Surrogate model of pressure swing adsorption process for efficient process optimization and evaluation

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Pressure swing adsorption (PSA) separates CO_2 from flue gas by difference of gas-adsorbent affinities between CO_2 and N_2. In order to unburden capture energy in a PSA process, it is essential to find an optimal operating pressure. The PSA process is modeled as a system of nonlinear partial differential equations (PDEs) to find a cyclic steady-state, making the process optimization numerically difficult and unstable. A surrogate model for the PSA process that captures the dynamic behavior allows finding the optimal operating condition without dynamic simulation. The dynamic models of Skarstorm cycle and vacuum cycle are modeled in gPROMS to investigate dynamic responses for operation above and below ambient pressure, respectively. Then a surrogate model expression as a system of few equations is proposed. The surrogate model predicts the key performance indicators of the PSA process, capture energy, rate, and purity, from the flue gas condition and operating pressure. Optimization of the PSA process is performed using the surrogate models as nonlinear programming (NLP). It is expected that the proposed surrogate model is an efficient evaluation tool of adsorbents for CO_2 capture.