

## **AN ABSTRACT OF A THESIS**

# **MODELING MULTICOMPONENT ADSORPTION BEDS USING THE SECOND VIRIAL SURFACE COEFFICIENTS AND THE ADVANCED CONTINUOUS SIMULATION LANGUAGE**

**Weijing Dang**

**Master of Science in Chemical Engineering**

The advanced continuous simulation language (ACSL) has been used to solve the partial differential equations that describe the behavior of adsorbent beds used to control the emission of volatile organic air pollutants. Five models were tested. These five models are isothermal beds with and without the local equilibrium, adiabatic beds with and without the local equilibrium, and finally a bed that is neither isothermal nor adiabatic. The second virial surface coefficients were used to describe the vapor-solid equilibrium. The derivation of Van Ness was used to obtain the second virial surface coefficients of the mixture from the isotherms of the pure components.

The method was tested with the same adsorption example as that of Johnson's thesis (MS, Tennessee Technological University, 1997) in which an equimolar mixture of benzene, cyclohexane, pentane, and acetone in air passes through a fixed bed of activated carbon. There is good agreement between results from this thesis and Johnson's thesis. The use of the second virial surface coefficients to obtain the vapor-solid equilibrium requires much less computer programming than the ideal adsorbed solution method used by Johnson.

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CONTINUOUS SIMULATION LANGUAGE**

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by

Weijing Dang

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MASTER OF SCIENCE

Chemical Engineering

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**CERTIFICATE OF APPROVAL OF THESIS**

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\_\_\_\_\_  
Chairperson

\_\_\_\_\_  
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Member

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Date

\_\_\_\_\_  
Member

\_\_\_\_\_  
Date

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\_\_\_\_\_  
Dean of Graduate Studies

\_\_\_\_\_  
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