AN ABSTRACT OF A THESIS

MODELING MULTICOMPONENT ADSORPTION BEDS USING THE ADVANCED CONTINUOUS SIMULATION LANGUAGE

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Master of Science in Chemical Engineering

A method has been developed for using the Advanced Continuous Simulation Language (ACSL) to model the dynamic behavior of multicomponent adsorption beds used to control emission levels of volatile organic air pollutants. Through the incorporation of the Dubinin Isotherm and the Ideal Adsorbed Solution (IAS) Theory, the amount of experimental data needed to accurately simulate the dynamic behavior of a given multicomponent adsorption bed is brought to a minimum. Aside from a basic knowledge of the physical properties of each component in a mixture of gaseous adsorbates, the only experimental data needed to simulate multicomponent adsorption bed behavior are the pure component isotherm of a single component in the adsorbate mixture.

To extend the applicability of this method to simulate multicomponent adsorption beds, ACSL models pertaining to five separate combinations of adsorption bed operating conditions have been developed and include: isothermal beds with fast mass transfer, isothermal beds with slow mass transfer, adiabatic beds with fast mass and heat transfer, adiabatic beds with slow mass and heat transfer, and nonadiabatic, nonisothermal beds with slow mass and heat transfer. The utility of these five multicomponent adsorption models in the design of industrial scale processes was demonstrated through the application of a general adsorption problem in which a mixture of benzene, cyclohexane, pentane, and acetone vapors are removed from an air stream by passing the gaseous mixture through a bed of activated carbon. Through a simple analysis of the results provided by the various simulations, important information regarding optimum operating specifications for the given adsorption bed were obtained. Verification of the accuracy of the results predicted by the five models was provided by way of a fractional material balance closure test. In passing this test, it was concluded that the method developed to model multicomponent adsorption beds is both accurate, and conducive in industrial scale adsorption bed design.

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