Use of a Rigorous Energy Balance Including Kinetic Energy in the Process Simulation of a Rapid Pressure Swing Adsorption

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Backgrounds and Objectives

➤ Industrial-scale adsorptive carbon capture processes should be designed to have a very short cycle time to reduce the unit size by maximising the bed productivity.

➤ To avoid an excessive energy consumption for feed gas compression, the fast cyclic adsorption process requires a vacuum regeneration step, i.e. Rapid Pressure Vacuum Swing Adsorption (RPVSA).

➤ The effect of kinetic energy change on the PSA performance is deemed negligible in most conventional adsorption processes but becomes important in case of a RPVSA experiencing rapid velocity changes with time and space.

➤ Detailed numerical simulations on CO_2 capture RPSA cycles have been carried out using gPROMS to see the effect of kinetic energy terms on the adsorption dynamics.
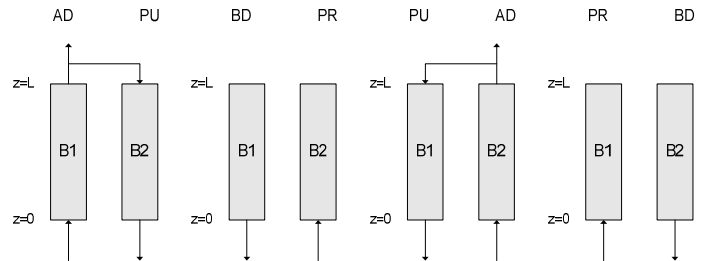

Figure 1. A two-bed, four-step Skarstrom cycle for RPVSA process.

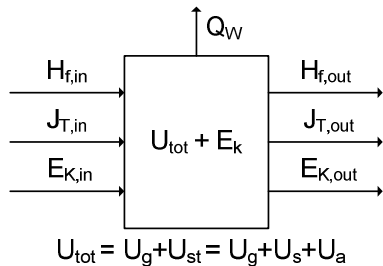## Rigorous Energy Balance Formulation and Model Validation

Figure 2. Block diagram for derivation of rigorous energy balance equation.

$$U_{tot} = U_g + U_{st} = U_g + U_s + U_a$$

Three energy balances have been compared:

➤ **Simplifed 1** [1]: Neglecting temporal pressure change and kinetic energy

➤ **Simplified 2** [2]: Neglecting kinetic energy only

➤ **Rigorous** : Including the kinetic energy terms

The model has been validated considering the limiting case of very high pressure drop along the adiabatic column with no adsorption, for which:

$$\Delta\left(H + \frac{1}{2}u^2\right) = 0 \qquad \Delta T = \frac{\left(\frac{1}{2}u_{in}^2 - \frac{1}{2}u_{out}^2\right)}{C_p}M$$
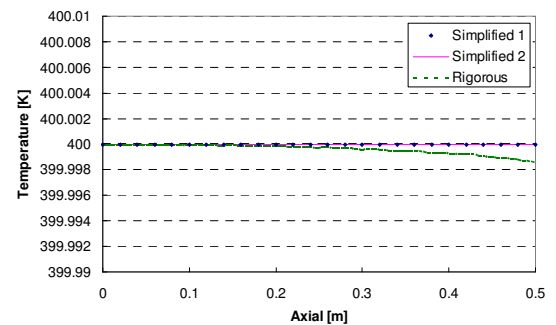

Figure 3. Temperature profiles along the column in the limiting case.

CO_2 Capture RPVSA Cycles – Simulation Results

➤ The operating conditions of a CO_2 capture RPVSA unit using Zeolite 13X.
P_{ads} = 1.5 bara, P_{des} = 0.1 bara, T_{feed} = 298.15 K

➤ CO_2 mixture gas feed (N_2/CO_2 = 0.85/0.15, molar basis).

➤ Pressure change during non-isobaric steps: $\dfrac{dP}{dt} = \alpha \cdot (P_f - P)$

➤ The rigorous energy balance shows a clear distinct from the others with a higher α.

➤ Testing Aspen Adsim confirms that Adsim uses Simplified 2 model neglecting kinetic energy effect, but the formulae of the energy balance shown in Adsim manual is not consistent with the actual equation.
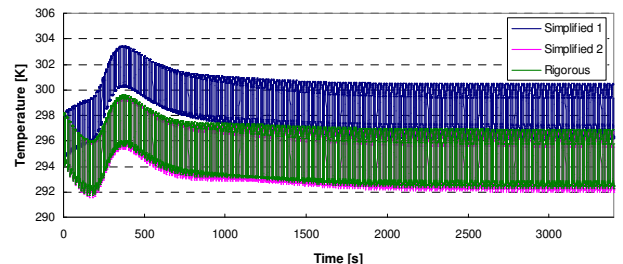

Figure 4. Temperature profiles over the cycles in the CO_2 capture RPVSA simulation.
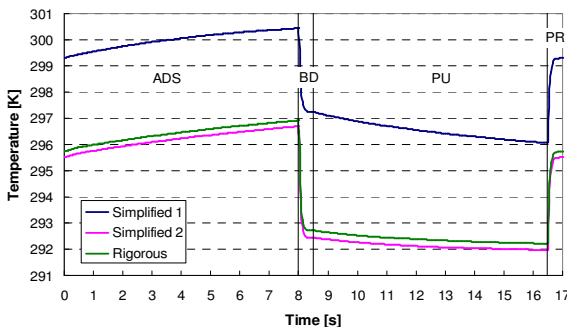
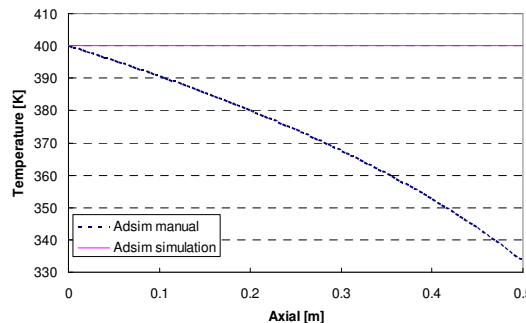

Figure 5. Temperature profiles during last cycle at CSS.

Figure 6. Temperature profiles in the limiting case of adiabatic, high pressure drop and no adsorption using Aspen Adsim manual formulae and actual Adsim simulator.

P/F = 0.025	Simplified 1	Simplified 2	Rigorous
α = 2 & t_{BD} = 4 s			
CO_2 Purity (%)	56.9324	56.9527	56.9534
CO_2 Recovery (%)	94.0662	93.9497	93.9489
CO_2 Productivity (mol$_{CO_2}$/kg$_{ads}$/h)	3.73	3.73	3.73
α = 10 & t_{BD} = 1 s			
CO_2 Purity (%)	56.7738	56.7804	56.7838
CO_2 Recovery (%)	94.7384	94.6707	94.6671
CO_2 Productivity (mol$_{CO_2}$/kg$_{ads}$/h)	5.12	5.11	5.11
α = 50 & t_{BD} = 0.5 s			
CO_2 Purity (%)	55.8499	55.1474	55.1985
CO_2 Recovery (%)	98.3544	99.4991	99.3971
CO_2 Productivity (mol$_{CO_2}$/kg$_{ads}$/h)	5.69	5.77	5.76

Table 1. RPVSA cycle performances.

Acknowledgements

References

[1] Ruthven D.M., 1984. Principles of adsorption and adsorption processes.

[2] Rodrigues et al., 2011. Separation & Purification Technology 81: 307-317.