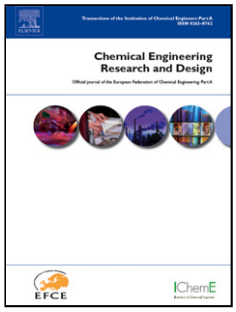

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Advanced Non-isothermal Dynamic Simulations of Dual Reflux Pressure Swing Adsorption Cycles

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Highlights

- An advanced non-isothermal numerical model was developed for dual reflux pressure swing adsorption process
- A dual convergence algorithm was developed to control the adsorption bed pressure profile
- A choked valve model was adopted to better capture gas flow characteristics
- Model validated against experimental data from two sources and could be used for further process studies

Abstract

An advanced non-isothermal dynamic model for the simulation of Dual Reflux Pressure Swing Adsorption (DR-PSA) cycles was constructed using Aspen Adsorption®. A new column pressure control method was developed to describe cycles that either continuously change pressure during the feed/purge steps or are held at constant pressure during these steps. This control method uses a dual convergence algorithm to adjust both the inlet volumetric flow of the compressor and the light product flow rate to achieve the desired pressure profile in the simulation. In addition, a choked flow valve after the compressor was employed to enable a high-fidelity simulation of the flows during the pressure reversal step in contrast to previous simulation approaches. To validate the model, predictions were benchmarked against the most detailed two sets experimental DR-PSA data available in the literature, which involved the separation of C_2H_6 + N_2 mixtures where bed pressures changed continuously during the feed/purge steps and the separation of CH_4 + N_2 mixtures where bed pressures were constant during these steps. At cyclic steady state, the standard deviations of the model's predictions from the experimental data involving C_2H_6 + N_2 mixtures separations were 0.003 mole fraction in a rich product stream with an average ethane composition of 0.63 mole fraction; and for the separation of CH_4 + N_2 mixtures, the standard deviation of the predicted product mole fractions from the experimental values