# MULTICOMPONENT ADSORPTION DYNAMICS CALCULATIONS EMPLOYING ADSORPTION POTENTIAL AND IDEAL ADSORBED SOLUTION THEORIES

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## Introduction

A model is described for predicting multicomponent adsorption equilibrium based on an approach combining the Adsorption Potential and the Ideal Adsorbed Solution (IAS) theories. This approach was mentioned briefly by Myers [1], who considered the Adsorption Potential theory in the form of the Dubinin-Radushkevich isotherm. Very recently, Stoeckli and coworkers extended the method to the Dubinin-Astakov isotherm [2,3]. They were able to predict breakthrough curves for the binary adsorption of several vapors on activated carbon, under isothermal conditions, using IAS and the Dubinin-Radushkevich isotherm [4]. Here, a different form of the characteristic curve is employed and the theory is applied to a gas mixture with several components under nonisothermal conditions.

## Theory

The analysis of single-gas isotherm data on the basis of the Adsorption Potential theory gives rise to a characteristic curve of adsorption on the carbon, which is the relationship between volume of the adsorbed phase,

$$W \equiv q V_A, \tag{1}$$

and adsorption potential,

$$\phi = R_g T \ln(P_s/P). \tag{2}$$

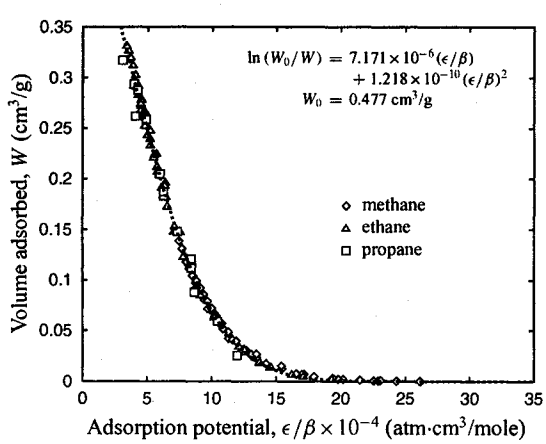


**Figure 1.** Characteristic curve of adsorption on AC.

It is assumed that for the species in the gas mixture an affinity coefficient $\beta$ can be used as a shifting factor to bring their characteristic curves on the same carbon into a single curve.

Although the functional form of the characteristic curve is adsorbent dependent, expressing the logarithm of $W$ as a truncated series development of $\phi/\beta$ has proved very versatile in fitting characteristic curves of various degrees of nonlinearity [5]:

$$\ln(W_0/W) = \sum_{i=1}^{n} k_i(\phi/\beta)^i. \tag{3}$$

Furthermore, a second-order polynomial ($n = 2$) usually gives a close fit of the experimental data.

In order to embed the IAS method in a dynamic simulation model, the spreading pressure of the gas mixture, $\Pi$, is treated as a dependent variable along with temperature and partial pressure of each adsorbate. The equation that $\Pi$ must ultimately satisfy is the condition

$$\sum_i^{NC} x_i = 1, \tag{4}$$

where the $x_i$ are the adsorbed-phase mole fractions, which are computed as follows. First, the adsorption potentials $\phi_i^0$, for which the pure-component adsorption equilibria yield the same value of $\Pi$, are calculated from the Gibbs adsorp-

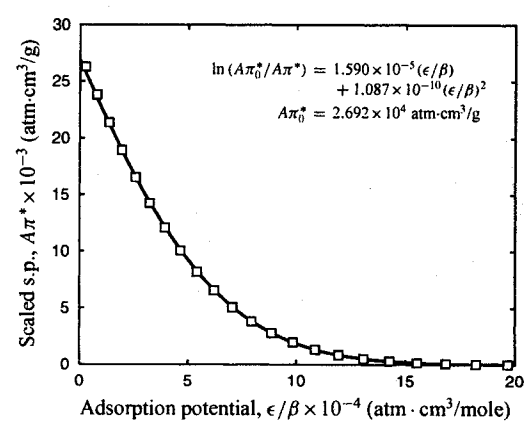


**Figure 2.** Scaled spreading pressure, $\Pi^* \equiv (V_A/\beta)\Pi A$, as a function of scaled adsorption potential, $\phi/\beta$.
The symbols denote values of $\Pi^*$ obtained by solving Eq. 5 numerically; the solid line is the least-squares fit of Eq. 8.

tion equation:

$$\int_{\phi_i^0/\beta_i}^{\infty} W(\phi^*)\, d\phi^* = \Pi_i^* \equiv (V_A/\beta)_i \Pi A \quad (\text{const. } T). \quad (5)$$

Then, the basic equation of IAS is employed to compute $x_i$:

$$x_i = \exp\left(\frac{\phi_i^0 - \phi_i}{R_g T}\right) = \frac{y_i P}{P_{s,i}} \exp\left(\frac{\phi_i^0}{R_g T}\right). \quad (6)$$

Once the correct value of $\Pi$ has been determined, the adsorbed-phase composition is calculated by the following expression:

$$1/q = \textstyle\sum_i x_i (V_A/W^0)_i, \quad q_i = x_i q, \quad W_i^0 \equiv W(\phi_i^0/\beta_i). \quad (7)$$

The advantage of writing Eq. 5 in terms of $\phi$ is that all species share the same integral function (the l.h.s. of the equation). This means that if the characteristic curves can be superposed using shifting factors, then the spreading pressure for the various species can be derived from a single curve also.

The author has observed that if the experimental characteristic curve can be fitted well by Eq. 3 with $n = 2$, then $\Pi^*$ can also approximated by a similar expression:

$$\ln(\Pi_0^*/\Pi^*) = s_1(\phi/\beta) + s_2(\phi/\beta)^2. \quad (8)$$

The most advantageous feature of Eq. 8 is that it can be rewritten explicitly for the scaled adsorption potential,

$$\phi/\beta = \frac{s_1}{2s_2}\left[\sqrt{1 + (4s_2/s_1^2)\ln(\Pi_0^*/\Pi^*)} - 1\right], \quad (9)$$

which reduces considerably the computational overhead introduced by the IAS method.

## Application example

The accuracy and computational efficiency of the equilibrium procedure was assessed by incorporating it in a dynamic, nonisothermal, nontrace column-breakthrough model. A linear driving force approximation is used for particle uptake, and it is assumed that there is no kinetic interaction between species for adsorption on the particles. A detailed description of the dynamic model is given in [6]. The model was solved numerically by the finite-volume method and a differential/algebraic equations solver [7].

The model was applied to the adsorption of a ternary hydrocarbon gas mixture from an inert carrier (He) in a packed bed of activated carbon. The experimental single-gas isotherm data [8] has been correlated on the basis of the Adsorption Potential theory. According to the theory, the characteristic curve should be temperature independent. As shown in Figure 1, this premise is fully verified by the experimental data. Furthermore, the individual characteristic curves have been sucessfully superposed by the use of shifting factors. Figure 2 shows the least-squares fit of Eq. 8 to the values of $\Pi^*$ obtained by solving numerically Eq. 5 using an adaptive quadrature procedure. The agreement between the fitted curve and the data is so good that the fitting is nearly an interpolation.

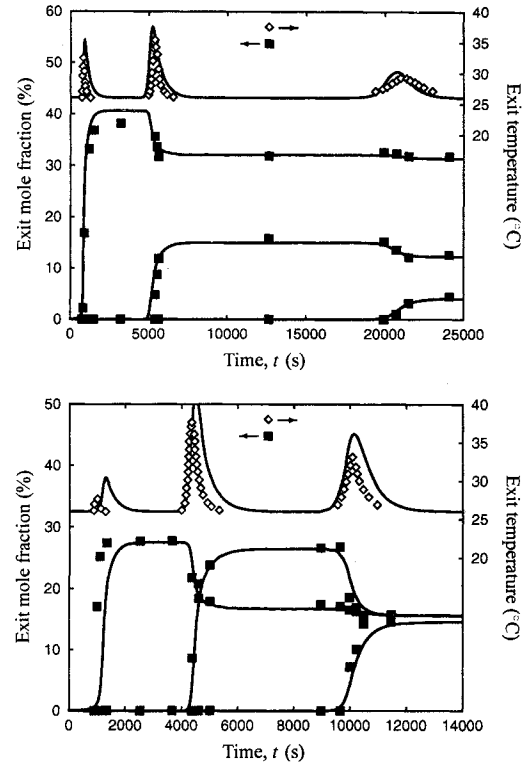


**Figure 3.** Breakthrough curves for methane (C1), ethane (C2), and propane (C3) mixture in activated carbon. Comparison between the measurements of [6] and model predictions.

Figure 3 shows the experimental and simulation breakthrough profiles for two runs corresponding to different operating conditions and feed concentrations. Each simulation run took less than a minute on a PC with a 300 MHz Pentium II processor. It is clear that the model gives a good agreement between its predictions and the experimental profiles. The test case demonstrates that the combined approach described here for predicting multicomponent adsorption equilibrium results in a computationally feasible procedure suitable for embedding in design and simulation models of adsorption on activated carbon.

## References

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