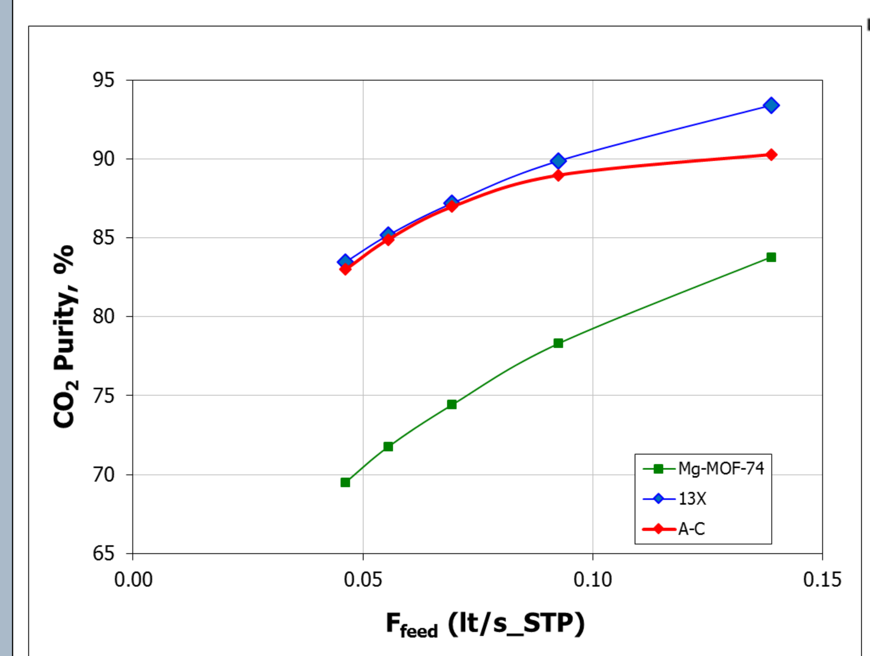
2. Process Superstructure

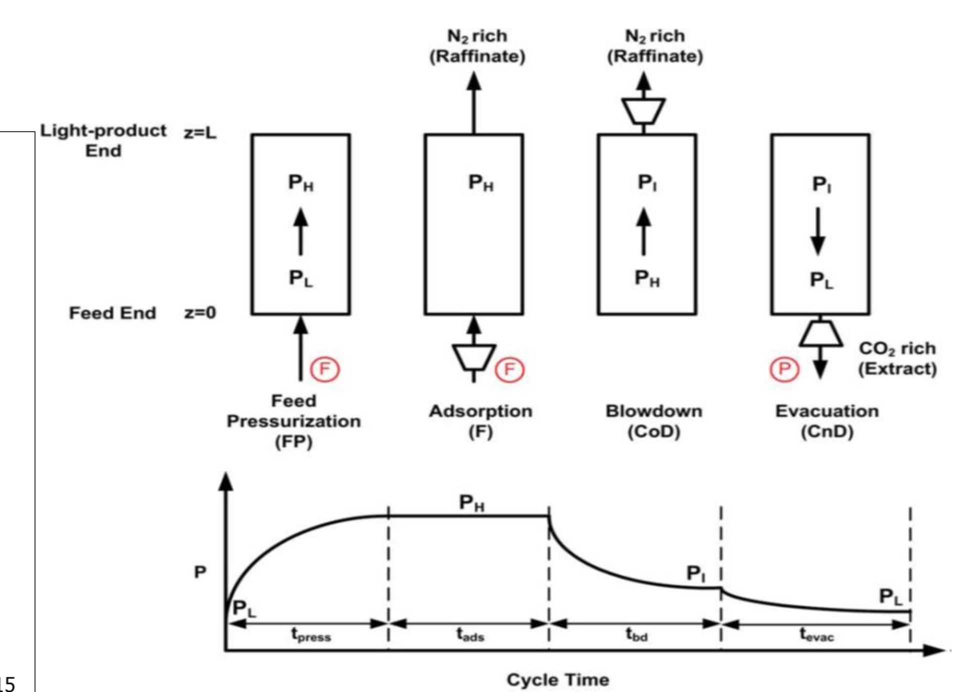


A typical four-bed PSA/VSA flowsheet.

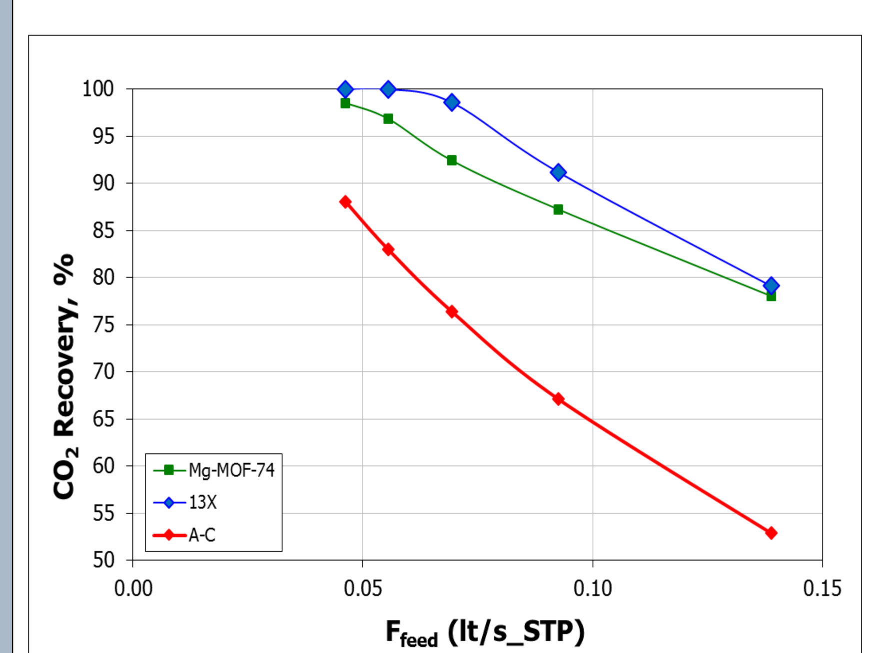
4. PSA/VSA Case Studies - Results

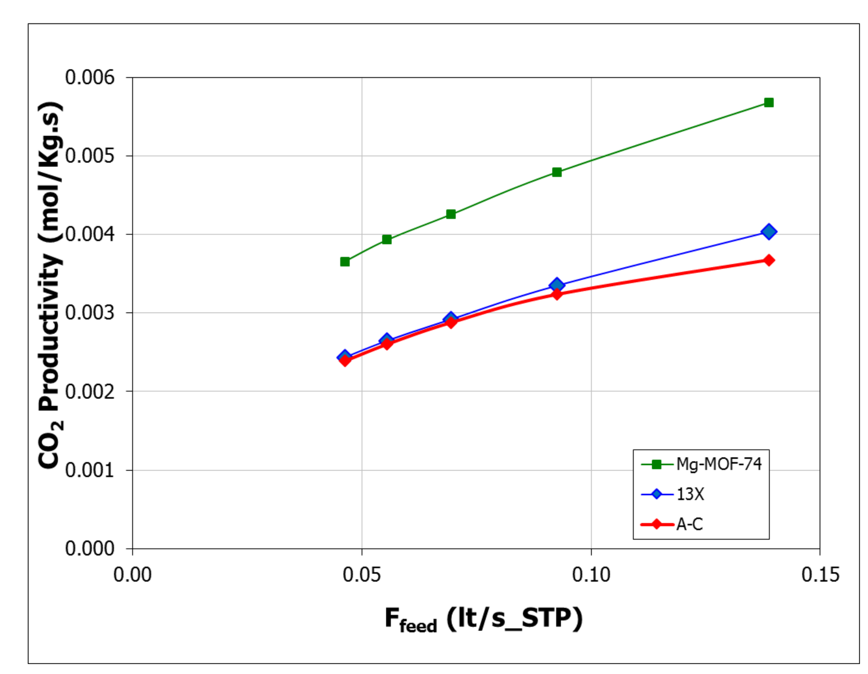
Case Study 1: Comparison of adsorbents



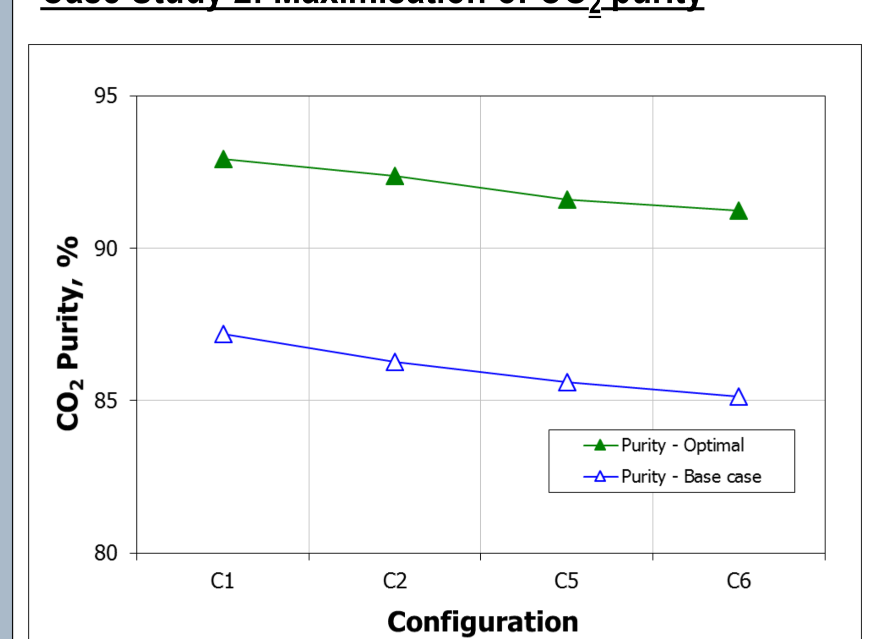


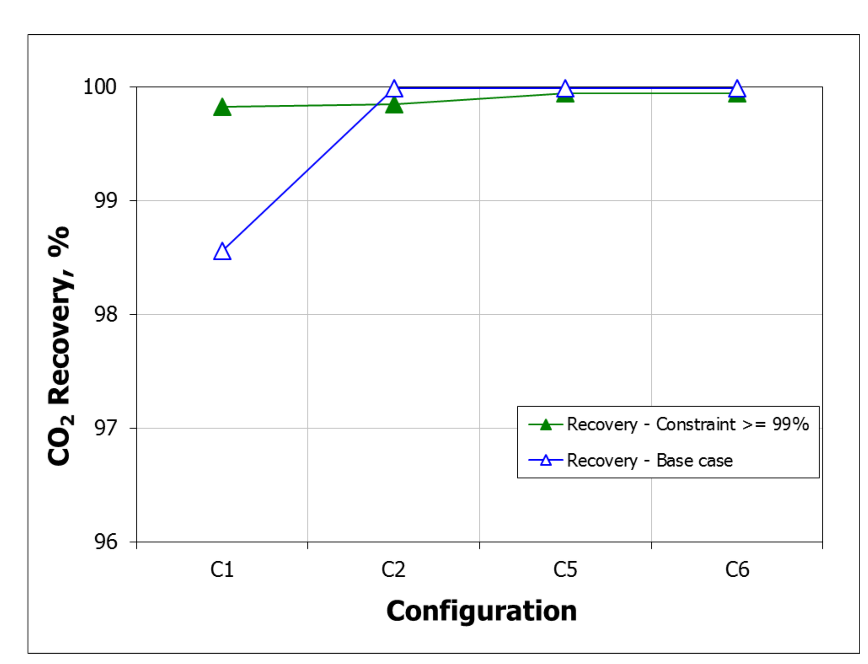
A 4-step PSA/VSA process with the pressure profiles[4].





Case Study 2: Maximisation of CO_2 purity





7. References

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8. Acknowledgements

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