PREDICTION OF LIQUID PHASE ADSORPTION EQUILIBRIA OF MULTI-SOLUTES IN WATER

MORIO OKAZAKI, HIROYUKI KAGE AND RYOZO TOEI
Department of Chemical Engineering, Kyoto University, Kyoto 606

For the purpose of exact prediction of multi-solute adsorption equilibrium from respective single-solute adsorption isotherms, we propose a new method which employs a modified Langmuir kinematic adsorption model, assuming that the adsorptive surface of the adsorbent is heterogeneous in energy of adsorption. The predictions of adsorption equilibria on activated carbon for ten kinds of aqueous solutions, involving two solutes, were performed. The prediction accuracy of the present method was the same or slightly better than the two modified Radke's methods, which were proposed by Jossens et al.

Introduction

Use of purification by adsorption for industrial and municipal wastewater treatment has become more prevalent in recent years. Adsorption equilibria for mixtures of organic pollutants are required for design of these processes. To reduce experimental work, it is desirable to be able to predict the adsorption equilibrium of mixed organic solutes in dilute aqueous solution by employing only experimental data from single-solute adsorption isotherms.

In spite of its industrial importance, there are few studies on the method of prediction or correlation of multi-solute adsorption equilibrium. Ockrent and Weber employed the Langmuir model extended to multi-solute system to predict two-solute adsorption. But their extended Langmuir model has a strong limitation on its application, because only a few organic aqueous solutions follow the Langmuir isotherm. Radke and Prausnitz extended the method of Myers and Prausnitz, which was proposed for mixed-gas adsorption, to multi-solute adsorption from dilute liquid solution. Their method is based on a formulation of the thermodynamics of adsorption, and it seems to be the most reliable one at present. Recently, Jossens et al. further improved its accuracy of prediction by applying their own correlation formula to single-solute adsorption isotherm, though the model still has some ambiguity in its accuracy.

1. Correlation of Single-Solute Adsorption Isotherm

We recognize a heterogeneous surface of adsorbent to be described by a distribution of adsorption energy. A “patch” of surface characterized by a given potential becomes the seat of an adsorbed phase, so that the surface is composed of infinitesimal patches of different energy. Now we adopt the Langmuir model (monolayer adsorption) on these individual patches, and further postulate the following assumptions.

Assumptions:

1. These patches adsorb independently of one another.
2. The Langmuir equation holds for each of these patches.
3. The ultimate uptake capacity \( Q_s \) is characterized by the combination of adsorbent and adsorbate. Then we assume that the configurations of adsorbed molecules is much the same as that of the molecules in liquid state, and that it doesn’t take any orientation. As a result, the surface area occupied by an adsorbed molecules can be ap-
approximated by the base area of a cube of the same volume as that occupied by an adsorbate molecule in liquid state. Therefore, \( Q_s \) is

\[
Q_s = S/q_m N_v = S/N_v (M/\rho N_v)^{2/3}
\]

**1.1 Definition of the energy distribution function on adsorption surface**

The Langmuir energy term "\( k \)" in Eq. (1) can be regarded as a function of adsorption energy. It becomes large as energy becomes large. Therefore, let the value of \( k \) designate the adsorption energy level. Introducing the distribution function of the patches against \( k \), \( f(k) \), which is represented by the number of adsorption sites per mole (that is, the number of adsorption sites divided by Avogadro's number), we get

\[
Q_s = \int_{k_{\min}}^{k_{\max}} f(k) dk
\]

The amount of adsorption on the patches having adsorption energy \( k \), \( q(k, C) \) is given by

\[
q(k, C) = f(k)kC/(1 + kC)
\]

or integration of Eq. (4) with respect to \( k \) gives

\[
Q(C) = \int_{k_{\min}}^{k_{\max}} q(k, C)dk = \int_{k_{\min}}^{k_{\max}} f(k)kC/(1 + kC) dk
\]

Finally, the adsorption isotherm for a single-solute system is represented by Eq. (5).

The next problem is how to identify the energy distribution function \( f(k) \) from the adsorption isotherm measured experimentally for the single-solute system.

**1.2 Identification of energy distribution function, \( f(k) \)**

To determine \( f(k) \), so as to fit the experimental data of single-solute adsorption equilibrium, \( Q(C) \) in Eq. (5), is essentially the same as "to solve integral equations". There are various methods to solve integral equations, but for simplicity of the following calculations, in the present study an analytical simulation formula which involves some unknown adjusting parameters was assumed as \( f(k) \), and the parameters which satisfied Eq. (5) were numerically searched. (When the density of adsorbate, \( \rho \), is unknown, \( Q_s \) becomes an unknown parameter, too. In this case, there are three unknown parameters to be identified.)

The next problem is how to choose an approximate formula for \( f(k) \). We can roughly consider this problem as follows. If the adsorption sites which have very low adsorption energy are taken into account, the number of sites draws toward infinity in general. And the intrinsic distribution curve of sites is thought to start from a certain maximum value of \( k \) and to increase gradually as \( k \) decreases, as curve A in Fig. 1. Further, the curve goes to infinity as \( k \) approaches 0, because there are sites which have zero energy everywhere on the adsorption surface. However, molecules adsorb on the sites from \( k_{\min} \) to \( k_{\max} \) in order of adsorption energy \( k \), and a molecule occupies the finite area around the site. Therefore, some sites which have lower value of \( k \) are covered with the adsorbed molecule which adsorbed on a higher \( k \) site and lose their adsorption capacity. According to the above consideration, the apparent distribution curve of patch for \( k \) increases gradually as \( k \) decreases from \( k_{\max} \), and has a maximum of \( f(k) \). Then it suddenly decreases as soon as it passes the maximum, and approaches \( f(k)=0 \), as \( k \) decreases. The form of the curve is qualitatively illustrated by curve B in Fig. 1.

Although various simulation formulas may be used for curve B in principle, Eq. (6), which corresponds to the broken line a-b in Fig. 1, is acceptable for the present problem from considerations of simplicity of analysis in spite of a small fault in accuracy of fitting.

\[
f(k) = A/k, \quad k_{\min} < k < k_{\max}
\]

There are three unknown adjusting parameters, \( A \), \( k_{\min} \), and \( k_{\max} \) in Eq. (6).

Substituting Eq. (6) into Eq. (3), we get

\[
Q_s = \int_{k_{\min}}^{k_{\max}} f(k) dk = A \ln (k_{\max}/k_{\min})
\]

Equation (7) can be used to eliminate one parameter, \( A \). Consequently, the unknown parameters become \( k_{\min} \) and \( k_{\max} \). Substitutions of Eqs. (6) and (7) into Eq. (5) and then integration of Eq. (5) with respect to \( k \) give

\[
Q(C) = \frac{Q_s}{\ln (k_{\max}/k_{\min})} - \ln 1 + k_{\max} C
\]

The optimum values of \( k_{\min} \) and \( k_{\max} \) should be determined by fitting Eq. (8) to the experimental equilibrium data for the single-solute system.

**2. Extension to Multi-Solute System**

Let us proceed to develop the prediction method of \( n \)-solute (multi-solute) adsorption equilibrium on the basis of single-solute equilibria. Now we postulate the following assumptions to simplify the succeed-

\* Equation (6) corresponds to the Frumkin-Temkin equation for a heterogeneous surface.
Assumptions:

4. The interaction among adsorbed molecules can be ignored irrespective of the species of the molecules. That is, adsorbed molecules can act in their occupied place independently of other molecules.

5. Although each patch has its peculiar values of $k$ corresponding to the respective species of adsorbate, the rank in the order of $k$ among the patches is independent of species of adsorbate.

2.1 The relationship among the values of $k$ for each adsorbate

The accumulated number of patches from $k^*$ to $k_{\text{max}}$ is given by

$$U(k^*) = \int_{k^*}^{k_{\text{max}}} f(k)\,dk$$  \hspace{1cm} (9)

When an arbitrary patch has adsorption energy $k^*_i$ for adsorbate 1, $k^*_i$ for adsorbate 2, and $k^*_i$ for adsorbate $i$, the relationship among $k^*_i$, $k^*_i$, ..., $k^*_i$ is described by Eq. (10) according to assumption (5).

$$U_i(k^*_i)/Q_{i\text{m}} = U_i(k^*_i)/Q_{i\text{m}} = \cdots = U_i(k^*_i)/Q_{i\text{m}}$$  \hspace{1cm} (10)

This relationship is schematically illustrated in Fig. 2. Combining Eqs. (7), (9) and (10), we get

$$\frac{\ln(k_{i\text{max}}/k^*_i)}{\ln(k_{i\text{max}}/k^*_i)} = \frac{\ln(k_{i\text{max}}/k^*_i)}{\ln(k_{i\text{max}}/k^*_i)} = \cdots$$  \hspace{1cm} (11)

2.2 The Langmuir adsorption isotherm for multisolute system

Surface coverage for component $i$ for a homogeneous surface, $\theta_i$, is

$$\theta_i = k_i C_i \left(1 - \sum_{j=1}^{n} \theta_j\right), \quad i = 1, 2, \ldots n$$  \hspace{1cm} (12)

Equation (12) can be solved with respect to $\theta_i$ to give Eq. (13).

$$\theta_i = k_i C_i \left(1 + \sum_{j=1}^{n} k_j C_j\right), \quad i = 1, 2, \ldots n$$  \hspace{1cm} (13)

On the other hand, the surface coverage for a heterogeneous surface is

$$\theta_i(C_i, k^*_i) = k^*_i C_i \left(1 + \sum_{j=1}^{n} k^*_j C_j\right), \quad i = 1, 2, \ldots n$$  \hspace{1cm} (14)

where $k^*_i$ in Eq. (14) should hold the relationship described by Eq. (11). Finally, the amount of adsorption for $i$, $Q_i$, can be expressed as follows:

$$Q_i(C_i) = \int_{k_{i\text{min}}}^{k_{i\text{max}}} f_i(k^*_i) \theta_i(C_i, k^*_i)\,dk^*_i$$

$$= \frac{Q_{i\text{m}} C_i}{\ln(k_{i\text{max}}/k_{i\text{min}})} \int_{k_{i\text{min}}}^{k_{i\text{max}}} \left\{dk^*_i \left(1 + \sum_{j=1}^{n} k^*_j C_j\right)\right\}$$  \hspace{1cm} (15)

Further, $k^*_i$ in Eq. (15) can be described as Eq. (16) from Eq. (11), by using $k^*_i$.

$$k^*_i = (k^*_i/k_{i\text{max}})k^*_i k_{j\text{max}}$$  \hspace{1cm} (16)

where

$$K_{i\text{d}} = \frac{\ln(k_{i\text{max}}/k_{i\text{min}})}{\ln(k_{i\text{max}}/k_{i\text{min}})}$$  \hspace{1cm} (17)

Substituting Eq. (16) into Eq. (15), we get

$$Q_i(C_i) = \frac{Q_{i\text{m}} C_i}{\ln(k_{i\text{max}}/k_{i\text{min}})} \int_{k_{i\text{min}}}^{k_{i\text{max}}} $$

$$\times \left\{dk^*_i \left(1 + \sum_{j=1}^{n} k^*_j (k_{i\text{max}}/k^*_i) k_{i\text{max}} C_j\right)\right\}$$  \hspace{1cm} (18)

Since $Q_{i\text{m}}$, $k_{i\text{min}}$, and $k_{i\text{max}}$ in Eq. (18) can be obtained from experimental data for each solute, the amounts of adsorption for all solutes at arbitrary concentrations, $C_i$, can be calculated by using Eq. (18).

3. Experiment

Experiments of adsorption equilibria on activated carbon (CAL, Calgon Corp.) for two-solute aqueous solution systems (phenol-p-nitrophenol, p-nitropheno1-p-cresol), were performed to verify the accuracy of the theoretical model. Before use, the carbon (14-16 mesh) was crushed, and the powdered carbon through 200 mesh was adopted. The powdered carbon was further washed and dried at 110°C for a day. Finally it was kept in a dessicator containing silica gel. Adsorption equilibria were obtained by contacting known weights of carbon with a given solution in flasks. The carbon was degassed for 30 minutes by aspirator as soon as it contacted the solution. The flasks were placed on a shaker and agitated for 1-4 days at 35°C. After equilibrium was attained a sample was taken from each flask. Prior to analysis, it was filtered through a 0.5 μm glass filter to be free of any trace of suspended carbon. The concentration of each solute at equilibrium was measured by ultraviolet spectrophotometry.

The equilibrium data for phenol-p-nitrophenol and p-cresol-p-nitrophenol systems are shown in Figs. 3 and 4, and Figs. 5 and 6, respectively.
4. Results of Prediction

The prediction of adsorption equilibria on activated carbon for ten kinds of adsorption system involving two solutes was performed by three methods, namely the two modified Radke’s methods, in which the Toth equation and the Jossens equation were adopted respectively, and the present method. The adsorption systems used for the predictions are summarized in Table 1.

4.1 Determinations of parameters for single-solute systems

Table 2 shows the values of parameters in Eq. (8), the Toth equation and the Jossens equation, which were determined from the equilibrium data for single-solute systems, together with the relative fitting errors. The value of \( Q_s \) in Eq. (8) obtained from Eq. (2) using \( \rho, M \) and \( S \) (B.E.T. surface area) are given in Table 3. \( Q_s, k_{max}, k_{min} \) were searched as parameters for only two systems, \( \alpha \)-phenyl phenol and dodecyl benzol sulfonic acid, because their densities were not available.

The fitting accuracies of Eq. (8) are somewhat worse than for the other two equations. The reason may be thought to be that the other two equations have three adjusting parameters, but Eq. (8) has only two parameters. If Eq. (8) is modified to have more parameters, the accuracy of fitting may be thought to become better. However, we dare to use a simulation formula having two parameters for simplicity of calculation.

4.2 Prediction for two-solute system

The relative errors of prediction for ten kinds of two-solute systems calculated by the two modified Radke’s methods, in which the Toth and Jossens equation were adopted respectively, and the method proposed here, are shown in Table 1, and comparisons between observed and predicted results for phenol-\( \alpha \)-nitrophenol and \( \beta \)-cresol-\( \beta \)-nitrophenol are given in Figs. 3 to 6.

From Table 1, we can find that our method has more stable accuracy than the others and that there is no system with especially inaccurate result by our method, in spite of a slight insufficiency of fitting for single-solute equilibrium.

Further, from the first, eighth and ninth columns...
The less adsorbable solutes are the reverse, except for experimental values for two-solute systems, and in the two-solute systems, are always predicted higher than the proposed model, while the less adsorbable solute might be underpredicted. Thus the more adsorbable solute is overpredicted, while the less adsorbable solute is underpredicted. Hence the present model has a possibility of improvement in exactitude by taking into account the effect of the interaction among adsorbate molecules, and this is a problem awaiting solution in future.

**Conclusion**

1. A Langmuir type single-solute adsorption equilibrium model for heterogeneous surface of adsorbent was proposed, and two parameters derived from the equilibrium data were obtained. Further, the model was extended to the multi-solute system, and two-solute adsorption equilibria were predicted by use of parameters for the single-solute system.

2. The prediction accuracy of the proposed method for the two-solute system was the same or a little better than the two modified Radke's methods, proposed by Jossens et al. (12) and This work.

- Table 1: Comparison of prediction accuracy of three methods for two-solute adsorption equilibrium

<table>
<thead>
<tr>
<th>Solute</th>
<th>Activated carbon</th>
<th>No. of exp. points</th>
<th>Av. relative difference $F$</th>
<th>Prediction errors $R(T)$</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>1* (A)/2(B)</td>
<td>35</td>
<td>CAL</td>
<td>21</td>
<td>0.235 0.204 0.223</td>
<td>This work</td>
</tr>
<tr>
<td>3(A)/2(B)</td>
<td>35</td>
<td>CAL</td>
<td>16</td>
<td>0.166 0.265 0.517</td>
<td>Jossens</td>
</tr>
<tr>
<td>2(A)/1(B)</td>
<td>20</td>
<td>B10-I</td>
<td>230</td>
<td>0.150 0.101 0.095</td>
<td>good</td>
</tr>
<tr>
<td>2(A)/4(B)</td>
<td>20</td>
<td>B10-I</td>
<td>64</td>
<td>0.158 0.109 0.111</td>
<td>good</td>
</tr>
<tr>
<td>2(A)/5(B)</td>
<td>20</td>
<td>B10-I</td>
<td>64</td>
<td>0.251 0.357 0.342</td>
<td>+ -</td>
</tr>
<tr>
<td>4(A)/6(B)</td>
<td>20</td>
<td>B10-I</td>
<td>64</td>
<td>0.179 0.185 0.214</td>
<td>+ -</td>
</tr>
<tr>
<td>7(A)/2(B)</td>
<td>20</td>
<td>B10-I</td>
<td>46</td>
<td>0.265 0.307 0.125</td>
<td>+ -</td>
</tr>
<tr>
<td>8(A)/9(B)</td>
<td>20</td>
<td>B10-II</td>
<td>16</td>
<td>0.224 0.784 0.780</td>
<td>+ -</td>
</tr>
<tr>
<td>4(A)/3(B)</td>
<td>25</td>
<td>Filtrasorb 300</td>
<td>29</td>
<td>0.102 0.220 0.119</td>
<td>good</td>
</tr>
<tr>
<td>10(A)/11(B)</td>
<td>25</td>
<td>Filtrasorb 300</td>
<td>19</td>
<td>0.149 0.043 0.055</td>
<td>good</td>
</tr>
</tbody>
</table>

- Table 2: Parameters and relative fitting errors of Eq. (8), the Toth equation and the Jossens equation

<table>
<thead>
<tr>
<th>Solute</th>
<th>$k_{min}$</th>
<th>$k_{max}$</th>
<th>$Q_1$</th>
<th>$F$</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
<th>$\delta$</th>
<th>$\epsilon$</th>
<th>$F^{\beta}$</th>
<th>$F^{\gamma}$</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>1*</td>
<td>8.15 x 10^{-5}</td>
<td>2.08 x 10^{-4}</td>
<td>5.48</td>
<td>2.64</td>
<td>4.02</td>
<td>0.234</td>
<td>0.304</td>
<td>2.36</td>
<td>6.70 x 10^{-5}</td>
<td>1.48 x 1.25</td>
<td>2.74</td>
<td>This work</td>
</tr>
<tr>
<td>2</td>
<td>1.03 x 10^{-5}</td>
<td>1.08 x 10^{-4}</td>
<td>5.27</td>
<td>6.70</td>
<td>273.</td>
<td>0.168</td>
<td>0.0326</td>
<td>1.46</td>
<td>5.17 x 10^{-15}</td>
<td>23.8</td>
<td>0.208</td>
<td>1.47</td>
</tr>
<tr>
<td>3</td>
<td>6.21 x 10^{-5}</td>
<td>7.21 x 10^{-4}</td>
<td>4.89</td>
<td>3.98</td>
<td>3.87</td>
<td>0.134</td>
<td>0.390</td>
<td>2.35</td>
<td>9.54 x 10^{-4}</td>
<td>0.412</td>
<td>2.29</td>
<td>3.39</td>
</tr>
<tr>
<td>1</td>
<td>1.07 x 10^{-5}</td>
<td>2.15 x 10^{-4}</td>
<td>8.99</td>
<td>16.9</td>
<td>18.4</td>
<td>0.325</td>
<td>0.130</td>
<td>2.73</td>
<td>4.02 x 10^{-4}</td>
<td>3.12</td>
<td>0.647</td>
<td>6.67</td>
</tr>
<tr>
<td>2</td>
<td>9.65 x 10^{-6}</td>
<td>2.44 x 10^{-5}</td>
<td>8.59</td>
<td>7.47</td>
<td>10.2</td>
<td>0.145</td>
<td>0.118</td>
<td>2.13</td>
<td>1.99 x 10^{-5}</td>
<td>5.56</td>
<td>0.581</td>
<td>1.88</td>
</tr>
<tr>
<td>3</td>
<td>3.52 x 10^{-7}</td>
<td>3.40 x 10^{-6}</td>
<td>8.33</td>
<td>7.28</td>
<td>11.3</td>
<td>0.187</td>
<td>0.133</td>
<td>3.08</td>
<td>6.64 x 10^{-5}</td>
<td>3.40</td>
<td>0.719</td>
<td>3.69</td>
</tr>
<tr>
<td>4</td>
<td>1.41 x 10^{-7}</td>
<td>4.63 x 10^{-6}</td>
<td>8.45</td>
<td>8.27</td>
<td>11.7</td>
<td>0.260</td>
<td>0.174</td>
<td>3.19</td>
<td>1.34 x 10^{-5}</td>
<td>3.02</td>
<td>0.623</td>
<td>3.68</td>
</tr>
<tr>
<td>5</td>
<td>1.84 x 10^{-7}</td>
<td>7.47 x 10^{-6}</td>
<td>7.11</td>
<td>10.1</td>
<td>103.</td>
<td>0.288</td>
<td>0.0568</td>
<td>3.17</td>
<td>8.85 x 10^{-5}</td>
<td>3.35</td>
<td>0.718</td>
<td>6.10</td>
</tr>
<tr>
<td>6</td>
<td>1.53 x 10^{-6}</td>
<td>5.97 x 10^{-6}</td>
<td>6.95</td>
<td>5.20</td>
<td>63.9</td>
<td>0.132</td>
<td>0.0445</td>
<td>1.66</td>
<td>1.08 x 10^{-5}</td>
<td>4.37</td>
<td>0.809</td>
<td>3.54</td>
</tr>
<tr>
<td>7</td>
<td>1.04 x 10^{-6}</td>
<td>2.34 x 10^{-6}</td>
<td>7.50</td>
<td>3.89</td>
<td>17.4</td>
<td>0.139</td>
<td>0.0876</td>
<td>1.25</td>
<td>1.58 x 10^{-5}</td>
<td>6.12</td>
<td>0.544</td>
<td>1.14</td>
</tr>
<tr>
<td>8</td>
<td>2.02 x 10^{-10}</td>
<td>8.17 x 10^{-6}</td>
<td>5.77</td>
<td>4.70</td>
<td>1.70</td>
<td>0.0538</td>
<td>0.272</td>
<td>2.82</td>
<td>4.78 x 10^{-5}</td>
<td>2.09</td>
<td>2.90</td>
<td>3.88</td>
</tr>
<tr>
<td>9</td>
<td>1.12 x 10^{-6}</td>
<td>6.29 x 10^{-6}</td>
<td>5.32</td>
<td>3.35</td>
<td>5.54</td>
<td>0.214</td>
<td>0.182</td>
<td>3.45</td>
<td>1.09 x 10^{-5}</td>
<td>3.97</td>
<td>0.742</td>
<td>3.73</td>
</tr>
<tr>
<td>10</td>
<td>8.41 x 10^{-6}</td>
<td>1.68 x 10^{-5}</td>
<td>5.46</td>
<td>4.16</td>
<td>10.1</td>
<td>0.183</td>
<td>0.106</td>
<td>2.79</td>
<td>2.04 x 10^{-5}</td>
<td>3.72</td>
<td>0.824</td>
<td>2.76</td>
</tr>
<tr>
<td>11</td>
<td>2.03 x 10^{-14}</td>
<td>1.61 x 10^{-12}</td>
<td>6.72</td>
<td>19.6</td>
<td>14.4</td>
<td>1.52</td>
<td>0.205</td>
<td>6.23</td>
<td>6.79 x 10^{-5}</td>
<td>3.16</td>
<td>0.469</td>
<td>7.34</td>
</tr>
<tr>
<td>12</td>
<td>4.66 x 10^{-11}</td>
<td>9.35 x 10^{-1}</td>
<td>6.91</td>
<td>19.2</td>
<td>100.</td>
<td>2.02</td>
<td>0.171</td>
<td>3.48</td>
<td>7.28 x 10^{-5}</td>
<td>5.02</td>
<td>0.138</td>
<td>5.69</td>
</tr>
</tbody>
</table>

- See Table 1.
- $F = \frac{[2][Q_{1, \text{cal}} - Q_{1, \exp}]^2}{[Q_{1, \text{exp}}]^2}$, $N$: No. of experimental points.
- $Q = \alpha C_0 \exp(\beta C_0)$, $\alpha$: [mol/kg], $\beta$: [mol/m^3]^{-1}$, $r$: [-].
- $C_0 = \frac{a C_0}{\exp(\beta C_0)}$, $a$: [mol/kg], $\beta$: [mol/m^3]^{-1}$, $r$: [-].

Each line of Table 1 shows that phenol is the more adsorbable solute for single-solute system, and its degree of adsorption for the two-solute system is overpredicted, while p-nitrophenol is underpredicted. The reason may be as follows. Although the more adsorbable solute occupies the wider portion on the adsorbent surface, the affinity among adsorbate molecules for different species is stronger than for the same species, so the less adsorbable solute might be enhanced. Thus the more adsorbable solute is overpredicted by the proposed model, while the less adsorbable solute is underpredicted. Hence the present model has a possibility of improvement in exactitude by taking into account the effect of the interaction among adsorbate molecules, and this is a problem awaiting solution in future.
Table 3 Characteristic properties of adsorbent and adsorbate, and ultimate uptake capacity of single-solute system by Eq. (2)

<table>
<thead>
<tr>
<th>Solute</th>
<th>$T$</th>
<th>Activated carbon</th>
<th>$M \times 10^3$</th>
<th>$S \times 10^{-3}$</th>
<th>$\rho \times 10^3$</th>
<th>$Q_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAL</td>
<td>35</td>
<td>110</td>
<td>920</td>
<td>1.06</td>
<td>5.48</td>
<td></td>
</tr>
<tr>
<td>CAL</td>
<td>35</td>
<td>139.11</td>
<td>920</td>
<td>1.48 (20°C)</td>
<td>5.27</td>
<td></td>
</tr>
<tr>
<td>CAL</td>
<td>35</td>
<td>30.10</td>
<td>920</td>
<td>1.03 (25°C)</td>
<td>5.27</td>
<td></td>
</tr>
<tr>
<td>B10-I</td>
<td>20</td>
<td>94.11</td>
<td>1500</td>
<td>1.05 (25°C)</td>
<td>1.05</td>
<td></td>
</tr>
<tr>
<td>B10-I</td>
<td>20</td>
<td>139.11</td>
<td>1500</td>
<td>1.48</td>
<td>1.05</td>
<td></td>
</tr>
<tr>
<td>B10-I</td>
<td>20</td>
<td>128.56</td>
<td>1500</td>
<td>1.35</td>
<td>1.05</td>
<td></td>
</tr>
<tr>
<td>B10-I</td>
<td>20</td>
<td>122.12</td>
<td>1500</td>
<td>1.27 (15°C)</td>
<td>1.05</td>
<td></td>
</tr>
<tr>
<td>B10-I</td>
<td>20</td>
<td>136.14</td>
<td>1500</td>
<td>1.09 (7°C)</td>
<td>1.05</td>
<td></td>
</tr>
<tr>
<td>B10-I</td>
<td>20</td>
<td>163.01</td>
<td>1500</td>
<td>1.41 (34°C)</td>
<td>1.05</td>
<td></td>
</tr>
<tr>
<td>Filtrasorb 300</td>
<td>110</td>
<td>920</td>
<td>1.05</td>
<td>1.05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Filtrasorb 300</td>
<td>128</td>
<td>920</td>
<td>1.27 (8°C)</td>
<td>1.05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Filtrasorb 300</td>
<td>136</td>
<td>920</td>
<td>1.09 (7°C)</td>
<td>1.05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Filtrasorb 300</td>
<td>163</td>
<td>920</td>
<td>1.41 (34°C)</td>
<td>1.05</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* When $\rho$ of solute was not available at experimental temperature, available value at the nearest temperature was adopted. In such cases, the temperatures are put in parentheses.

** See Table 1.

Jossens et al. The model used in the proposed method was derived by a different approach from the modified Radke's models, and its calculation was simpler than the others. Specifically, although the present model needs the data of density of solutes, it has only two parameters.

Acknowledgment

The authors are grateful to Messrs. H. Tanaka, Y. Miyoshi, T. Takahashi and Miss K. Yamanaka for their assistance in the experimental work, to Dr. M. Kitagawa and Dr. S. Nakano of Osaka Municipal Technical Research Institute for various suggestions for experimental procedure and to the Ministry of Education, Science and Culture of Japan for the awards of Grant-in-Aid for Scientific Research, Special Project Research No. 011917 (1975), 112123 (1976) and 210416 (1977).

Nomenclature

- $C$ = concentration of solution [mol/m^3]
- $f(k)$ = distribution function of patches [mol^2/m^3 kg]
- $k$ = adsorption energy [m^2/mol]
- $M$ = molecular weight [kg/mol]
- $N_o$ = Avogadro's number [1/mol]
- $Q$ = amount of adsorption [mol/kg]
- $Q_s$ = amount of adsorption on patches which have adsorption energy $k$ [mol/kg]
- $Q_i$ = ultimate uptake capacity [mol/kg]
- $Q_{ik}$ = ultimate uptake capacity on patches which have adsorption energy $k$ [mol/kg]
- $q(k,C)$ = amount of adsorption on patches which have adsorption energy $k$ [mol/m^3 kg]
- $q_m$ = base area of an adsorbed molecule [m^2]
- $S$ = surface area of adsorbent [m^2/kg]
- $T$ = temperature [° C]
- $U(k^*)$ = accumulated number of patches [mol/kg]
- $\theta$ = surface coverage [-]
- $\rho$ = density [kg/m^3]

<Subscripts>

- $i$ = component
- $\max$ = maximum
- $\min$ = minimum

<Superscript>

- * = equivalent

Literature Cited


(A part of this paper was presented at the 11th Autumn Meeting of The Soc. of Chem. Engrs., Japan, at Tokyo, October, 1977).