Optimization of a Pressure Swing Adsorption Process with Different Adsorbents Properties for CO₂ Capture

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In spite of many types of adsorbents being developed for CO_2 capture with the aim of using in an industrial pressure swing adsorption (PSA) process, the lack of a systematic methodology connecting the experimental data in a lab-scale system to an industrial-scale system stands as a major challenge. As a step toward building such a methodology, we present a method to find optimal operating conditions of a PSA for varying parameters representing physic-chemical properties of adsorbents. The operation optimization is based on a solution of a PSA model at cyclic steady state (CSS) obtained by successive substitution. To alleviate the high computational cost in calculation of the CSS solution, we use a procedure in spirit of the *homotopy continuation*, where we use the solution of a similar set of parameters previously tried as an initial condition. A trend of the optimal operating conditions with respect to the adsorbent parameters is discussed as a basis for a further study, where the aim will be to relate the material design parameters to the performance of an industrial process unit.