Surrogate Model Construction of Pressure Swing Adsorption Process

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Carbon capture technologies act as significant keys to climate change issues. Pressure swing adsorption (PSA) is a promising process for carbon capture. Since a PSA model consists of partial differential-algebraic equations, it is a computationally intensive challenge to use the rigorous model in reaching a cyclic-steady-state and finding an optimal operating condition. To relieve the computational burden, a first-principle-based surrogate model is proposed which holds the dynamic features of the rigorous system. The case study in this work is the design of a surrogate PSA model for CO2 capture from flue gas. Overall operating conditions are obtained as solutions of the simplified equations when adsorbent parameters and pressure values are given. Also, the surrogate system provides a simple calculation method for performance indicators such as energy efficiency, capture rate, and purity. The surrogate model is validated by comparing the results of the surrogate model with those of the rigorous one. The application of the surrogate PSA model to various adsorbents is expected to directly calculate and compare the performance of each material.