Chemical Engineering Thesis Defense

Prediction of Multicomponent Gas Adsorption Equilibrium for Direct Air Capture Using Ideal Adsorbed Solution Theory

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Abstract

Adsorption equilibrium is an important metric used to assess adsorbent performance for gas mixture separation processes. Gas adsorption processes such as carbon capture are becoming more urgent as climate change and global warming accelerate. To speed up and reduce the cost of research on adsorbent materials and adsorption processes, we developed an open-source Python code that generates mixed-gas adsorption equilibrium data using pure gas adsorption isotherms based on the ideal gas adsorption theory (IAST). The major efforts of this M.S. research were placed on adding additional components to the mixture models since most other publications focused on just binary gas mixtures. Generated mixed-gas equilibrium data were compared to experimentally collected data in order to validate the multicomponent IAST model and to determine the accuracy of the computer codes developed in this work. Additional mixed-gas equilibrium data were then generated and analyzed for trends in the data, with a specific emphasis placed on carbon capture application conditions.

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