Choosing Adsorbent Materials for Separation from their Isotherms on Perfect Crystals: Application to n-Butane/iso-Butane Separation with All-silica Zeolites

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Complete binary adsorption isotherms are obtained on all-silica zeolites in the IZA-database using Gibbs ensemble Monte Carlo (GEMC) simulations. The vast majority of these isotherms can be fit to multi-site Langmuir isotherms. A mathematical model is developed for a pressure-swing adsorption (PSA) process, a breakthrough process, and a single-stage equilibrium process. By assuming local equilibrium between the fluid and solid phases, no parameter estimation is required in the models. Instead, the separation results only depend on the isotherm developed from the GEMC simulations. The results reveal that ranking adsorbents by the breakthrough approach cannot correctly rank adsorbents by the PSA process. However, the single-stage equilibrium process appears to rank materials in an order much more in line with a PSA process. These results suggest that using batch experiments or GEMC simulations to rank materials for an equilibrium-based adsorption separation is advantageous to other approaches, since the former approaches can perform a single-stage equilibrium process.