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Modelling of Pressure Swing Adsorption (PSA) Processes for post-combustion Carbon Dioxide (CO_2) capture from flue gas

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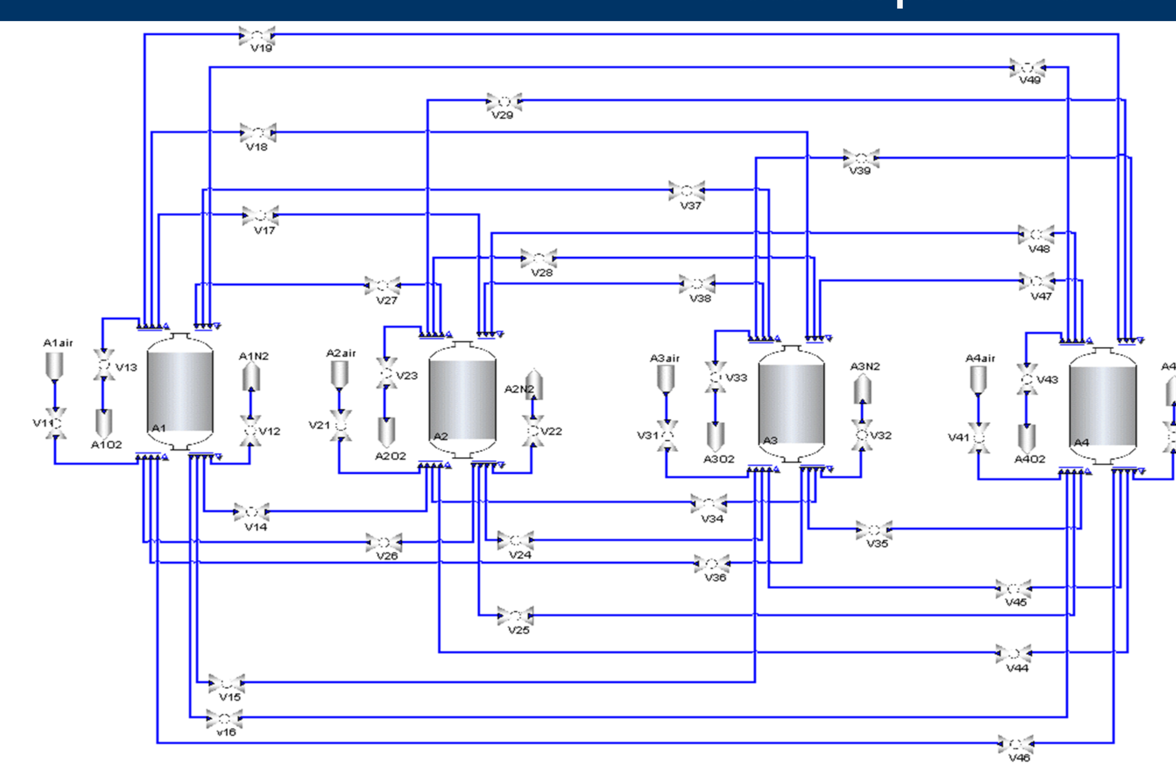
1. Aim Of Research

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 for Pressure Swing Adsorption (PSA) for gas separations is presented. The PSA concept has been applied on the process of post-combustion Carbon Dioxide (CO_2) capture from flue gas. We present the development of a modelling framework for efficient simulation and optimization strategies for the design of PSA/VSA processes with detailed adsorption and transport models. 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.

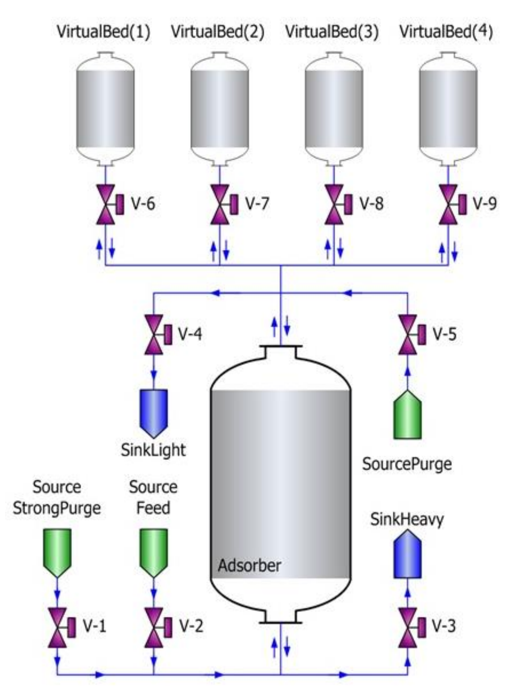
2. Process Superstructure



A typical four-bed PSA/VSA flowsheet.

3. Mathematical Modelling

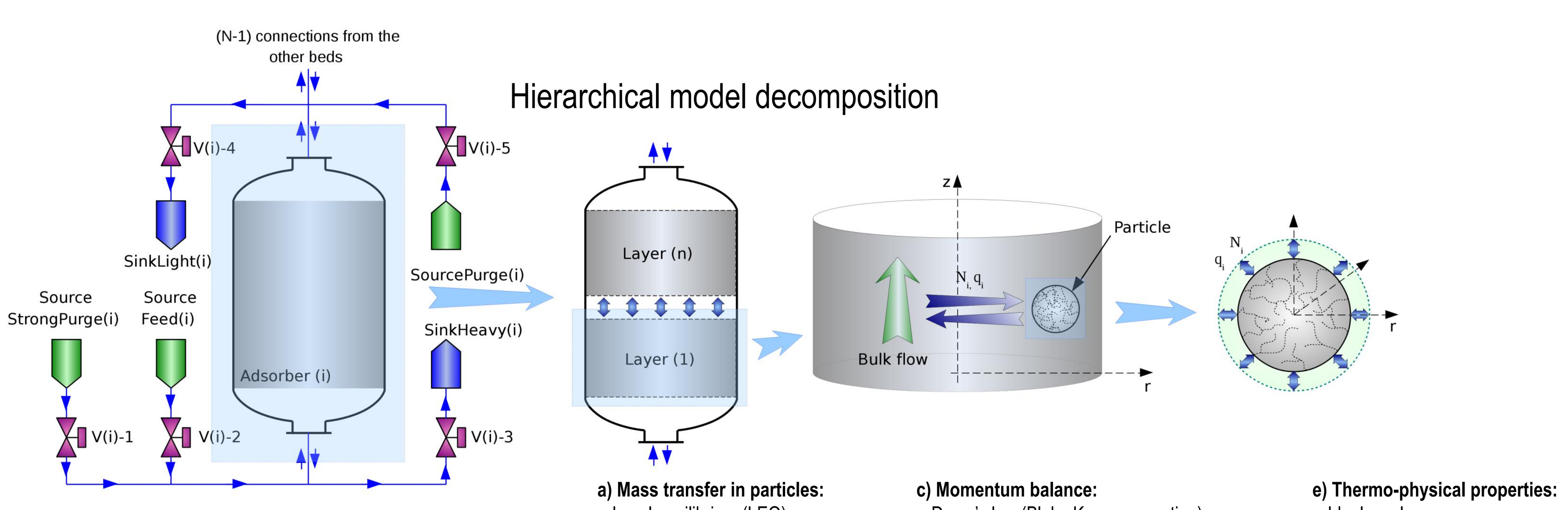
Pressure Swing Adsorption



The following model equations describe each step in the process:

- A mass balance for each component in gas phase.
- An energy balance that includes gas, solid and adsorbed phase.
- A momentum balance that predicts the pressure drop along the bed.
- A transport model describing non-selective mass transfer in the macropores of the adsorbent, and surface or activated diffusion of the adsorbate (gas mixture) in the micropores of the adsorbent.
- An equilibrium isotherm describing the thermodynamic relationship between the gas mixture and adsorbed phase.

Hierarchical model decomposition



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 and at the particle level, only changes in the radial direction of the partcile occur.

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:
- Darcy's law (Blake Kozeny equation)
- Ergun's equation

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

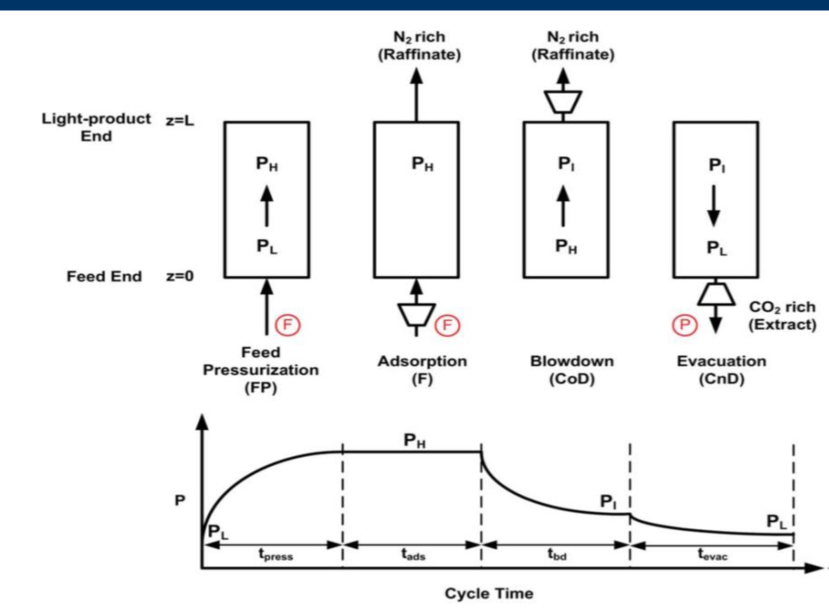
e) Thermo-physical properties:
- Ideal gas law
- Equation of state

f) Transport properties:
- Constant values
- Correlations

4. PSA/VSA Case Studies - Results

Case 1: PSA/VSA Model validation

Capture of CO_2 from dry flue gas (15% CO_2, 85% N_2) using Zeolite 13X as the adsorbent



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

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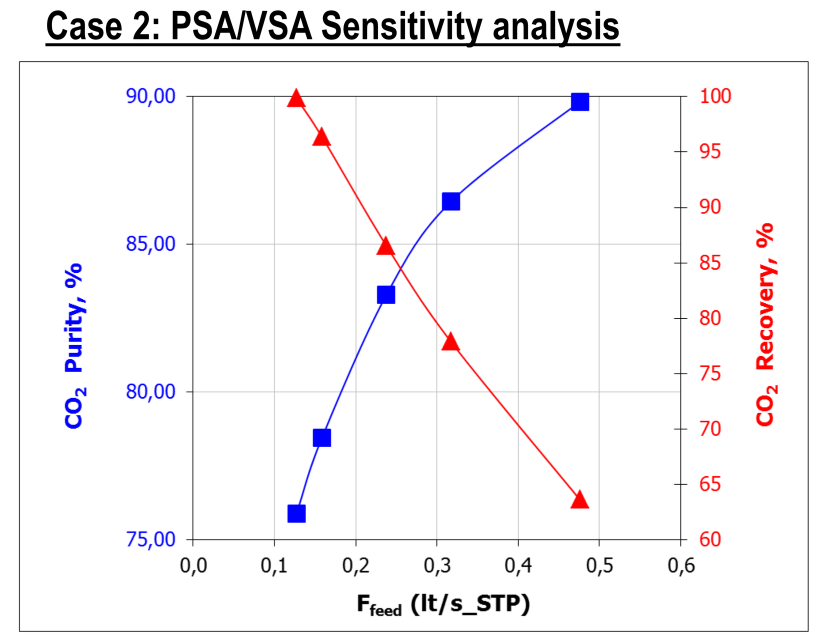
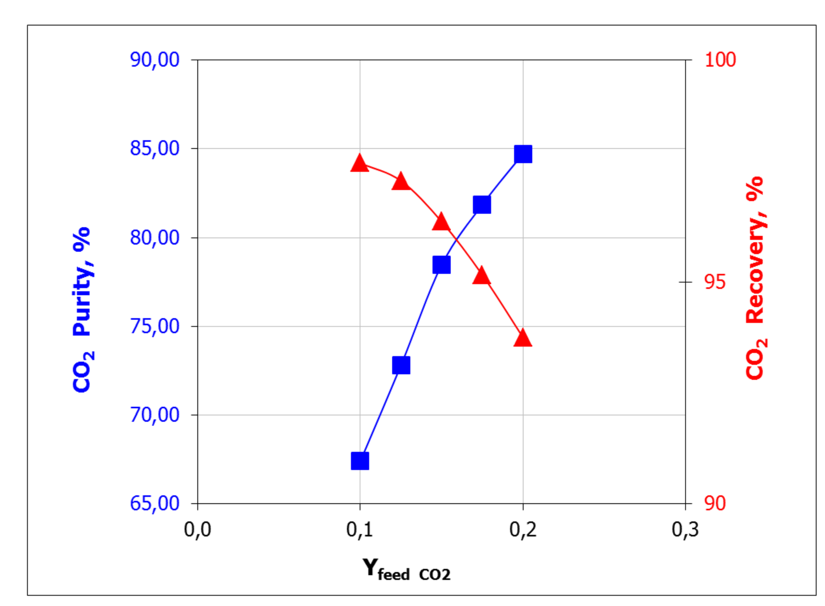
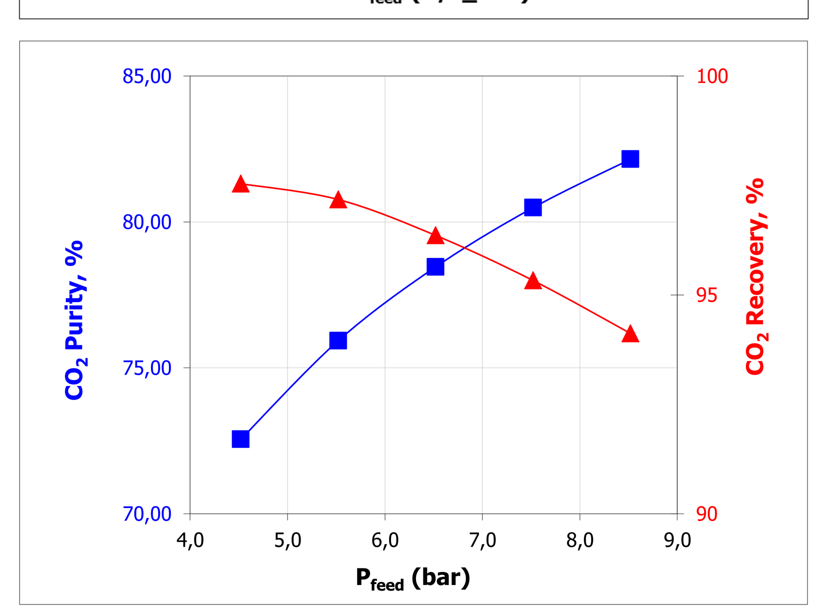
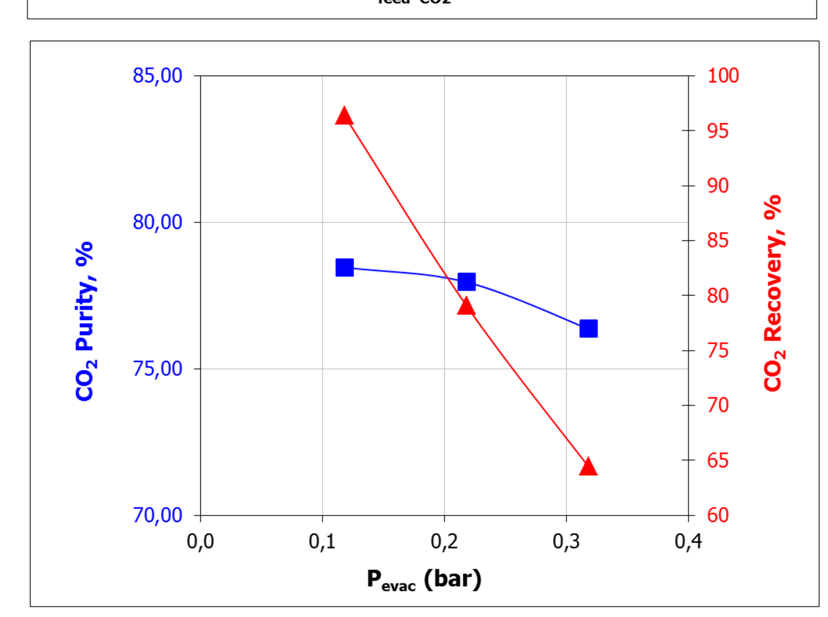
Reference	**Pfeed (bar)**	**Tfeed (K)**	**L/D**	**Number of cycles (CSS)**	**Discretization method**	**Purity CO_2**	**Recovery CO_2**	**Purity CO_2**	**Recovery CO_2**	**Deviation Purity CO_2**	**Deviation Recovery CO_2**
4	6,52	370,00	11,36	100	CFDM,2,40	88,94	96,90	82,22	95,15	-7,56	-1,81
4	6,94	365,32	11,36	100	CFDM,2,40	95,46	15,00	90,82	14,74	-4,86	-1,73
4	8,69	364,42	17,64	100	CFDM,2,40	92,29	80,00	95,74	78,22	3,73	-2,22
						Ko et al	Ko et al	this work	this work		
Reference	**Pfeed (bar)**	**Tfeed (K)**	**L/D**	**Number of cycles (CSS)**	**Discretization method**	**Purity N_2**	**Recovery N_2**	**Purity N_2**	**Recovery N_2**	**Deviation Purity N_2**	**Deviation Recovery N_2**
4	6,52	370,00	11,36	100	CFDM,2,40	99,45	97,87	95,91	96,71	-3,56	-1,19
4	6,94	365,32	11,36	100	CFDM,2,40	97,75	100,00	85,90	99,56	-12,12	-0,44
4	8,69	364,42	17,64	100	CFDM,2,40	99,00	100,00	96,28	99,46	-2,75	-0,54

Case 2: PSA/VSA Sensitivity analysis









5. Conclusions

- A gPROMS-based modelling framework for multi-bed PSA/VSA flowsheets.
- Formulation of detailed mathematical models at different scales in the adsorbent bed.
- Complex gas-valves control bed interactions.
- Customized gPROMS Output Channel Interface for real time plotting and user friendly visualization of key variables in the PSA/VSA plant.
- 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).
- Results of sensitivity analysis illustrate the typical trade-offs between process performance indicators (CO_2 purity and CO_2 recovery).

6. Current Work

- Multilayer adsorbent studies.
- Optimization studies of the PSA/VSA process in order to maximize purity and recovery for both top light product (raffinate) N_2 and bottom heavy product (extract) CO_2.
- Investigation studies of the optimal structural properties of the selected adsorbent based on the equilibrium and mass transfer characteristics imposed by the previous optimization studies.
- Synergies between material design and process design will be systematically explored.
- Extension of the modelling framework with other types of adsorbents such as Metal Organic Frameworks (MOFs)
- Software development activities.

7. References

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8. Acknowledgements

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SEVENTH FRAMEWORK PROGRAMME

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