ON THE POTENTIAL OF PHASE-CHANGE ADSORBENTS FOR CO_2 CAPTURE BY TEMPERATURE SWING ADSORPTION

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We investigate the potential of a class of recently discovered metal–organic-framework materials for their use in temperature swing adsorption (TSA) processes for CO_2 capture; the particularity of the considered materials is their reversible and temperature dependent step-shaped CO_2 adsorption isotherm. Specifically, we present a comprehensive modeling study, where the performance of five different materials with step-shaped isotherms [McDonald et al., Nature, 2015, 519, 303] in a four step TSA cycle is assessed. The specific energy requirement of the TSA process operated with these materials is lower than for a commercial 13X zeolite, and a smaller temperature swing is required to reach similar levels of CO_2 purity and recovery. The effect of a step in the adsorption isotherm is illustrated and discussed, and design criteria that lead to an optimal and robust operation of the considered TSA cycle are identified. The presented criteria could guide material scientists in designing novel materials whose step position is tailored to specific CO_2 separation tasks.