Batch Adsorption: Intraparticle Adsorbate Concentration Profile Models

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Several models proposed describe the adsorbate concentration profile in an adsorbent particle. A theoretical consideration is made in this work to see what bulk concentration-time curves are predicted by these models when applied to a batch adsorption. A similar, but experimental, comparison was made in terms of parameter estimation by Kaguei et al. (1989).

Mass balance for batch adsorption with a linear isotherm is expressed:

$$\frac{\partial A}{\partial \tau}=\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial A}{\partial x}\right) \tag{1a}$$

$$\frac{dA_b}{d\tau}=-N\left(\frac{\partial A}{\partial x}\right)_{x=1} \tag{1b}$$

$$\text{at } \tau=0,\ A=0,\ A_b=1 \tag{1c}$$

$$\text{at } x=1,\ \frac{\partial A}{\partial x}=Bi(A_b-A) \tag{1d}$$

Exact Solution (Do and Rice, 1986)

$$(A_b)_{\text{exact}}=(A_b)_\infty+\sum_{n=1}^{\infty}A_n\exp(-\lambda_n^2\tau) \tag{2a}$$

where

$$(A_b)_\infty=\frac{3}{3+N} \tag{2b}$$

$$A_n=\left[1+\frac{N}{2}\left(1-\frac{\lambda_n^2}{NBi}\right)^2\left(\frac{1}{\sin^2\lambda_n}-\frac{\cot\lambda_n}{\lambda_n}\right)\right]^{-1} \tag{2c}$$

and λ_n is an nth positive root of the following equation:

$$\lambda\cot\lambda-1=\frac{\lambda^2}{N-\dfrac{\lambda^2}{Bi}} \tag{2d}$$

Nth-Order Concentration Profile Model

Do and Mayfield (1987) assumed

$$A=a_0+a_nx^n \tag{3a}$$

and found the exponent to be approximately:

$$n=0.123\tau^{-0.68} \tag{3b}$$

Their study on the batch adsorption with an infinitely large volume of tank is modified to that with a finite volume of tank. The loss of adsorbate from the bulk fluid equals the gain of the adsorbent:

$$\frac{dA_b}{d\tau}=-\frac{N}{3}\frac{d\overline{A}}{d\tau} \tag{4a}$$

where $\overline{A}$ is the average concentration in a particle.

$$\overline{A}=3\int_0^1 Ax^2dx \tag{4b}$$

An integration then gives:

$$A_b-1=-\frac{N\overline{A}}{3} \tag{4c}$$

$$=-N\left(\frac{a_0}{3}+\frac{a_n}{n+3}\right) \tag{4d}$$

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Combining Eq. 4d with Eqs. 1b and 1d in which Eq. 3a is substituted, one obtains:

$$\left(\frac{1}{Bi}+\frac{1}{n+3}\right)\frac{dA_b}{d\tau}=3-(3+N)A_b \qquad (5)$$

Hence, let us approximate the power " − 0.68" by " − 2/3" so that Eq. 3b becomes (in the range of $\tau = 0.001$-0.2):

$$n=0.133\tau^{-2/3} \qquad (6)$$

As a matter of fact, with the aid of Eq. 6, Eq. 5 is analytically solved to give:

$$(A_b)_{nth}=(A_b)_\infty\left\{1+\frac{N}{3}\exp\left[-\left(1+\frac{N}{3}\right)\psi\right]\right\} \qquad (7a)$$

where

$$\psi=\frac{9}{1+\dfrac{3}{Bi}}\left\{\tau+\gamma^2 Bi\left[\tau^{1/3}-\gamma\tan^{-1}\left(\frac{\tau^{1/3}}{\gamma}\right)\right]\right\} \qquad (7b)$$

$$\gamma=\sqrt{\frac{0.133}{3+Bi}} \qquad (7c)$$

Some other models examined in our note are discussed below.

Parabolic Concentration Profile Model

Liaw et al. (1979) and Rice (1982) assumed

$$A=a_0+a_2x^2 \qquad (8a)$$

and obtained

$$(A_b)_{par}=(A_b)_\infty\left[1+\frac{N}{3}\exp\left(-\frac{3+N}{\dfrac{1}{Bi}+\dfrac{1}{5}}\tau\right)\right] \qquad (8b)$$

Quartic Concentration Profile Model

Do and Rice (1986) assumed

$$A=a_0+a_2x^2+a_4x^4 \qquad (9a)$$

and obtained

$$(A_b)_{quar}=(A_b)_\infty+D_1\exp(-d_1\tau)+D_2\exp(-d_2\tau) \qquad (9b)$$

where

$$d_1,d_2=\frac{u_1}{2u_2}\left(1\pm\sqrt{1-\frac{4u_2}{u_1^2(A_b)_\infty}}\right) \qquad (9c)$$

$$D_i=\frac{1-(A_b)_\infty[1+3Nd_i/140]}{2-(A_b)_\infty u_1 d_i} \quad (i=1,2) \qquad (9d)$$

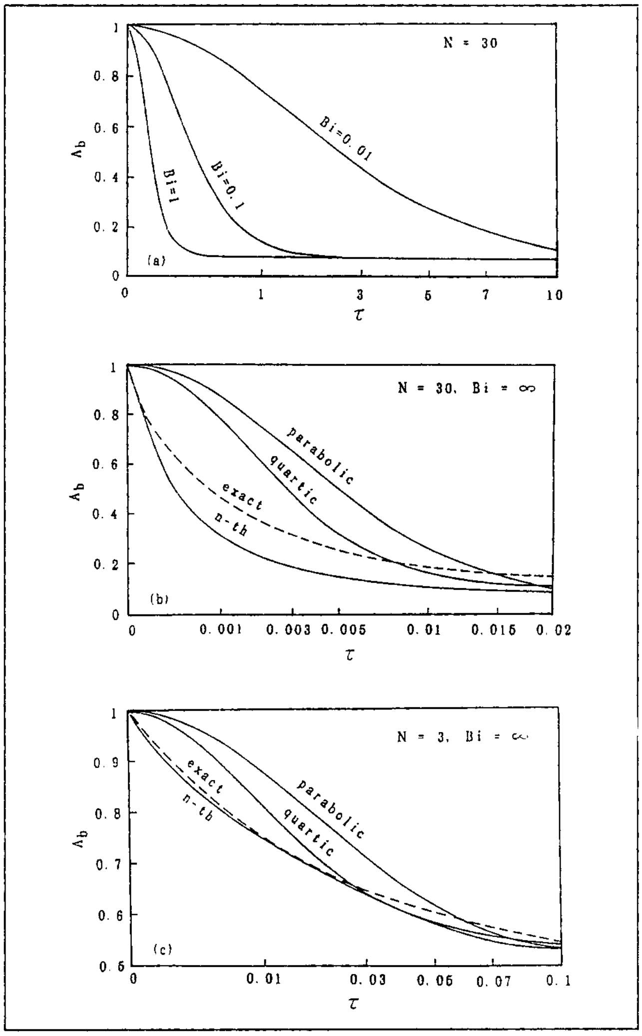

Figure 1. Exact solution $(A_b)_{exact}-\tau$ vs. $A_b-\tau$ curves for nth-order, parabolic and quartic concentration models: (a) $N=30$, $Bi\leq 1$; (b) $N=30$, $Bi=\infty$; (c) $N=3$, $Bi=\infty$.

$$u_1=\frac{11}{84}+\frac{3}{140}N+\frac{1}{3Bi} \qquad (9e)$$

$$u_2=\frac{1}{420}+\frac{9}{420Bi} \qquad (9f)$$

Figures 1a-1c (abscissa proportional to $\sqrt{\tau}$) illustrate $A_b-\tau$ curves calculated from Eqs. 2a, 7a, 8b, and 9b, respectively. As shown in Figure 1a, when $Bi\leq 1$, there is no appreciable difference between all the curves, $(A_b)_{par}-\tau$, $(A_b)_{quar}-\tau$, $(A_b)_{nth}-\tau$ and $(A_b)_{exact}-\tau$. Figures 1b and 1c show the curves with $Bi=\infty$: When $N=30$, all the curves for concentration profile models differ considerably from the $(A_b)_{exact}-\tau$ curve. The deviation becomes larger increasingly in the order of that with $(A_b)_{nth}-\tau$, $(A_b)_{quar}-\tau$, and $(A_b)_{par}-\tau$. When $N=3$, the $(A_b)_{nth}-\tau$ curve is close to the $(A_b)_{exact}-\tau$ curve, but the other two curves differ from the $(A_b)_{exact}-\tau$ curve. The deviation is again the largest with $(A_b)_{par}-\tau$ curve.

It is obvious that the intraparticle concentration profile becomes less significant when Bi is small: fluid-to-particle mass-transfer controls the overall rate. On the other hand, the concentration profile plays an important role when Bi is large: the overall rate is controlled by the diffusion of adsorbate in particle. In the latter case, as far as the prediction of bulk concentration in a batch tank is concerned, none of the concentration profile models so far proposed are satisfactory.

Rice and Do will propose a new approximation for the situation when $Bi \to \infty$ in their book titled *Applied Mathematics and Modeling for Chemical Engineers*, which will be published in 1994.

Notation

A = dimensionless intraparticle concentration, $q/(KC_0)$
A_b = dimensionless bulk fluid concentration, C/C_0
Bi = Biot number, $k_m R/(KD_s)$
C = bulk fluid concentration
C_0 = initial bulk fluid concentration
D_s = surface diffusivity
K = linear equilibrium adsorption constant
k_m = particle-fluid mass-transfer coefficient
m_p = mass of adsorbent
N = $3m_pK/(V\rho_p)$
q = adsorbed concentration
R = radius
t = time
V = liquid volume
x = dimensionless radial distance variable

Greek letters

ρ_p = particle density
τ = $D_s t/R^2$

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