

New Models for Evaluating the Adsorption Rate of an Adsorbent*

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Abstract Four models for the rate of adsorption in an adsorbent (slab-like, cylindrical or spherical) are presented. The parabolic profile (PP) model is obtained by assuming a parabolic intraparticle concentration profile. The shell-core (SC) model is based on a shell-core type profile. The modified shell-core (MSC) model is an extension of the SC model. And the general driving force (GDF) model is a weighted average of the PP and MSC models. Sample calculations show that the GDF model provides the best approximation.

Keywords adsorption rate, adsorption, adsorbent

1 INTRODUCTION

In the design and study of adsorption processes, the uptake rate of the adsorbent particles (slab-like, cylindrical or spherical) is an important parameter. In principle, the adsorption rate can be obtained by solving the intraparticle mass transfer equation which, for simultaneous pore and surface diffusions, may be written as

$$\frac{\partial q}{\partial t} + \epsilon_p \frac{\partial c}{\partial t} = \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[r^{n-1} \left(D_p \frac{\partial c}{\partial r} + D_s \frac{\partial q}{\partial r} \right) \right] \quad (1)$$

with the initial and boundary conditions

$$t = 0, \quad c = c_0, \quad q = q_0 \quad (2)$$

$$r = 0, \quad \frac{\partial c}{\partial r} = \frac{\partial q}{\partial r} = 0 \quad (3)$$

$$r = R, \quad D_p \frac{\partial c}{\partial r} + D_s \frac{\partial q}{\partial r} = k_f(c_b - c_R) \quad (4)$$

and the assumption of local equilibrium in the adsorbent

$$q = f(c) \quad \text{or} \quad c = g(q) \quad (5)$$

where c and q are the pore fluid and the adsorbed (surface) phase concentrations respectively.

The meanings of all other symbols are given in the section on Nomenclature.

Integrating Eq. (1) through the volume of an adsorbent pellet and applying Eq. (3), one has

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$$\frac{d}{dt}(\bar{q} + \epsilon_p \bar{c}) = \frac{n}{R} \left(D_p \frac{\partial c}{\partial r} + D_s \frac{\partial q}{\partial r} \right)_R \quad (6)$$

where \bar{q} and \bar{c} are the average values of q and c respectively, defined as

$$\bar{q} = \frac{n}{R^n} \int_0^R q r^{n-1} dr \quad \text{and} \quad \bar{c} = \frac{n}{R^n} \int_0^R c r^{n-1} dr \quad (7)$$

The left hand side of Eq. (6) is usually known as the rate of adsorption (or accumulation) by the adsorbent and is the prime parameter that we are concerned with here.

It is noted that the problem considered here is a fairly general one. Simpler cases result when one or more of the following assumptions are adopted; (1) linear adsorption equilibrium; (2) pore diffusion control; (3) surface diffusion control; (4) negligible external film mass transfer resistance; and (5) $q \gg \epsilon_p c$.

Solving Eq. (1), in general, will enable the determination of the adsorption rate. Such an approach, however, will involve extensive numerical computation in cases where repetitive solution of the intraparticle diffusion equation is necessary. In order to reduce computational work, a number of approximate expressions or models for the adsorption rate have been proposed. Among them the most popular one is Glueckauf's linear driving force (LDF) model^[1]

$$\frac{d\bar{q}}{dt} = \frac{15D_s}{R^2} (q_R - \bar{q}) \quad (8)$$

for the case of spherical adsorbents, surface diffusion control and $q \gg \epsilon_p c$. As shown by Liaw *et al.*^[2] and Do and Rice^[3], Eq. (8) corresponds to the presence of a parabolic surface concentration profile. Other approximations have been proposed and discussed by, for example, Scott^[4], Carta^[5], Kikkinides and Yang^[6], Alpay and Scott^[7], Buzanowski and Yang^[8, 9], Do and Nguyen^[10], Do and Mayfield^[11], Hills^[12], Nakao and Suzuki^[13].

In two earlier papers^[14, 15], we presented two different approximations, named as Models I and II, and demonstrated their applications in modeling batch, continuous-flow stirred tank and fixed-bed adsorption processes. The present work can be considered a further generalization of our earlier work in the sense that the approximations or models derived here are more general and have a better theoretical foundation.

2 DERIVATION OF MODELS

2.1 Parabolic Profile (PP) Model

As noted above, Glueckauf's approximation, *e. g.* Eq. (8), is for a special case. We are now going to present results for the general case based on the parabolic profile assumption. Within an adsorbent pellet, there exist two types of concentrations: the pore (fluid) concentration, c , and the surface concentration, q . In most cases, c and q are assumed to be in equilibrium and the equilibrium relationship may be non-linear. Accordingly, the parabolic profile assumption may be applied either to c or q . The two cases will be treated separately.

2.1.1 Parabolic profile model in pore concentration c or $(PP)_c$ model

In this case the pore concentration is assumed to have the form

$$c = a + b(r/R)^2 \quad (9)$$

where a and b are undetermined coefficients. Then by definition

$$c_R = a + b \quad (10)$$

$$\bar{c} = a + [n/(n+2)]b \quad (11)$$

From Eqs. (10) and (11) one has

$$a = c_R - [(n+2)/2](c_R - \bar{c}) \quad (12a)$$

$$b = [(n+2)/2](c_R - \bar{c}) \quad (12b)$$

which, upon the substitution into Eq. (9), give

$$c = c_R - [(n+2)/2](c_R - \bar{c})[1 - (r/R)^2] \quad (13)$$

Then

$$\left. \frac{\partial c}{\partial r} \right|_R = \frac{n+2}{R}(c_R - \bar{c}) \quad (14)$$

From Eqs. (6) and (14) one obtains

$$\frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} = \frac{n(n+2)}{R^2} (D_p + D_s \frac{dq_R}{dc_R})(c_R - \bar{c}) \quad (15)$$

Which is the parabolic profile (PP) model in pore concentration c or, simply, $(PP)_c$ model.

Since Eq. (15) contains four dependent variables \bar{q} , \bar{c} , q_R and c_R , in actual calculations it is to be solved together with the following three equations

$$\frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} = \frac{n}{R} k_f (c_b - c_R) \quad (16)$$

$$q_R = f(c_R) \quad \text{or} \quad c_R = g(q_R) \quad (17)$$

$$\bar{q} \approx f(\bar{c}) \quad \text{or} \quad \bar{c} \approx g(\bar{q}) \quad (18)$$

Eq. (16) results from Eqs. (4) and (6), Eq. (17) expresses the adsorption equilibrium at $r=R$, and Eq. (18) is only an approximation, as seen from the definition in Eq. (7), except for the special case of linear adsorption equilibrium.

2.1.2 Parabolic profile model in surface concentration q or $(PP)_q$ model

Here q is expressed as

$$q = a + b(r/R)^2 \quad (19)$$

Following the same procedure as in the previous case, one obtains eventually

$$\frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} = \frac{n(n+2)}{R^2} (D_p \frac{dq_R}{dq} + D_s)(q_R - \bar{q}) \quad (20)$$

which is the parabolic profile (PP) model in surface concentration q or, simply, $(PP)_q$ model.

It can be readily shown that Eq. (20) reduces to Eq. (8) for the special case of $q \gg \epsilon_p c$, $n=3$ (spherical adsorbents) and $D_s \gg D_p \frac{dq_R}{dq}$ (surface diffusion control).

2.2 Shell-Core (SC) Model

The assumption that intraparticle concentration profile is parabolic is probably reasonable when the concentration gradient (or driving force) in the adsorbent is "small" (e.g. as in a fixed-bed adsorption process where the bulk phase concentration changes gradually).

This assumption is likely to fail, however, when the concentration gradient in the adsorbent is "large" (e. g. as in a batch process where a step change is effected initially in the bulk phase concentration). In our earlier work^[14], we used the "concentration layer" concept to describe "large" concentration gradient. In the present work we employ instead the "shell-core" concept, meaning that the adsorbent is divided into a shell where the concentration gradient is "large" and a core where there is no concentration gradient. The thickness of the shell is designated by δR with δ being a dimensionless parameter. It is further assumed that the concentration profile within the shell is parabolic.

Depending on whether the pore or surface concentration is the primary variable, we again have two cases here.

2.2.1 Shell-core model in pore concentration c or (SC)_c model

In this case we assume the pore concentration profile to be

$$c - c_0 = a + b(r/R) + d(r/R)^2, \quad (1 - \delta)R \leq r \leq R \quad (21a)$$

$$c - c_0 = 0, \quad 0 \leq r \leq (1 - \delta)R \quad (21b)$$

To determine the coefficients a , b and d , the following conditions are used

$$c = c_R \quad \text{at} \quad r = R \quad (22a)$$

$$c = c_0 \quad \text{at} \quad r = (1 - \delta)R \quad (22b)$$

$$\frac{\partial c}{\partial r} = 0 \quad \text{at} \quad r = (1 - \delta)R \quad (22c)$$

Substituting Eq. (21a) into Eqs. (22a)–(22c) and solving for a , b and d , one has

$$a = (1 - \delta)^2 (c_R - c_0) / \delta^2 \quad (23a)$$

$$b = -2(1 - \delta)(c_R - c_0) / \delta^2 \quad (23b)$$

$$d = (c_R - c_0) / \delta^2 \quad (23c)$$

Then, Eq. (21a) becomes

$$c - c_0 = (1 - \delta - \frac{r}{R})^2 \frac{c_R - c_0}{\delta^2}, \quad (1 - \delta)R \leq r \leq R \quad (24)$$

From Eqs. (7), (21b) and (24), one obtains

$$\begin{aligned} \bar{c} - c_0 &= \frac{n(c_R - c_0)}{\delta^2} \int_{1-\delta}^1 (1 - \delta - \frac{r}{R})^2 (\frac{r}{R})^{n-1} d(\frac{r}{R}) \\ &= \frac{n(c_R - c_0)}{\delta^2} \left[\frac{1}{n+2} - \frac{2(1-\delta)}{n+1} + \frac{(1-\delta)^2}{n} - \frac{2(1-\delta)^{n+2}}{n(n+1)(n+2)} \right] \end{aligned} \quad (25)$$

which may be simplified to

$$\bar{c} - c_0 = \frac{n}{3} (c_R - c_0) \delta \left[1 - \frac{n-1}{4} \delta + \frac{(n-1)(n-2)}{20} \delta^2 \right] \quad (26)$$

It is interesting to note that if $\delta = 1$, that is, when the shell domain occupies the entire pellet, Eq. (26) gives

$$\frac{\bar{c} - c_0}{c_R - c_0} = \begin{cases} 1/3 & \text{for } n=1 \\ 1/2 & \text{for } n=2 \\ 3/5 & \text{for } n=3 \end{cases} \quad (27)$$

Thus one may expect that the shell-core model is valid when the dimensionless driving

force satisfies

$$\frac{c_R - \bar{c}}{c_R - c_0} > \begin{cases} 2/3 & \text{for } n=1 \\ 1/2 & \text{for } n=2 \\ 2/5 & \text{for } n=3 \end{cases} \quad (28)$$

Eq. (26) provides the equation for determining δ , the dimensionless shell thickness. For $n=1$ (slab-like particles) the solution is very simple. For $n=2$ (cylindrical particles) analytical solution can be obtained but is not very simple. For $n=3$ (spherical particles) numerical method has to be used for its exact solution. To keep the final expression for the adsorption rate in a relatively simple form, we derive an approximate solution for δ in the form of a truncated series of $\frac{(\bar{c}-c_0)}{(c_R-c_0)}$ (which is less than unity for the shell-core profile). The final results are

$$\delta = \frac{3}{n} \frac{\bar{c}-c_0}{c_R-c_0} \left(1 + \frac{3n-3}{4n} \frac{\bar{c}-c_0}{c_R-c_0} + \dots \right) \quad (29)$$

or

$$\frac{1}{\delta} = \frac{n}{3} \frac{c_R-c_0}{\bar{c}-c_0} \left(1 - \frac{3n-3}{4n} \frac{\bar{c}-c_0}{c_R-c_0} + \dots \right) \approx \frac{n}{3} \frac{c_R-c_0}{\bar{c}-c_0} - \frac{n-1}{4} \quad (30)$$

It is seen that, to a first approximation, δ is proportional to $\frac{(\bar{c}-c_0)}{(c_R-c_0)}$.

From Eqs. (24) and (30), one gets

$$\left. \frac{\partial c}{\partial r} \right|_R = \frac{2n}{3R} (c_R - c_0) \left(\frac{c_R - c_0}{\bar{c} - c_0} - \frac{3n - 3}{4n} \right) \quad (31)$$

which, upon substitution into Eq. (6), gives the adsorption rate

$$\frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} = \frac{2n^2}{3R^2} \left(D_p + D_s \frac{dq_R}{dc_R} \right) (c_R - c_0) \left(\frac{c_R - c_0}{\bar{c} - c_0} - \frac{3n - 3}{4n} \right) \quad (32)$$

Eq. (32) is the shell-core (SC) model in pore concentration c or, simply, $(SC)_c$ model. It is expected that this equation will give a reasonable approximation when the driving force for adsorption in the adsorbent is "large". It will not be valid, however, when the driving force is "small", as seen from the fact that the right hand side of Eq. (32) remains finite as $\bar{c} \rightarrow c_R$ while in reality the adsorption rate must vanish as adsorption equilibrium is approached.

2.2.2 Shell-core model in surface concentration q or $(SC)_q$ model

Here q is expressed as

$$q - q_0 = a + b \left(\frac{r}{R} \right) + d \left(\frac{r}{R} \right)^2, \quad (1 - \delta)R \leq r \leq R \quad (33a)$$

$$q - q_0 = 0, \quad (1 - \delta)R \leq r \leq R \quad (33b)$$

The adsorption rate is obtained as

$$\frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} = \frac{2n^2}{3R^2} \left(D_p \frac{dq_R}{dc_R} + D_s \right) (q_R - q_0) \left(\frac{q_R - q_0}{\bar{q} - q_0} - \frac{3n - 3}{4n} \right) \quad (34)$$

which is the counterpart of Eq. (32).

2.3 Modified shell-core (MSC) model

As mentioned earlier, the shell-core model represented by Eqs. (32) or (34) is not valid for "small" driving force. This problem can be overcome, to a certain extent, by

introducing the following modification. First we write

$$1 = \frac{c_R - \bar{c}}{c_R - c_0} \frac{1}{1 - (\bar{c} - c_0)/(c_R - c_0)} \approx \frac{c_R - \bar{c}}{c_R - c_0} \left(1 + \frac{\bar{c} - c_0}{c_R - c_0} \right) \quad (35)$$

It is noted that the approximation introduced in Eq. (35) is consistent with that in Eq. (30), *i. e.* retaining only the first two terms in a power series of $(\bar{c} - c_0)/(c_R - c_0)$.

Multiplying Eq. (32) with Eq. (35) and neglecting higher order terms, one has

$$\frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} = \frac{2n^2}{3R^2} \left(D_p + D_s \frac{dq_R}{dc_R} \right) \left(\frac{c_R - c_0}{\bar{c} - c_0} + \frac{n+3}{4n} \right) (c_R - \bar{c}) \quad (36)$$

which is the modified shell-core (MSC) model in pore concentration c or, simply, (MSC)_c model. It is at least qualitatively valid for "small" driving force.

Similarly Eq. (34) can be modified to give the (MSC)_q model

$$\frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} = \frac{2n^2}{3R^2} \left(D_p \frac{dq_R}{dc_R} + D_s \right) \left(\frac{q_R - q_0}{\bar{q} - q_0} + \frac{n+3}{4n} \right) (q_R - \bar{q}) \quad (37)$$

We would like to mention at this point that Model I suggested by Yao and Tien^[14, 15] is a special form of the modified shell-core model.

2.4 General driving force (GDF) model

As noted earlier, the assumption of a parabolic intraparticle concentration profile and, therefore, the PP model may be reasonable when the driving force for adsorption within the pellet is "small" or when $(\bar{c} - c_0)/(c_R - c_0)$ is close to unity. On the other hand, when the driving force is "large" or when $(\bar{c} - c_0)/(c_R - c_0)$ is much less than unity, the MSC model (also the SC model) is expected to be valid. To construct a general approximation, we take a weighted average of the PP model [Eq. (15)] and the MSC model [Eq. (36)] with the weighting factor on the former being $(\bar{c} - c_0)/(c_R - c_0)$ and that on the latter being $[1 - (\bar{c} - c_0)/(c_R - c_0)]$. The result is

$$\begin{aligned} \frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} &= \frac{2n^2}{3R^2} \left(D_p + D_s \frac{dq_R}{dc_R} \right) \\ &\cdot \left(\frac{c_R - c_0}{\bar{c} - c_0} - \frac{3n-3}{4n} + \frac{5n+9}{4n} \frac{\bar{c} - c_0}{c_R - c_0} \right) (c_R - \bar{c}) \end{aligned} \quad (38)$$

which is the general driving force (GDF) model in pore concentration c or, simply, (GDF)_c model.

Similarly, a weighted average of Eqs. (20) and (37) gives the (GDF)_q model

$$\begin{aligned} \frac{d(\bar{q} + \epsilon_p \bar{c})}{dt} &= \frac{2n^2}{3R^2} \left(D_p \frac{dq_R}{dc_R} + D_s \right) \\ &\cdot \left(\frac{q_R - q_0}{\bar{q} - q_0} - \frac{3n-3}{4n} + \frac{5n+9}{4n} \frac{\bar{q} - q_0}{q_R - q_0} \right) (q_R - \bar{q}) \end{aligned} \quad (39)$$

3 AN EXAMPLE OF APPLICATION

To demonstrate the utility of the models presented above, we apply them to the simple problem of an adsorbent pellet (slab-like, cylindrical or spherical) adsorbing from an infinite

solution with $q \gg \epsilon_p c$, surface diffusion control and negligible external film mass transfer resistance. In dimensionless variables

$$y = \frac{q - q_0}{q_R - q_0}, \quad x = \frac{r}{R} \quad \text{and} \quad \tau = \frac{D_s t}{R^2}$$

the intraparticle mass transfer equation can be written as

$$\frac{\partial y}{\partial \tau} = \frac{1}{x^{n-1}} \frac{\partial}{\partial x} \left(x^{n-1} \frac{\partial y}{\partial x} \right) \quad (40)$$

with the initial and boundary conditions

$$\tau = 0, \quad y = 0 \quad (41)$$

$$x = 0, \quad \frac{\partial y}{\partial x} = 0 \quad (42)$$

$$x = 1, \quad y = 1 \quad (43)$$

3.1 Exact solution

The exact solution to Eqs. (40)–(43) can be found in reference [16] and the average value of y , \bar{y} , is given by

$$\bar{y} = 1 - \frac{8}{\pi^2} \sum_{i=1}^{\infty} \frac{1}{(2i-1)^2} \exp\left[-\frac{(2i-1)^2 \pi^2 \tau}{4}\right] \quad \text{for } n=1 \quad (44a)$$

$$\bar{y} = 1 - 4 \sum_{i=1}^{\infty} \frac{1}{\beta_i^2} \exp(-\beta_i^2 \tau) \quad \text{for } n=2 \quad (44b)$$

$$\bar{y} = 1 - \frac{6}{\pi^2} \sum_{i=1}^{\infty} \frac{1}{i^2} \exp(-i^2 \pi^2 \tau) \quad \text{for } n=3 \quad (44c)$$

where β_i is root of $J_0(\beta) = 0$ ($\beta_1 = 2.4048$, $\beta_2 = 5.5201$, $\beta_3 = 8.6537$, ...).

For very small τ , the exact asymptotic solution is

$$\bar{y} = 2n \sqrt{\tau/\pi} \quad (45)$$

3.2 Approximate solution with the PP model

In dimensionless form the model equation is

$$\frac{d\bar{y}}{d\tau} = n(n+2)(1-\bar{y}) \quad (46)$$

which, upon integration with $\bar{y} = 0$ at $\tau = 0$ gives

$$\bar{y} = 1 - \exp[-n(n+2)\tau] \quad (47)$$

For very small τ , Eq. (47) can be approximated by

$$\bar{y} = n(n+2)\tau \quad (48)$$

which is totally different from Eq. (45), indicating that the PP model is not valid for small times or large driving force.

3.3 Approximate solution with the SC model

Here the dimensionless model equation is

$$\frac{d\bar{y}}{d\tau} = \frac{2n^2}{3} \left(\frac{1}{\bar{y}} - \frac{3n-3}{4n} \right) \quad (49)$$

By integration one has

$$\bar{y} = 2 \sqrt{\tau/3} \quad \text{for } n = 1 \quad (50a)$$

$$\bar{y} + \frac{8}{3}\ln(1 - \frac{3}{8}\bar{y}) + \tau = 0 \quad \text{for } n = 2 \quad (50b)$$

$$\bar{y} + 2\ln(1 - \frac{1}{2}\bar{y}) + 3\tau = 0 \quad \text{for } n = 3 \quad (50c)$$

For very small τ (thus small \bar{y}), Eqs. (50b) and (50c) can be approximated by

$$\bar{y} = 2n \sqrt{\tau/3} \quad (51)$$

which is in close agreement with the exact asymptotic solution Eq. (45). Eq. (51) can in fact be obtained by retaining only the leading (first) term on the right hand side of Eq. (49) followed by integration.

It is worth noting that as $\tau \rightarrow \infty$, Eqs. (50a)–(50c) mean respectively

$$\bar{y} \rightarrow \infty \quad \text{for } n = 1 \quad (52a)$$

$$\bar{y} \rightarrow 8/3 \quad \text{for } n = 2 \quad (52b)$$

$$\bar{y} \rightarrow 2 \quad \text{for } n = 3 \quad (52c)$$

which are in obvious contradiction with reality and show clearly that the SC model is not valid for large times or small driving force.

3.4 Approximate solution with the MSC model

In this case one has

$$\frac{d\bar{y}}{d\tau} = \frac{2n^2}{3} \left(\frac{1}{\bar{y}} + \frac{n+3}{4n} \right) (1-\bar{y}) \quad (53)$$

which can be integrated to give

$$\ln(1 - \bar{y}^2) + \frac{4}{3}\tau = 0 \quad \text{for } n = 1 \quad (54a)$$

$$\ln(1 - \bar{y}) + \frac{8}{5}\ln(1 + \frac{5}{8}\bar{y}) + \frac{13}{3}\tau = 0 \quad \text{for } n = 2 \quad (54b)$$

$$\ln(1 - \bar{y}) + 2\ln(1 + \frac{1}{2}\bar{y}) + 9\tau = 0 \quad \text{for } n = 3 \quad (54c)$$

For very small τ (small \bar{y}) Eqs. (54a)–(54c) can also be simplified to Eq. (51), as expected, since the MSC and SC models have the same leading term on the right hand side.

3.5 Approximate solution with the GDF model

Here the model equation is

$$\frac{d\bar{y}}{d\tau} = \frac{2n^2}{3} \left(\frac{1}{\bar{y}} - \frac{3n-3}{4n} + \frac{5n+9}{4n} \bar{y} \right) (1-\bar{y}) \quad (55)$$

Upon the integration with $\bar{y}=0$ at $\tau=0$, one gets

$$\ln(1-\bar{y}) - \frac{1}{2}\ln(1 + \frac{7}{2}\bar{y}^2) + \frac{2}{\sqrt{14}}\arctan \frac{7\bar{y}}{\sqrt{14}} + 3\tau = 0 \quad \text{for } n=1 \quad (56a)$$

$$\ln(1-\bar{y}) - \frac{1}{2}\ln(1 - \frac{3}{8}\bar{y} + \frac{19}{8}\bar{y}^2) + \frac{13}{\sqrt{599}} \left[\arctan \frac{3}{\sqrt{599}} - \arctan \frac{3-38\bar{y}}{\sqrt{599}} \right] + 8\tau = 0 \quad \text{for } n=2 \quad (56b)$$

$$\ln(1-\bar{y}) - \frac{1}{2} \ln\left(1 - \frac{1}{2}\bar{y} + 2\bar{y}^2\right) + \frac{3}{\sqrt{31}} \left[\arctan \frac{1}{\sqrt{31}} - \arctan \frac{1-8\bar{y}}{\sqrt{31}} \right] + 15\tau = 0 \quad \text{for } n=3 \quad (56c)$$

which can again be simplified to Eq. (51) for very small τ as the GDF model has the same leading term as the MSC and SC models.

In Table 1, the values of \bar{y} as a function of τ obtained according to the exact solution and different approximations are listed. It can be seen that the GDF model provides a good approximation throughout and the MSC model is slightly inferior. The SC model is valid for relatively small τ but greatly overestimates the adsorption rate for large τ . The PP model underestimates the adsorption rate for small τ and may be considered acceptable for relatively large τ .

Table 1 Values of y as a function of τ obtained by different methods

n	τ	Exact	PP	SC	MSC	GDF
1	0.001	0.036	0.003	0.037	0.037	0.036
	0.01	0.113	0.030	0.115	0.115	0.112
	0.05	0.252	0.139	0.258	0.254	0.248
	0.1	0.357	0.259	0.365	0.353	0.350
	0.2	0.504	0.451	0.516	0.484	0.498
	0.5	0.764	0.777	0.816	0.698	0.767
	1.0	0.931	0.950	1.150	0.858	0.943
	2.0	0.994	0.998	1.630	0.965	0.997
	∞	1	1	∞	1	1
2	0.001	0.07	0.008	0.072	0.072	0.071
	0.005	0.155	0.039	0.160	0.159	0.154
	0.01	0.215	0.077	0.225	0.223	0.214
	0.02	0.299	0.148	0.313	0.308	0.296
	0.05	0.452	0.330	0.477	0.464	0.455
	0.1	0.606	0.551	0.665	0.615	0.623
	0.2	0.782	0.798	0.904	0.777	0.818
	0.5	0.962	0.982	1.320	0.946	0.982
	∞	1	1	8/3	1	1
3	0.001	0.104	0.015	0.107	0.107	0.104
	0.002	0.145	0.030	0.151	0.150	0.145
	0.005	0.224	0.072	0.236	0.233	0.223
	0.01	0.309	0.139	0.327	0.322	0.307
	0.02	0.419	0.259	0.450	0.438	0.420
	0.05	0.607	0.528	0.678	0.632	0.628
	0.1	0.770	0.777	0.905	0.791	0.815
	0.2	0.915	0.950	1.180	0.922	0.957
	∞	1	1	2	1	1

4 CONCLUSIONS

We have presented four different approximations or models for the rate of adsorption in an adsorbent pellet (slab-like, cylindrical or spherical). The parabolic profile (PP) model is based on the assumption of a parabolic intraparticle (pore or surface) concentration profile and is essentially a generalization of the linear driving force (LDF) model of Glueckauf's. The shell-core (SC) model is obtained by considering the adsorbent to consist of a shell (where there is "large" concentration gradient) and a core (where there is no concentration gradient). The modified shell-core (MSC) model is an extension of the SC model so as to make the adsorption rate proportional to the driving force for adsorption in the adsorbent. Finally the general driving force (GDF) model is constructed by taking a weighted average of the PP and MSC models.

It is demonstrated that the GDF model provides the best approximation and the MSC model is somewhat inferior to the GDF model. The PP model is acceptable only in the cases of "small" driving force. The SC model, though good for relatively large driving force, is not recommended since it can lead to erroneous results in the case of "small" driving force.

NOMENCLATURE

a	coefficient in concentration profile
b	coefficient in concentration profile
c	pore fluid concentration, $\text{mol} \cdot \text{m}^{-3}$
D_p	pore diffusivity, $\text{m}^2 \cdot \text{s}^{-1}$
D_s	surface diffusivity, $\text{m}^2 \cdot \text{s}^{-1}$
d	coefficient in concentration profile
$f(c)$	denotes adsorption isotherm $q = f(c)$
$g(q)$	denotes adsorption isotherm $c = g(q)$
$J_0(\beta)$	Bessel function of zero order
k_t	external fluid film mass transfer coefficient, $\text{m} \cdot \text{s}^{-1}$
n	dimensionality of the adsorbent, $n=1, 2, 3$ for a slab-like, cylindrical or spherical pellet
q	surface (adsorbed phase) concentration, $\text{mol} \cdot \text{m}^{-3}$
R	size of the adsorbent, equal to half the thickness (slab-like pellet) or to the radius (cylindrical or spherical pellet), m
r	spacial coordinate, m
t	time coordinate, s
β_i	root of $J_0(\beta) = 0$
δ	dimensionless shell thickness
ϵ_p	porosity of the adsorbent

Superscript

— average value

Subscripts

b	bulk phase value
c	in terms of pore concentration c
q	in terms of surface (adsorbed phase) concentration q
R	value at $r=R$

0 initial value

REFERENCE

- 1 Glueckauf, E. , *Trans. Faraday Soc.* , **51**, 1540(1955).
- 2 Liaw, C.H. , *et al.* , *AIChE J.* , **25**, 376(1979).
- 3 Do, D.D. , Rice, R.G. , *AIChE J.* , **32**, 149(1986).
- 4 Scott, D.M. , *Chem. Eng. Sci.* , **49**, 914(1994).
- 5 Catra, G. , *Chem. Eng. Sci.* , **48**, 622(1993).
- 6 Kikkinides, E.S. , Yang, R.T. , *Chem. Eng. Sci.* , **48**, 1169(1993).
- 7 Alpay, E. , Scott, D.M. , *Chem. Eng. Sci.* , **47**, 499(1992).
- 8 Buzanowski, M.A. , Yang, R.T. , *Chem. Eng. Sci.* , **44**, 2683(1989).
- 9 Buzanowski, M.A. , Yang, R.T. , *Chem. Eng. Sci.* , **46**, 2589(1991).
- 10 Do, D.D. , Nguyen, T.S. , *Chem. Eng. Comm.* , **72**, 171(1988).
- 11 Do, D.D. , Mayfield, P.L.J. , *AIChE J.* , **33**, 1397(1982).
- 12 Hills, J.H. , *Chem. Eng. Sci.* , **41**, 2779(1986).
- 13 Nakao, S. , Suzuki, K. , *J. Chem. Eng. Japan* , **16**, 114(1983).
- 14 Yao, C. , Tien, C. , *Chem. Eng. Sci.* , **48**, 187(1993).
- 15 Yao, C. , Tien, C. , *Sep. Technol.* , **4**, 67(1994).
- 16 Crank, J. , *The Mathematics of Diffusion*, Clarendon Press, Oxford(1956).