

Dynamic and Equilibrium Mixed Vapor Adsorption Studies on Activated Carbon

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Single vapor adsorption isotherms can often be predicted at equilibrium, subject to some limitations, from the physical properties of the adsorbate vapors, by techniques based upon the Dubinin-Polanyi concept of affinity co-efficient¹⁻⁴.

It is often necessary to predict the adsorption behavior of specific vapors in the presence of other vapors and gas species in multicomponent or binary mixtures. The other species may or may not compete with the adsorption of the vapor species of interest. Techniques and approaches for predicting the equilibrium adsorption of one vapor component in a multicomponent or even a binary mixture are much less developed. Previous results have indicated that the following models have some potential for application to multicomponent adsorption by microporous carbon adsorbents.

1. Dubinin-Polanyi pore filling theory¹
2. John's mixture isotherm model⁵
3. Myer's ideal adsorption solution theory⁶

In this study, these theories have been evaluated. In all the models, single vapor isotherm data are used to predict multicomponent adsorption on BPL activated carbon.

The Dubinin-Polanyi theory has been used much less to predict multicomponent adsorption. The results that are available indicate, however, that the theory may have some potential for application to multicomponent adsorption. Bering et al^{7,8} extended the Dubinin-Polanyi equation to the adsorption of mixtures by means of the following equation:

$$\Sigma a_i = \frac{W_0}{\Sigma \bar{V}_i} \exp \left[-BT^2 \left(\frac{\Sigma \bar{V}_i \log (P_i/P_{si})}{\Sigma \bar{V}_i \beta_i} \right)^2 \right] \quad (1)$$

where \bar{V}_i = the partial molar volume of mixture component i.
 β_i = the partial molar affinity coefficient of mixture component i
 P_{si} = the saturated vapor pressure of component i
 P_i = the equilibrium pressure of component i
 a_i = the number of g. moles of component i adsorbed per gram of adsorbent
 N_i = the mole fraction of component i in the adsorbed phase
 W_0 & B = Constants characterizing the adsorbent.

The second model and the associated isotherm equation, which was developed by John et al⁵, is very similar, in principal, to the Dubinin-Polanyi model:

$$\log \log P_{12} = C_{12} + D_{12} \log W_{12} \quad (2)$$

where C_{12} and D_{12} are constants obtained from single vapor isotherms that depend upon the composition of the mixture.

$$P_{12} = \frac{\Sigma P_i}{\Sigma P_{si}} \cdot 10^N \quad (3)$$

N = an integer between 2 and 6

W_{12} = the total amount of mixed adsorbate.

Figure 1 shows a comparison of experimental equilibrium isotherm data with both the Dubinin-Polanyi model and John's isotherm model. Figure 1 indicates that these two models can be applied with some degree of success to calculate mixed adsorption isotherm. Agreement is better at low pressures but significant discrepancies occur at higher equilibrium pressures with the models underestimating the amount adsorbed. These two methods do not predict the equilibrium adsorption of one vapor component in a multicomponent system. However, they allow prediction of the total amount adsorbed.

The ideal adsorption solution theory has also been used to predict mixed gas adsorption with some success at low coverages/low relative pressure⁶. The method assumes that the adsorbed phase forms an ideal solution and involves determination of "spreading pressure" from the single vapor isotherms.

Figure 2 shows a comparison between data obtained from kinetic studies on the breakthrough/penetration of $\text{CHCl}_3/\text{CCl}_4$ vapor mixtures through BPL activated carbon beds with the predictions of the ideal adsorbed solution theory. Mole fraction of one component in the vapor phase is plotted against mole fraction of the same component in the adsorbed phase. Normal liquid-vapor equilibria data are also shown in Figure 2. The $\text{CHCl}_3/\text{CCl}_4$ experimental data shows a linear relationship between gas phase composition and adsorbed phase composition. The ideal adsorbed solution theory predicts a non-linear relationship, however. Thus, it appears that adsorbed $\text{CHCl}_3/\text{CCl}_4$ mixtures do not form an

ideal solution. Preliminary results on n-hexane/benzene and $\text{CH}_2\text{Cl}_2/\text{CHCl}_3$ mixtures indicate that the adsorption results agree more closely with both the predictions of the ideal adsorbed solution theory and the normal vapor-liquid equilibria.

In conclusion, the ideal adsorbed solution theory can be applied with some degree of success to binary vapor mixtures adsorbed on BPL activated carbon depending upon the mixture selected.

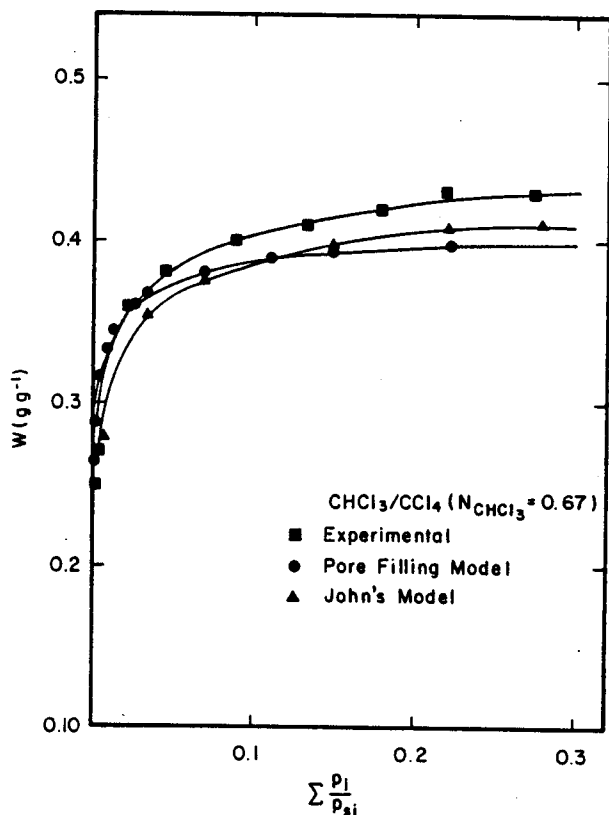


Figure 1. Experimental and Predicted Isotherms (BPL Activated Carbon, 25°C).

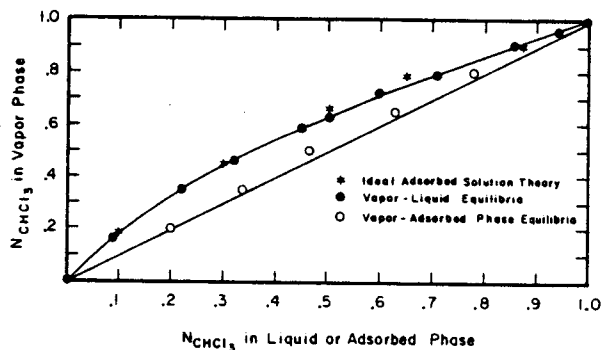


Figure 2. Vapor-Liquid and Vapor-Adsorbed Phase Equilibria for $\text{CHCl}_3/\text{CCl}_4$ Binary Systems (BPL Activated Carbon, 25°C).

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