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New Approximate Model for Nonlinear Adsorption and Concentration Dependent Surface Diffusion in a Single Particle

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Abstract. A new approximate model for nonlinear adsorption (Langmuir model) and concentration dependent surface diffusion (HIO model) in a single particle was derived, based on a parabolic concentration profile assumption for the summation of the gas and adsorbed phases. The surface diffusivity was approximated with the adsorbed phase concentration evaluated at the surface of the particle, as the average of the adsorbed phase concentration, and as the average of the first two approximations. Overall, the approximate model based on the average of the first two approximations compared the best with the exact solution for a wide variety of systems and conditions.

Keywords: langmuir isotherm, parabolic profile, pore diffusion, concentration dependent surface diffusion, HIO

Introduction

Surface diffusion is the transport of a substance within the adsorbed phase, and it occurs simultaneously with gas phase or pore diffusion. Moreover, although the mobility of molecules in the adsorbed phase is smaller than in the gas phase, the adsorbed phase concentration is usually much higher; thus, significant surface fluxes are possible. In fact, under certain conditions, surface diffusion can contribute significantly to the overall intraparticle mass transport (Kapoor and Yang, 1990), especially in microporous adsorbents (like activated carbon) which necessarily promote large adsorbed phase concentrations. This point has been raised by Doong and Yang (1986), where they found that surface diffusion contributed as much as 50% to the total flux in the pores of activated carbon during the pressure swing separation of CO_2, H_2 and CH_4.

Moreover, it has been shown that the surface diffusivity increases rather significantly with an increase in the adsorbed phase concentration (Kapoor et al., 1989). Several models have been suggested in the literature to describe concentration dependent surface diffusion. These models have been thoroughly reviewed by Kapoor et al. (1989). Among them, the HIO model developed by Hihashi et al. (1963) has been widely used to account for concentration-dependent surface diffusion in spherical adsorbent particles (Doong and Yang, 1986; Sun and Meunier, 1987; and Kapoor and Yang, 1991). Many approximate expressions have also been developed to simplify the mathematical complexities associated with an exact description of intraparticle diffusion in spherical adsorbent particles (Liaw et al., 1979; Wakao and Kaguei, 1982; Do and Rice, 1986; Hills, 1986; Do and Mayfield, 1987; Tomida and McCoy, 1987; Do and Nguyen, 1988; Buzanowski and Yang, 1989; Kim, 1989; Goto et al., 1990; Lai and Tan, 1991; Goto and Hirose, 1993; Xiu and Wakao, 1993; Yao and Tien, 1993; Zhang and Ritter, 1997; Carta and Cincotti, 1998; Botte et al., 1998). However, none of these approximate models have accounted for concentration dependent surface diffusion.

In this paper, a new approximate model based on a concentration-dependent surface diffusivity (HIO), nonlinear adsorption isotherm (Langmuir) and parabolic concentration profile assumption for the summation of gas and adsorbed phases (Lai and Tan, 1991; Zhang and Ritter, 1997) is developed to simplify the pore-surface diffusion model. Three different approximations are examined to evaluate the concentration-dependent surface diffusivity in terms of the HIO model. Uptake curves from these three approximations are compared with those from the exact (numerical) solution to the pore-surface diffusion model using three different adsorbate-adsorbent systems that cover a broad range of isotherm nonlinearity, and pore and surface diffusivities.

Theory

The mass balance and Fickian flux equations in a spherical adsorbent particle are written in dimensionless form as (Zhang and Ritter, 1997)

$$\frac{\partial \psi}{\partial \tau} = -\frac{1}{\xi^2}\frac{\partial}{\partial \xi}(\xi^2 N_\xi) \tag{1}$$

$$N_\xi = -\frac{\partial C}{\partial \xi} - \lambda(Q)\frac{\partial Q}{\partial \xi} \tag{2}$$

where $\tau = D_g t/R^2$, $\xi = r/R$, $C = c/c_{b0}$, $Q = \gamma q/c_{b0}$, $\gamma = \rho_p/\varepsilon_p$, $\lambda(Q) = D_a(Q)/D_g$, and $\psi = C + Q$. ψ accounts for the total moles inside the adsorbent particle in both the gas and adsorbed phases; and the values of D_g and $D_a(q)$ include their corresponding tortuosity factors. The corresponding dimensionless initial and boundary conditions are given by

$$\psi = 0 \quad @\,\tau = 0 \tag{3}$$

$$\frac{\partial \psi}{\partial \xi} = 0 \quad @\,\xi = 0 \tag{4}$$

$$\psi = \psi_s \quad @\,\xi = 1 \tag{5}$$

For mathematical simplicity, a parabolic profile is assumed for ψ. Inside the particle, this leads to

$$\psi = A + B\xi^2 \tag{6}$$

and on the external surface of the particle, it leads to

$$\psi_s = A + B \tag{7}$$

The volume-average sum of ψ is written as

$$\bar{\psi} = 3\int_0^1 \psi\xi^2\, d\xi = A + \frac{3}{5}B \tag{8}$$

From the definition and parabolic concentration profile assumption of ψ, the mass flux across the external surface is expressed by

$$\left.\frac{\partial \psi}{\partial \xi}\right|_{\xi=1} = \left.\frac{\partial C}{\partial \xi}\right|_{\xi=1} + \left.\frac{\partial Q}{\partial \xi}\right|_{\xi=1} = 2B \tag{9}$$

Integrating Eq. (1) gives the rate of change in $\bar{\psi}$ as

$$\frac{\partial \bar{\psi}}{\partial \tau} = -3N_\xi|_{\xi=1} \tag{10}$$

where $N_\xi|_{\xi=1}$ is given by Eq. (2) evaluated at the external surface of the particle. This casts Eq. (10) as

$$\frac{\partial \bar{\psi}}{\partial \tau} = 3\left.\frac{\partial C}{\partial \xi}\right|_{\xi=1} + 3(Q)\left.\frac{\partial Q}{\partial \xi}\right|_{\xi=1} \tag{11}$$

Assuming that equilibrium exists at every local position inside the particle, i.e., $Q = f(C)$, leads to

$$\left.\frac{\partial Q}{\partial \xi}\right|_{\xi=1} = f'(C)|_{C_s}\left.\frac{\partial C}{\partial \xi}\right|_{\xi=1} \tag{12}$$

Substituting Eq. (12) into Eq. (9), and rearranging gives

$$\left.\frac{\partial Q}{\partial \xi}\right|_{\xi=1} = \frac{2B}{\left(\frac{1}{f'(C)|_{C_s}} + 1\right)} \tag{13}$$

and substituting Eqs. (12) and (13) into Eq. (11) leads to

$$\frac{d\bar{\psi}}{d\tau} = \frac{6B\left(\frac{1}{f'(C)|_{C_s}} + \lambda(Q)|\right)}{\left(\frac{1}{f'(C)|_{C_s}} + 1\right)} \tag{14}$$

The following relation is obtained from Eqs. (7) and (8):

$$2B = 5(\psi_s - \bar{\psi}) \tag{15}$$

Substitution into Eq. (14) gives a new approximate model of Eq. (1) as

$$\frac{d\bar{\psi}}{d\tau} = 15(\psi_s - \bar{\psi})\frac{\left(1 + \lambda(Q)|\, f'(C)|_{C_s}\right)}{\left(1 + f'(C)|_{C_s}\right)} \tag{16}$$

which is similar to that developed by Zhang and Ritter (1997), except for the concentration-dependent surface diffusivity. Equation 16 is now written in terms of $\frac{d\bar{Q}}{d\tau}$ as follows.

According to the definition of ψ, $\bar{\psi}$ and ψ_s are expressed as

$$\bar{\psi} = \bar{C} + \bar{Q} \tag{17}$$

$$\psi_s = C_s + Q_s \tag{18}$$

Subtracting these equations gives

$$\psi_s - \bar{\psi} = (C_s - \bar{C}) + (Q_s - \bar{Q}) \tag{19}$$

The gas and adsorbed phases are related to their corresponding average values, by assuming that (Yao and Tien, 1993; Zhang and Ritter, 1997):

$$\bar{Q} = f(\bar{C})$$

and according to the chain rule,

$$\frac{\partial \bar{\psi}}{\partial \tau} = \left(\frac{1}{f'(\bar{C})} + 1\right)\frac{\partial \bar{Q}}{\partial \tau} \tag{20}$$

Substituting Eqs. (19) and (20) into (16), leads to

$$\frac{d\bar{Q}}{d\tau} = \frac{15 f'(\bar{C})[(C_s - \bar{C}) + (Q_s - \bar{Q})]\left[1 + f'(C)|_{C_s}\lambda(Q)\right]}{[1 + f'(\bar{C})]\left[1 + f'(C)|_{C_s}\right]} \tag{21}$$

The Langmuir adsorption isotherm and its derivative are given by

$$Q = \frac{Q_m b' C}{1 + b' C} \tag{22}$$

$$f'(C)|_{C_s} = Q_m b'\left(1 - \frac{Q_s}{Q_m}\right)^2 \tag{23}$$

With the assumption $\bar{Q} = f(\bar{C})$, Eqs. (22) and (23) become

$$\bar{Q} = \frac{Q_m b' \bar{C}}{1 + b' \bar{C}} \tag{24}$$

$$f'(\bar{C}) = Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2 \tag{25}$$

Substituting Eqs. (22)–(25) into Eq. (21) gives

$$\begin{aligned}\frac{d\bar{Q}}{d\tau} &= 15(Q_s - \bar{Q})\frac{Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2}{\left(1 + Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2\right)} \\ &\quad \times \frac{\left(1 + \lambda(Q) Q_m b'\left(1 - \frac{Q_s}{Q_m}\right)^2\right)}{\left(1 + Q_m b'\left(1 - \frac{Q_s}{Q_m}\right)^2\right)} \\ &\quad \times \left(1 + \frac{Q_m}{b'(Q_m - Q_s)(Q_m - \bar{Q})}\right)\end{aligned} \tag{26}$$

In terms of the HIO model (Yang et al., 1973; Kapoor et al., 1989).

$$D_a(q) = \frac{D_{a0}}{1 - \theta} \tag{27}$$

where $\theta = q/q_m = Q/Q_m$. Equation (32) shows that the surface diffusivity is a function of the amount adsorbed, which changes with the radial position in the particle. To eliminate this radial dependence, three different approaches are evaluated. The first approach is given by

$$\lambda(Q)|_{Q_s} = \frac{\lambda_0}{1 - \frac{Q_s}{Q_m}} \tag{28}$$

where $\lambda_0 = \frac{D_{a0}}{D_g}$. Equation (28) assumes that Q is given by Q_s, the adsorbed phase loading at the external surface of the of the particle. This casts Eq. (26) into

$$\begin{aligned}\frac{d\bar{Q}}{d\tau} &= 15(Q_s - \bar{Q})\frac{Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2}{\left(1 + Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2\right)} \\ &\quad \times \frac{\left(1 + \lambda_0 Q_m b'\left(1 - \frac{Q_s}{Q_m}\right)\right)}{\left(1 + Q_m b'\left(1 - \frac{Q_s}{Q_m}\right)^2\right)} \\ &\quad \times \left(1 + \frac{Q_m}{b'(Q_m - Q_s)(Q_m - \bar{Q})}\right)\end{aligned} \tag{29}$$

and is referred to as the Q_s model (Q_s-M). The second approach is given by

$$\lambda(Q)|_{Q_s} = \frac{\lambda_0}{1 - \frac{\bar{Q}}{Q_m}} \tag{30}$$

which assumes that Q is given by $\bar{Q}$, the average adsorbed-phase loading in the particle. This gives

Eq. (26) as

$$\frac{d\bar{Q}}{d\tau} = 15(Q_s - \bar{Q})\frac{Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2}{\left(1 + Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2\right)} \times \frac{\left(1 + \frac{\lambda_0 Q_m b'}{\left(1 - \frac{\bar{Q}}{Q_m}\right)}\left(1 - \frac{Q_s}{Q_m}\right)^2\right)}{\left(1 + Q_m b'\left(1 - \frac{Q_s}{Q_m}\right)^2\right)} \times \left(1 + \frac{Q_m}{b'(Q_m - Q_s)(Q_m - \bar{Q})}\right) \quad (31)$$

and is referred to as the $\bar{Q}$ model ($\bar{Q}$-M). A superficial analysis of Eqs. (29) and (31) (dividing Eq. (29) by Eq. (31)) shows that the solution given by Eq. (31) always under-predicts the solution given by Eq. (29). Therefore, it is worth trying another approximation that gives a solution in between the predictions given by Eqs. (29) and (31), and compare it with the exact solution. From a mathematical point of view, an approximation that fits the requirements mentioned above is obtained by taking an average of the two models used before to approximate λ. This third approach is given by

$$\lambda(Q)|_{Q_s} = \frac{\lambda_0}{2}\left[\frac{1}{1 - \frac{\bar{Q}}{Q_m}} + \frac{1}{1 - \frac{Q_s}{Q_m}}\right] \quad (32)$$

which assumes Q is represented by the average of Q_s and $\bar{Q}$. This gives Eq. (26) as

$$\frac{d\bar{Q}}{d\tau} = 15(Q_s - \bar{Q})\frac{Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2}{\left(1 + Q_m b'\left(1 - \frac{\bar{Q}}{Q_m}\right)^2\right)} \times \frac{\left(1 + \frac{\lambda_0 Q_m b'}{2}\left(\frac{1}{1 - \frac{\bar{Q}}{Q_m}} + \frac{1}{1 - \frac{Q_s}{Q_m}}\right)\left(1 - \frac{Q_s}{Q_m}\right)^2\right)}{\left(1 + Q_m b'\left(1 - \frac{Q_s}{Q_m}\right)^2\right)} \times \left(1 + \frac{Q_m}{b'(Q_m - Q_s)(Q_m - \bar{Q})}\right) \quad (33)$$

and is referred to as the Q_s-$\bar{Q}$ model (Q_s-$\bar{Q}$-M). Equations (29), (31) and (33) are very convenient, ordinary differential equation forms of Eq. (1) in terms of the Langmuir adsorption isotherm and the HIO concentration-dependent surface diffusivity. The validity and utility of these new approximate models are examined below by computing uptake curves in a spherical porous adsorbent particle and comparing them to the exact (numerical) solution of Eq. (1).

Results and Discussion

For the approximate models, the average amount adsorbed $\bar{Q}$, was obtained by solving Eqs. (29), (31) and (33), using Maple and a fourth-fifth order Runge-Kutta routine. The numerical solution to Eq. (1) was obtained by applying a three level-finite difference scheme for the spatial coordinates and implicit stepping for the temporal coordinates, and using the Band (J) subroutine (Newman, 1973). The overall uptake in the adsorbent particle for the exact solution at any time t, was calculated using the equation (Kapoor and Yang, 1991):

$$\frac{M_t}{M_\infty} = \frac{3}{Q_s + 1}\int_0^1 Q\left[1 + \frac{1}{b'(Q_m - Q)}\right]\xi^2\, d\xi \quad (34)$$

Equation (34) was solved numerically, using the trapezoid rule. For the three approximate models (Q_s-M, $\bar{Q}$-M and Q_s-$\bar{Q}$-M), the overall uptakes were approximated by

$$\frac{M_t}{M_\infty} = \frac{\bar{Q}}{Q_s + 1}\left(1 + \frac{1}{b'(Q_m - \bar{Q})}\right) \quad (35)$$

To evaluate the uptake curves from the new models, three different systems that include contributions of both pore and concentration-dependent surface diffusion inside the particles were examined. These three systems covered a sufficient range of adsorption isotherms, and pore and surface diffusivities to verify the accuracy of the new model and to disclose subtle effects of isotherm nonlinearity. They include hexane on activated carbon at 298 K (adopted from Kapoor and Yang, 1991), and carbon dioxide and methane on activated carbon at 298 K (adopted from Doong and Yang, 1986; Ritter and Yang, 1987). The values of the surface diffusivities in the limit of zero fractional surface coverage (D_{a0}) were calculated using the correlation by Sladek et al. (1974), corrected by a mean tortuosity factor of 50 (Doong and Yang, 1986). The heats of adsorption used in the Sladek correlation were obtained from Doong and Yang (1986) and Kapoor and Yang (1991). These systems were also evaluated at three different external particle surface concentrations

Table 1. Physical parameters used for uptake curve computations.[a]

	System		
Parameter	*A*	*B*	*C*
ε_p —	0.61	0.61	0.61
ρ_p (kg/m^3)	850	850	850
R (m)	0.001	0.0028	0.0028
b (m^3/kg)	148.02	0.1697	0.2824
q_m (kg/kg)	0.2208	0.4162	0.0947
D_g (m^2/s)	1.79×10^{-9}	4.10×10^{-9}	6.89×10^{-9}
D_{a0} (m^2/s)	1.05×10^{-10}	7.40×10^{-10}	7.40×10^{-10}
c_b (kg/m^3)	7.51×10^{-4}	6.54×10^{-1}	3.93×10^{-1}
	4.50×10^{-3}	3.92×10^{0}	2.36×10^{0}
	1.58×10^{-2}	1.38×10^{1}	8.26×10^{0}

[a] *A*: hexane-activated carbon at 298 K (Kapoor and Yang, 1991; and assuming a tortuosity of 50).

B: carbon dioxide-activated carbon at 298 K (Doong and Yang, 1986; Ritter and Yang, 1987).

C: methane-activated carbon at 298 K (Doong and Yang, 1986; Ritter and Yang, 1987).

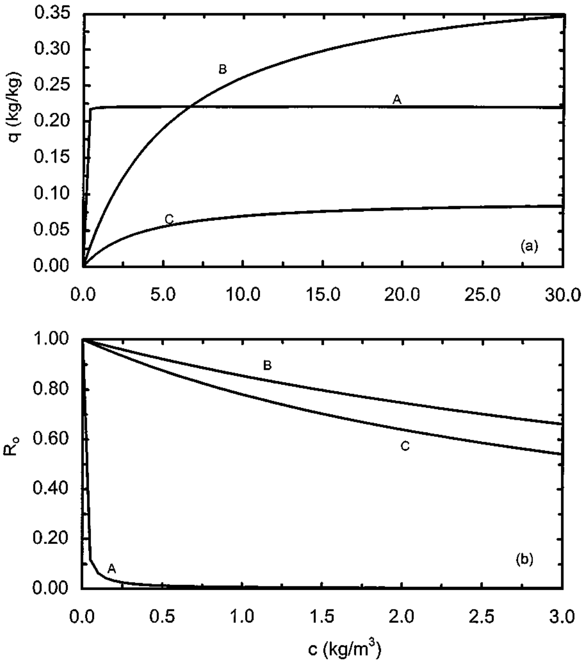

Figure 1. Adsorption isotherms at 298 K for the (*A*) hexane-activated carbon system (Kapoor and Yang, 1991), (*B*) carbon dioxide-activated carbon and (*C*) methane-activated carbon system (Doong and Yang, 1986; and Ritter and Yang, 1987): (a) shapes of the isotherms in terms of q and c, and (b) shapes of the isotherms according to the non-linearity parameter, R_0 (see Eq. (36)).

($q_s/q_m = 0.1, 0.4$ and 0.7), which are in the range where the HIO model is valid (Yang et al., 1973).

The complete set of adsorption isotherm, kinetic and adsorbent parameters for the three systems are given in the Table 1. The corresponding adsorption isotherms for each system are shown in Fig. 1. Figure 1(a) shows the conventional adsorption isotherms for the different systems; Fig. 1(b) shows the same information plotted in terms of the non-linearity parameter, R_0, which is defined as (Weber and Chakravorti, 1974)

$$R_0 = \frac{1}{1 + bc} \tag{36}$$

Steeper curves in Fig. 1(b) correspond to isotherms with a higher degree of non-linearity. Clearly, the hexane system is highly nonlinear and very strongly adsorbed, followed by the methane system, and then the carbon dioxide system, which is the least non-linear and only weakly adsorbed. According to this designation the effect of the concentration on the surface diffusivity should be most apparent for the hexane-activated carbon system and least apparent for the carbon dioxide-activated carbon system. It is interesting that in terms of Fig. 1(a), the carbon dioxide isotherm appears to be more non-linear than the methane isotherm, but not in terms of R_0.

Figures 2–4 show the comparison of the fractional uptake curves from the three approximations and the exact solution at three different bulk concentrations: 7.51×10^{-4}, 4.50×10^{-3} and 1.58×10^{-2} kg/m^3 for the hexane-activated carbon system, 6.54×10^{-1}, 3.92×10^{0} and 1.38×10^{1} kg/m^3 for the carbon dioxide-activated carbon system, and 3.93×10^{-1}, 2.36×10^{0} and 8.26×10^{0} kg/m^3 for the methane-activated carbon system, corresponding to $q_s/q_m = 0.1$, 0.4 and 0.7, respectively. From all three figures it is noticed that except for the hexane-activated carbon system at the highest bulk concentration, the new approximate model performs reasonable well for all three of the approaches that were used to evaluate the concentration dependence of the surface diffusivity. It is also shown in the figures that in all cases the approximate solutions under-predict and over-predict the exact solution at different points. This behavior is due to the parabolic profile assumption (see Eq. (6)) and is in agreement with the results reported by Botte et al. (1998). Botte et al. (1998) showed that for a linear isotherm the solution obtained using the parabolic profile intercepts the exact solution at three different points; therefore, the approximate solution under-predicts and over-predicts the exact solution in some region along the uptake curves. They calculated the dimensionless times at which this behavior takes place in a linear isotherm, and they

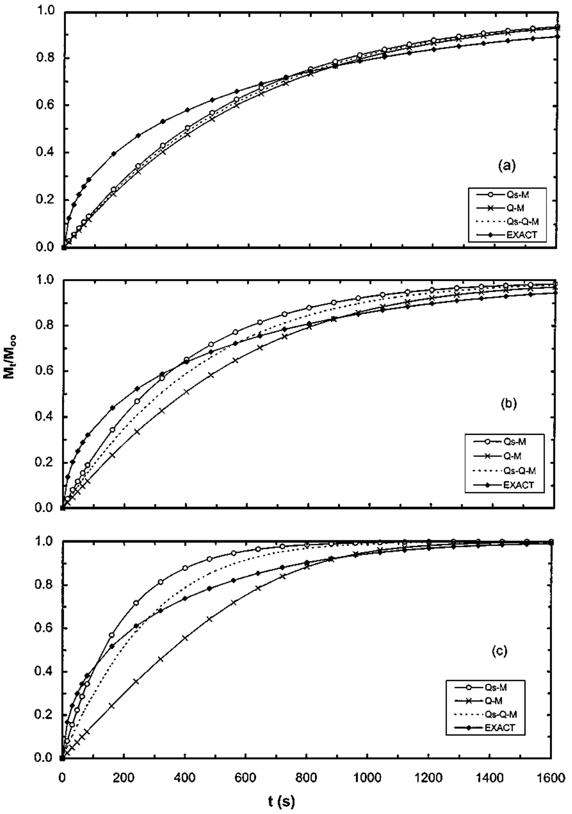

Figure 2. Comparison of fractional uptake curves from the exact and three different approximate solutions of the pore-surface diffusion equation with concentration-dependent surface diffusivity (HIO) for the hexane-activated carbon system at bulk concentrations corresponding to q_s/q_m equal to (a) 0.1, (b) 0.4 and (c) 0.7.

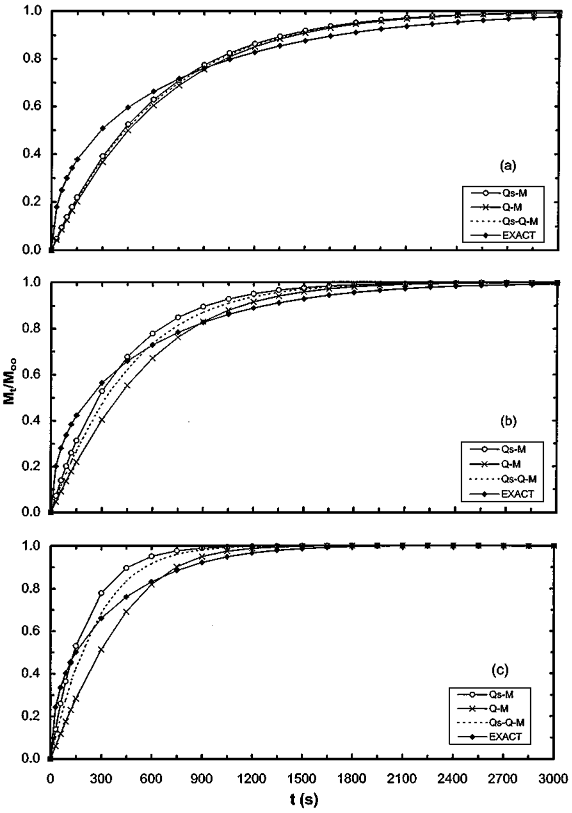

Figure 3. Comparison of fractional uptake curves from the exact and three different approximate solutions of the pore-surface diffusion equation with concentration-dependent surface diffusivity (HIO) for the carbon dioxide-activated carbon system at bulk concentrations corresponding to q_s/q_m equal to (a) 0.1, (b) 0.4 and (c) 0.7.

showed that the same behavior is also observed for nonlinear isotherms. However for nonlinear isotherms, the crossover points are different than those for a linear isotherm and they depend on the bulk concentration and the model used for the parabolic profile approximation.

Also, as anticipated, in all cases the results given by Q_s-M over predict those given by $\bar{Q}$-M, and the results given by Q_s-$\bar{Q}$-M fall in between those given by Q_s-M and $\bar{Q}$-M. Moreover, in all cases, Q_s-M performs very well at short times but severely over predicts the exact solution at long times; and $\bar{Q}$-M performs very well at long times but severely under predicts the exact solution at short times. So it is reasonable to expect Q_s-$\bar{Q}$-M to compare better with the exact solution over the entire uptake curve than either Q_s-M or $\bar{Q}$-M. The results in Figs. 2–4 show this to be true, and relatively independent of the bulk concentration and isotherm non-linearity. For example, although for the highly non-linear and strongly adsorbed hexane-activated carbon system, Q_s-M compares much better with the exact solution than $\bar{Q}$-M, Q_s-$\bar{Q}$-M appears to represent the exact solution better than Q_s-M over the entire ranges of the three uptake curves; similarly for the other two systems.

As the isotherms become more linear, or at lower bulk concentrations, all three approximations appear to perform equally well; but on average Q_s-$\bar{Q}$-M still does better in representing the exact solution. The fact that the predictions from all three models improve and agree with each other with decreasing non-linearity or increasing bulk concentration is not surprising since in both cases, the dependence of the uptake curve on the adsorbed phase concentration diminishes. In contrast, when the adsorbed phase concentration is high, giving rise to a marked dependence of the uptake curve on $\bar{Q}$, the three different models disagree widely, as seen

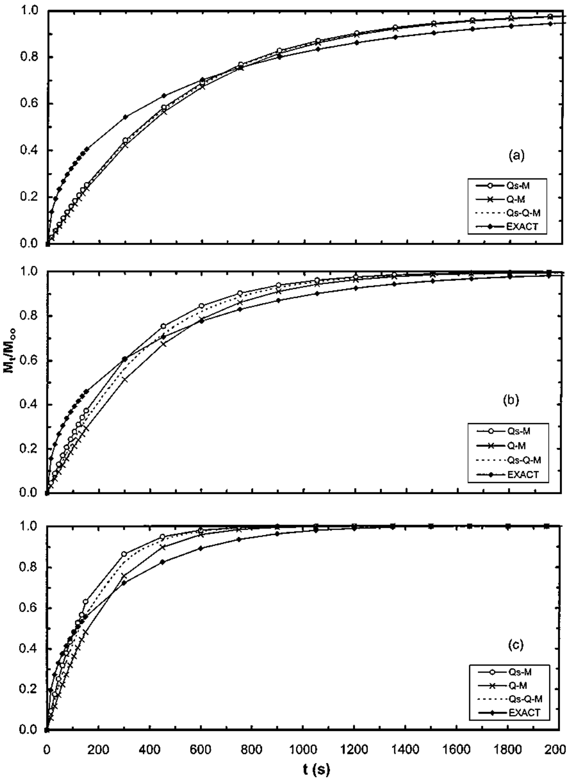

Figure 4. Comparison of fractional uptake curves from the exact and three different approximate solutions of the pore-surface diffusion equation with concentration-dependent surface diffusivity (HIO) for the methane-activated carbon system at bulk concentrations corresponding to q_s/q_m equal to (a) 0.1, (b) 0.4 and (c) 0.7.

for the hexane-activated carbon system at $q_s/q_m = 0.7$ (Fig. 2(c)).

Conclusions

A new approximate model of the pore-surface diffusion equation that accounts for non-linear (Langmuir) adsorption, gas phase pore diffusion and concentration-dependent adsorbed phase surface diffusion, in a single adsorbent particle was derived. The new approximate model employs the parabolic concentration profile assumption for the summation of the gas and adsorbed phases; it also employs three different approximations to evaluate the concentration-dependent surface diffusivity using the HIO model. The surface diffusivity was approximated with the adsorbed phase concentration evaluated: 1) at the surface of the particle (Q_s-M), 2) as the average adsorbed phase concentration ($\bar{Q}$-M), and 3) as the average of the first two approximations (Q_s-$\bar{Q}$-M). In terms of particle uptake curves, for strongly adsorbed systems, Q_s-M compared better with the exact solution than $\bar{Q}$-M, whereas for less strongly adsorbed systems, both Q_s-M and $\bar{Q}$-M compared well with the exact solution. However, for all of the systems evaluated, on average, Q_s-$\bar{Q}$-M compared the best with the exact solution; thus, this model should prove to be useful in saving computation time when both pore diffusion and concentration-dependent surface diffusion must be taken into account.

Nomenclature

A	Parameter in the parabolic profile assumption
B	Parameter in the parabolic profile assumption
b	Langmuir isotherm parameter, m^3/kg
b'	Dimensionless Langmuir isotherm parameter, $b \times c_b$
C	Dimensionless concentration in the void fraction of the adsorbent particle, c/c_b
$\bar{C}$	Dimensionless volume averaged concentration in the void fraction of the adsorbent particle, $\bar{c}/c_b$
C_s	Dimensionless surface concentration, c_s/c_b
c	Concentration in the void fraction of the adsorbent particle, kg/m^3
$\bar{c}$	Volume averaged concentration in the void fraction of the adsorbent particle, kg/m^3
c_b	Bulk concentration outside the adsorbent particle, kg/m^3
D_g	Gas phase (pore) diffusivity, m^2/s
D_a	Adsorbed phase (surface) diffusivity, m^2/s
D_{a0}	Adsorbed phase (surface) diffusivity at zero fractional surface coverage, m^2/s
M	Total uptake (gas and adsorbed phases) at radial position r, kg/m^3
M_t	Total uptake at time t, kg/m^3
M_∞	Total uptake at infinite time, kg/m^3
N_r	Total flux at radial position r, mol/m^2 s
N_ξ	Dimensionless total flux at radial position ξ
Q	Dimensionless adsorbed phase concentration, $\gamma q/c_b$
$\bar{Q}$	Dimensionless volume averaged adsorbed phase concentration, $\gamma \bar{q}/c_b$
Q_s	Dimensionless adsorbed phase concentration in equilibrium with gas surrounding the adsorbent particle, $\gamma q_s/c_b$
Q_m	Dimensionless Langmuir isotherm parameter, $\gamma q_m/c_b$
q	Adsorbed phase concentration, kg/kg
$\bar{q}$	Volume averaged adsorbed phase concentration, kg/kg

q_m	Langmuir isotherm parameter, kg/kg
q	Adsorbed phase concentration in equilibrium with the gas surrounding the adsorbent particle, kg/kg
R	Radius of the adsorbent particle, m
R_0	Isotherm non linearity parameter, $1/(1+bc)$
r	Radial coordinate, m
t	Time, s

Greek Letters

ε_p	Intraparticle void fraction
ρ_p	Density of adsorbent particle, kg/m^3
γ	Ratio of particle density to intraparticle void fraction
λ_0	Ratio of adsorbed phase (surface) diffusivity at zero fractional coverage to gas phase (pore) diffusivity
τ	Dimensionless time, $D_g t/R^2$
θ	Fractional surface coverage
ξ	Dimensionless radial distance
ψ	Dimensionless sum of the adsorbates in the gas and adsorbed phases
$\bar{\psi}$	Dimensionless average sum of the adsorbates in the gas and adsorbed phases
ψ_s	Dimensionless sum of the adsorbates at the surface of the adsorbent particle, $\psi\|_{\xi=1}$

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