

Fixed-Bed Irreversible Adsorption with Pore Diffusion and Axial Dispersion

A. E. Rodrigues, J. M. Loureiro, and M. Rendueles de la Vega

Laboratory of Separation and Reaction Engineering (LSRE), Depto. de Engenharia Química, Faculdade de Engenharia da Universidade do Porto, 4200-465 Porto, Portugal

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In 1966, Hall et al.¹ studied the breakthrough behavior for favorable equilibrium adsorption in isothermal conditions with solid-diffusion or pore-diffusion resistances. They developed numerical solutions for both cases; moreover, in the case of irreversible equilibrium they were able to develop analytical solutions, even in the presence of film mass-transfer resistances.

Apart from the work of Hall et al.,¹ the case of rectangular isotherms (irreversible equilibrium) in combination with solid-diffusion resistances was approximately and exactly solved by Vermeulen² under the constant-pattern assumption and Cooper,³ respectively, whereas the same equilibrium coupled with pore-diffusion was tackled by Cooper and Liberman⁴; Yoshida et al.⁵ present a review of the previous works and consider the case of external fluid film plus an internal homogeneous resistance simulated by a “solid film” or by solid diffusion.

The objectives of this paper are

(1) To develop a new mathematical solution for fixed-bed adsorption with irreversible equilibrium and pore diffusion including axial dispersion.

(2) To develop an equivalence with a simpler model that lumps pore diffusion and axial dispersion in an apparent pore diffusivity.

Mathematical Development

Consider a column packed with an adsorbent in which a solute adsorbs irreversibly; the process is supposed to be isothermal; axial dispersed plug flow through the bed is further

assumed. The solute material balances in a bed volume element and inside the particles are, respectively,

$$\varepsilon D_{ax} \frac{\partial^2 c}{\partial z^2} = u_0 \frac{\partial c}{\partial z} + \varepsilon \frac{\partial c}{\partial t} + (1 - \varepsilon) \frac{\partial \bar{q}}{\partial t} \quad (1)$$

$$\frac{\partial q}{\partial t} = \varepsilon_p \frac{\partial c_p}{\partial t} + (1 - \varepsilon_p) \frac{\partial q'}{\partial t} = D_{epore} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_p}{\partial r} \right) \right] \quad (2)$$

In these equations c and c_p are the solute concentrations in the fluid phases in the bed and in the particles voids, respectively; q' is the adsorbed concentration in equilibrium with c_p and \bar{q} is the average concentration inside particles; u_0 is the superficial fluid velocity in the bed; ε and ε_p are the bed and particle porosities, respectively; D_{ax} is the axial dispersion coefficient and D_{epore} is the effective pore diffusivity; r is the radial coordinate in the particles; z is the axial coordinate in the bed; and t is time. In the following, the amount of solute in the pores of the particles will be neglected in comparison with the adsorbed amount, that is, the instantaneous solid concentration will be taken as $q = \varepsilon_p c_p + (1 - \varepsilon_p) q' \approx (1 - \varepsilon_p) q'$.

Introducing the dimensionless concentrations $F = c/c_0$ and $\bar{y} = \bar{q}/q_0$ with q_0 in equilibrium with c_0 , and replacing the axial by the time coordinate with the aid of the concentration velocity

$$w = \frac{dz}{dt} = \frac{u_i}{1 + \xi}$$

where $u_i = u_0/\varepsilon$ is the bed interstitial velocity and

Correspondence concerning this article should be addressed to A. E. Rodrigues.

$$\xi = \frac{1 - \varepsilon q_0}{\varepsilon c_0}$$

is the column capacity factor, the bed material balance becomes

$$\frac{\tau(1 + \xi)^2}{\xi \text{Pe}} \frac{\partial^2 F}{\partial t^2} + \frac{\partial F}{\partial t} - \frac{\partial \bar{y}}{\partial t} = 0 \quad (3)$$

where $\tau = L/u_i$ is the space time and $\text{Pe} = u_i(L/D_{ax})$ is the axial Peclet number. The above change of coordinates assumes that a constant pattern concentration wave develops inside the column. The numerical solution of the model Eqs. 1 and 2 shows that this assumption is reasonable when the Peclet number is sufficiently high ($\text{Pe} \geq 10$) and $\tau/\tau_p \geq 0.45$ with $\tau_p = R_0^2/D_{epore}$. Note that for an irreversible isotherm the concentration q_0 in equilibrium with c_0 is $q_0 = (1 - \varepsilon_p)q_s$, where q_s is the maximum (saturation) solid (adsorbed) concentration.

When dealing with the saturation step of the column, Eq. 3 can be integrated once, subject to the conditions that before breakthrough occurs both F and \bar{y} are zero, as well as the time derivative of F , leading to

$$\frac{\tau(1 + \xi)^2}{\xi \text{Pe}} \frac{\partial F}{\partial t} + F - \bar{y} = 0 \quad (4)$$

Introducing further the throughput parameter⁶ T , with

$$T = \frac{c_0(Ut - \varepsilon V)}{(1 - \varepsilon)q_0V} = \frac{1}{\xi} \left(\frac{t}{\tau} - 1 \right)$$

the bed material balance is finally written as

$$\frac{(1 + \xi)^2}{\xi^2 \text{Pe}} \frac{dF}{dT} + F - \bar{y} = 0 \quad (5)$$

When $\text{Pe} \rightarrow \infty$, this equation gives the common constant-pattern condition $F = \bar{y}$, valid for sufficiently long times with favorable equilibrium in the absence of axial dispersion. It shows that when axial dispersion is not negligible, such an assumption is surely not safe.

Introducing the dimensionless variables $y = q/q_0$ and $F_p = c_p/c_0$, the particle mass balance becomes

$$\frac{\partial y}{\partial t} = D_{epore} \frac{c_0}{q_0} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial F_p}{\partial r} \right) \quad (6)$$

For irreversible isotherms, the solute entering the particles saturates each spherical shell before advancing as a front, the adsorbed solid concentration of which is q_s (the saturation concentration) wherever $c_p > 0$. The pore concentration varies between $c_p = c$ at the particle surface $r = R_0$ (R_0 is the particle radius), and $c_p = 0$ for $r \leq r_i$, where the front is located. The solid dimensionless concentration $y = q/q_0 = 1$ for the saturated outer shell $r_i \leq r \leq R_0$ and $y = 0$ for the inner core $0 \leq r \leq r_i$. The average solid concentration is then

$$\bar{y} = \frac{3}{R_0^3} \int_0^{R_0} r^2 y dr = \frac{3}{R_0^3} \int_{r_i}^{R_0} r^2 dr = 1 - \left(\frac{r_i}{R_0} \right)^3 \quad (7)$$

whereas, from Eqs. 6 and 7, taking into account the symmetry condition at the particle center, the time derivative of the average concentration \bar{y} is given by

$$\frac{\partial \bar{y}}{\partial t} = \frac{3}{R_0} D_{epore} \frac{c_0}{q_0} \left(\frac{\partial F_p}{\partial r} \right)_{r=R_0} \quad (8)$$

On the other hand, in the region $r_i \leq r \leq R_0$ the y derivative with respect to time, $\partial y/\partial t = 0$ because $y = 1$; the result from Eq. 6 is that in this region, the product $r^2(\partial F_p/\partial r) = \text{constant}$. With the conditions that for $r = R_0$, $F_p = F$ and for $r = r_i$, $F_p = 0$, this enables the calculation of the pore concentration F_p as a function of the fluid concentration F in the bed voids; the result is

$$F_p = F \frac{1 - \frac{r_i}{r}}{1 - \frac{r_i}{R_0}} = F \frac{R_0(r - r_i)}{r(R_0 - r_i)} \quad (9)$$

The derivative of this pore concentration with respect to r can then be calculated; replacing the time variable with the throughput parameter

$$T = \frac{1}{\xi} \left(\frac{t}{\tau} - 1 \right)$$

introducing the number of mass-transfer units by intraparticle pore diffusion

$$N_p = \frac{1 - \varepsilon}{\varepsilon} \frac{15}{R_0^2} D_{epore} \tau$$

and substituting the F_p derivative with respect to r at the particle surface, the differential equation giving the average particle concentration, Eq. 8, finally becomes

$$\frac{d\bar{y}}{dT} = \frac{N_p}{5} \frac{F}{(1 - \bar{y})^{-1/3} - 1} \quad (10)$$

Equations 5 and 10 are the model equations for the saturation of the adsorbent bed, with rectangular isotherm and in the presence of axial dispersion; they give the fluid F and average solid \bar{y} concentrations as functions of the throughput parameter T ; a simplification, valid for high ξ will be further made, that is, the approximation $(1 + \xi)^2/\xi^2 \approx 1$ in Eq. 5. Equation 10, together with the following resulting equation, constitute a system of ordinary differential equations in the independent variable T

$$\frac{1}{\text{Pe}} \frac{dF}{dT} + F - \bar{y} = 0 \quad (11)$$

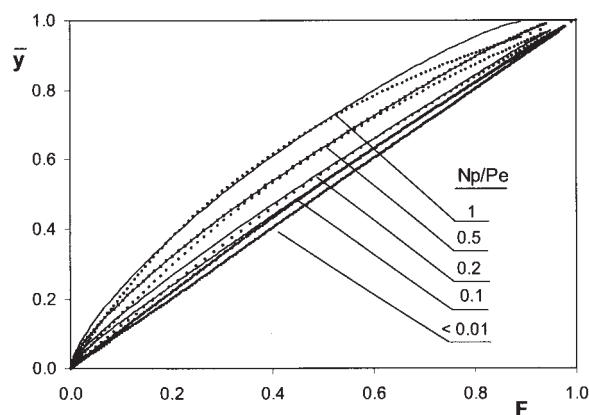


Figure 1. Average adsorbed phase concentration (\bar{y}) as a function of dimensionless fluid phase concentration (F) with N_p/Pe as a parameter.

—: Numerical solution; ···: calculated with $\alpha = \beta = 1.4 N_p/Pe$ in Eq. 14.

These equations must be integrated so that the concentrations F and \bar{y} are determined. The initial conditions for the solution should be

$$T \leq T_{Bp} \quad F = \bar{y} = 0 \quad (12)$$

where T_{Bp} stands for breakthrough “time.” The problem is that this breakthrough time is not known a priori. A methodology based on the definition of the throughput parameter is then used; first, the equations are integrated with $T_{Bp} = 0$ in Eq. 12 conditions, giving values of F and \bar{y} that coexist for the same T ; then, as by definition of T , the breakthrough curve, F vs. T , should be centered at $T = 1$. The following equality should hold for the breakthrough curve

$$\int_0^\infty (1 - F) dT = \int_0^1 T dF \quad (13)$$

which enables the determination of the T_{Bp} that, by displacement, correctly centers the breakthrough curve around $T = 1$.

Numerical Solution

Equations 10 and 11 were numerically solved using subroutine DGEAR from the IMSL library; the zero initial conditions were used. Fluid (F) and average solid (\bar{y}) concentrations for the same value of the throughput parameter are represented in Figure 1 for different values of the parameter ratio N_p/Pe . In fact, if Eqs. 10 and 11 are divided, it is clearly seen that the relation between the fluid and average solid concentrations is a function of this parameter ratio only. It is worth noting that, for high values of the N_p/Pe ratio, the particles saturate before the bed, that is, the average concentration inside particles, \bar{y} , reaches the unit value while the concentration in the bed voids, F , is still increasing. As a consequence, the computer stops with an error message from the package DGEAR before $F = 1$, a little after $\bar{y} = 1$.

The shape of the curve \bar{y} vs. F suggests a functional dependency of the type

$$\bar{y} = \frac{(1 + \alpha)F}{1 + \beta F} \quad (14)$$

This curve, for $\alpha = \beta = 1.4 N_p/Pe$, is also represented in Figure 1 for comparison. It is seen that the simulation of the real $\bar{y}(F)$ dependency is reasonable, at least for small values of the ratio N_p/Pe , given that for $\alpha = \beta$ both \bar{y} and F go simultaneously for the unit value (saturation). A better simulation of the observed \bar{y} vs. F behavior is obtained when the same value is used for α , but $\beta = 1.3 N_p/Pe$ is used instead; this can be seen in Figure 2, where the numerical solution is compared with this new analytical approach, which takes into account the observed behavior that $\bar{y} = 1$ before $F = 1$; with this approach, $F = 1/(1 + \alpha - \beta)$ when \bar{y} reaches the unit value.

Equation 14 was used to develop an approximate analytical solution for Eqs. 10 and 11. The procedure used is outlined in the following.

Approximate Analytical Solution

The value of F from Eq. 14 is used to replace the F variable in Eq. 10. With the auxiliary change of dependent variable

$$x^3 = 1 - \bar{y} \quad \text{or} \quad F = \frac{1 - x^3}{\gamma + \beta x^3} \quad (15)$$

Equation 10 is transformed in the following differential equation with separated variables

$$N_p dT = -15 \frac{x(\gamma + \beta x^3)}{x^2 + x + 1} dx \quad (16)$$

where $\gamma = 1 + \alpha - \beta$.

The analytical integration of this ordinary differential equation gives

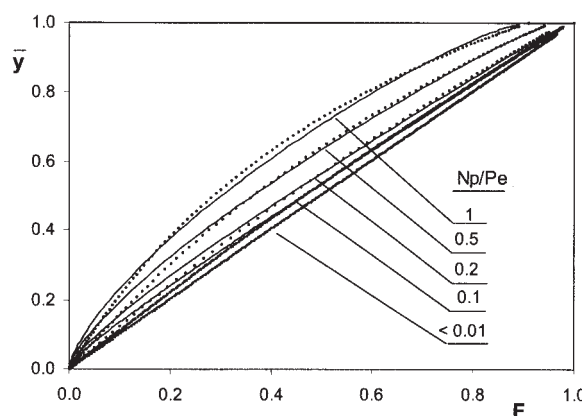


Figure 2. Average adsorbed phase concentration (\bar{y}) as a function of dimensionless fluid phase concentration (F) with N_p/Pe as a parameter.

—: Numerical solution; ···: calculated with $\alpha = 1.4 N_p/Pe$ and $\beta = 1.3 N_p/Pe$ in Eq. 14.

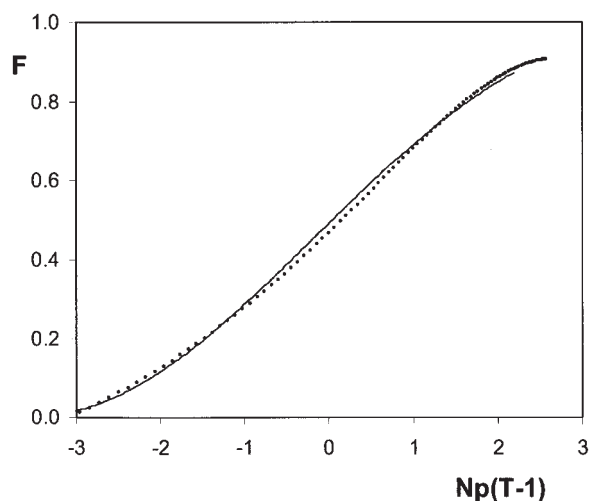


Figure 3. Breakthrough curves in terms of F vs. $N_p(T-1)$ for $N_p/Pe = 1$.

—: Numerical solution; ···: analytical solution with $\alpha = 1.4 N_p/Pe$ and $\beta = 1.3 N_p/Pe$.

$$N_p T = -\frac{5\beta x^2}{2}(2x-3) - \frac{15(1+\alpha)}{2} \ln(x^2+x+1) + 5\sqrt{3}(1+\alpha)\tan^{-1}\left(\frac{2x+1}{\sqrt{3}}\right) + C \quad (17)$$

The constant of integration C is to be determined with the help of condition Eq. 13; replacing T in Eq. 13 for its value given by Eq. 17 and performing the integration between $F_0 = 0$ and $F_1 = 1$, that is, between $x_0 = 1$ and $x_1 = [(1-\gamma)/(1+\beta)]^{1/3}$, the following value of C is obtained

$$C = N_p + \frac{5}{2} + \frac{5x_1^2}{2}(2x_1-3) + \frac{1-x_1^3}{\gamma+\beta x_1^3} \left[\frac{5\beta x_1^2}{2}(2x_1-3) + \frac{15(1+\alpha)}{2} \ln(x_1^2+x_1+1) - 5\sqrt{3}(1+\alpha)\tan^{-1}\left(\frac{2x_1+1}{\sqrt{3}}\right) \right] \quad (18)$$

When $\alpha = \beta$, $\gamma = 1$ and then $x_1 = 0$; in this case the value of C is given simply by

$$C = N_p + \frac{5}{2} - \frac{5(1+\alpha)\pi}{2\sqrt{3}} \quad (19)$$

The analytical curves (dashed lines) F vs. $N_p(T-1)$ for $N_p/Pe = 1$, obtained using the values of C given by Eqs. 18 and 19 with $\alpha = 1.4 N_p/Pe$ and $\beta = 1.3 N_p/Pe$, are compared in Figure 3 with the numerical solution (full lines); although this is the worst simulated case, the differences are only slight; for all other cases the curves are practically coincident. Taking this into account and the facts that Eq. 19 is much simpler than Eq. 18, and that $x_1 = [(1-\gamma)/(1+\beta)]^{1/3}$ for the given values of α and β corresponds to $\bar{y} < 0$, which has no physical meaning, the value of C given by Eq. 19 will be used throughout.

Replacing this value of the integration constant in the equa-

tion for T , Eq. 17, the following approximated value is then obtained

$$N_p(T-1) = -\frac{5\beta}{2}(2x^3-3x^2) - \frac{15(1+\alpha)}{2} \ln(x^2+x+1) + 5\sqrt{3}(1+\alpha)\tan^{-1}\left(\frac{2x+1}{\sqrt{3}}\right) - \frac{5(1+\alpha)\pi}{2\sqrt{3}} + \frac{5}{2} \quad (20)$$

This equation is equivalent to the one given by Hall et al.¹ in the case of $Pe \rightarrow \infty$, that is, when axial dispersion is negligible; this limit is obtained by replacing the values $\alpha = \beta = 0$ in Eq. 20.

Breakthrough occurs when $F = 0$, that is, $x = 1$; then, the value of the throughput parameter at breakthrough can be calculated from Eq. 20 to be

$$T_{Bp} = 1 + \frac{5}{2N_p} \left[(1+\beta) - (1-\alpha) \left(3 \ln 3 - \frac{\pi}{\sqrt{3}} \right) \right] \quad (21)$$

Similarly, the final time, that is, the value of the throughput parameter corresponding to the complete saturation of the particles is obtained from Eq. 20 for $x = 0$ ($\bar{y} = 1$, $F = 1/\gamma$); if $\alpha = \beta$ this time also corresponds to $F = 1$ (complete saturation of the bed)

$$T_F = 1 + \frac{5}{2N_p} \quad (22)$$

From Eq. 20, with F given by Eq. 15, the analytical solution in the form of an F vs. T curve can be obtained. This analytical response is compared with the numerical one in Figure 4, for different values of the parameter N_p/Pe ; the response is made independent of N_p by the chosen representation of $N_p(T-1)$ instead of T as abscissa. The comparison is very good, even for relatively high values of N_p/Pe , showing that the approximation used is reasonable.

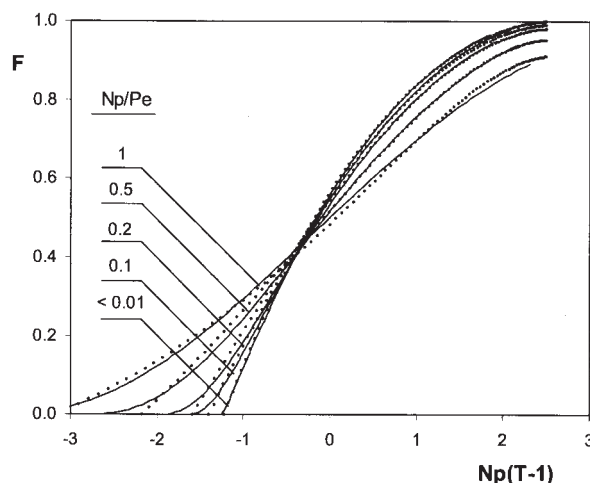


Figure 4. Influence of N_p/Pe on the F vs. $N_p(T-1)$ curve.

—: Numerical solution; ···: analytical solution.

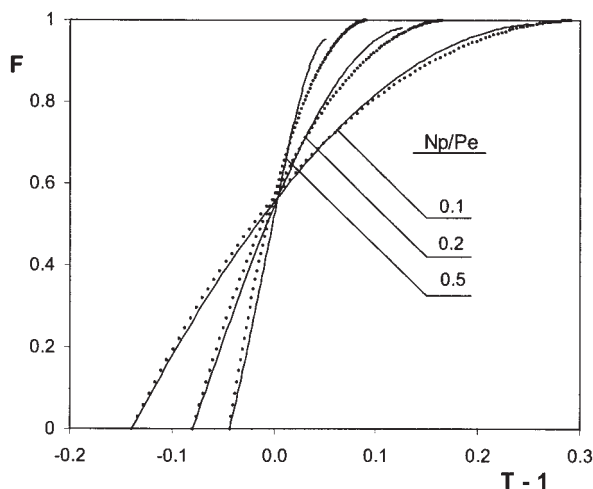


Figure 5. F vs. $(T - 1)$ curves.

Comparison between the complete model solution for pore diffusion plus axial dispersion (full lines) and lumped model using \tilde{N}_p given by Eq. 24.

Equivalent Effective Pore Diffusivity

Based on the equality of the breakthrough times with and without axial dispersion, an equivalent effective pore diffusivity can be developed. In fact, if the effect of axial dispersion is not explicitly considered, that is, if axial dispersion and pore diffusion are lumped into an apparent effective pore diffusivity $\tilde{D}_{e_{pore}}$, the value of the throughput parameter at breakthrough is calculated from

$$T_{Bp} = 1 + \frac{5}{2\tilde{N}_p} \left(1 - 3 \ln 3 + \frac{\pi}{\sqrt{3}} \right) \quad (23)$$

This equation results from Eq. 21 for $\alpha = \beta = 0$; because axial dispersion was lumped together with pore diffusion, an apparent number of transfer units by pore diffusion \tilde{N}_p was further introduced.

If $N_p(T_{Bp} - 1)$ with axial dispersion, given by Eq. 21, is divided by $\tilde{N}_p(T_{Bp} - 1)$, given by Eq. 23, imposing further that $(T_{Bp} - 1)$ is the same in both situations (equality of breakthrough times), the following relation, defining the equivalent diffusivity $\tilde{D}_{e_{pore}}$ is obtained

$$\frac{\tilde{N}_p}{N_p} = \frac{\tilde{D}_{e_{pore}}}{D_{e_{pore}}} \approx \frac{1}{1 + 1.61 \frac{N_p}{Pe}} \quad (24)$$

This equivalent diffusivity $\tilde{D}_{e_{pore}}$ can be used with the model equations valid in the absence of axial dispersion, enabling the prediction of the system behavior in the presence of axial dispersion, measured by the Peclet number (Pe), as a function of the parameter N_p/Pe . Equivalently, for given values of N_p and Pe, the equation developed by Hall et al.,¹ corresponding to Eq. 20 with $\alpha = \beta = 0$, can be used with \tilde{N}_p replacing N_p . Curves F vs. T analytically calculated with Eq. 20 using \tilde{N}_p , and with the Hall et al.¹ equation using \tilde{N}_p are represented in Figure 5 for $Pe = 100$. The analysis of this figure shows that

the latter approach is reasonable as far as $N_p/Pe \leq 0.2$.

Equation 24 is represented in Figure 6; the analysis of this figure shows that the influence of axial dispersion on the observed effective pore diffusivity can be neglected if $N_p/Pe \leq 0.07$ because then $0.9 \leq \tilde{D}_{e_{pore}}/D_{e_{pore}} \leq 1$.

Equivalent Effective Solid Diffusivity

Using similar approaches, the breakthrough behavior of an irreversible isotherm system with axial dispersion and solid diffusion control was studied by Convers and Defives⁷ and Ikeda et al.⁸; Ozil and Bonnetain⁹ further extended their results, thus enabling the development of an equivalence between the diffusivities with and without axial dispersion when solid diffusion controls.

The developed equivalence for pore diffusion control can be compared with the equivalence for solid diffusion control, both in the presence of axial dispersion; in fact, using the present notation, the breakthrough time of a solid diffusion controlled system is⁹

$$t_{Bp} = \xi \tau \left(1 - \frac{1}{Pe} - \frac{1}{N_s} \right) \quad (25)$$

An equivalence can then be obtained, in the same way as before, giving for solid diffusion control

$$\frac{\tilde{N}_s}{N_s} = \frac{\tilde{D}_{e_{solid}}}{D_{e_{solid}}} \approx \frac{1}{1 + \frac{N_s}{Pe}} \quad (26)$$

In this equation, $\tilde{D}_{e_{solid}}$ and $D_{e_{solid}}$ are the equivalent (from a model that lumps solid diffusion and axial dispersion) and the effective (from a model that explicitly separates the contributions of solid diffusion and axial dispersion) solid diffusivities, respectively; \tilde{N}_s and $N_s = 15 \xi \tau \tilde{D}_{e_{solid}}/R_0^2$ are the equivalent and the real numbers of mass-transfer units by intraparticle (homogeneous) solid diffusion and ξ is the adsorption (ion exchange) column capacity factor.

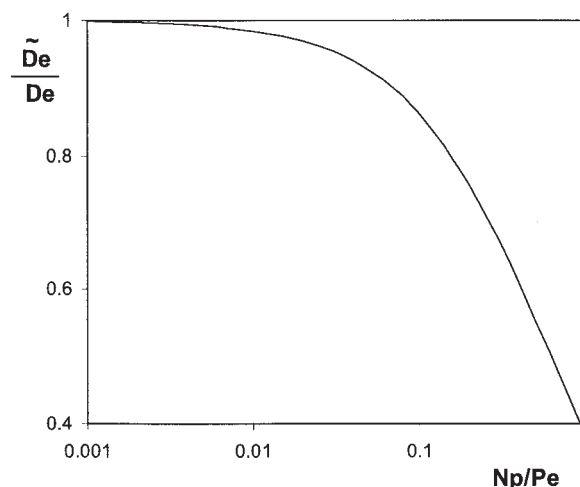


Figure 6. Plot of \tilde{D}_e/D_e vs. N_p/Pe .

Conclusions

In this article, the analytical solution of Hall et al.¹ for irreversible equilibrium with pore diffusion is extended for the case where axial dispersion is present. This is accomplished by an approximation that relates the concentration in the fluid phase with the average concentration in the solid phase, given that the constant-pattern assumption establishing the equality of these concentrations is no longer valid. The analytical solution obtained is then compared with a numerical solution of the equations using the Gear method,¹⁰ showing that the approximation used is reasonable. When the Peclet number tends to infinity (absence of axial dispersion), the solution consistently reduces to the solution in Hall et al.¹

This new solution is used for the development of an equivalent pore diffusivity, valid when a model that lumps pore diffusion and axial dispersion is considered. Results in terms of breakthrough curves from both models are similar for $N_p/Pe \leq 0.2$.

When solid diffusion controls, solutions taken from the literature also establish an apparent solid diffusivity.

Notation

c = fluid concentration in the bulk fluid phase, mol/m³
 c_0 = feed fluid concentration, mol/m³
 c_p = fluid concentration inside pores, mol/m³
 D_{ax} = axial dispersion coefficient, m²/s
 $D_{e_{pore}}$ = effective pore diffusivity, m²/s
 $\bar{D}_{e_{pore}}$ = apparent pore diffusivity, m²/s
 $D_{e_{solid}}$ = solid diffusivity, m²/s
 $\bar{D}_{e_{solid}}$ = apparent solid diffusivity, m²/s
 F = dimensionless concentration in the bulk fluid phase ($=c/c_0$)
 F_p = dimensionless concentration in the pores ($=c_p/c_0$)
 L = bed length, m
 N_p = number of transfer units by pore diffusion
 \bar{N}_p = number of transfer units by apparent pore diffusion
 N_s = number of transfer units by solid diffusion
 \bar{N}_s = number of transfer units by apparent solid diffusion
 q = adsorbed concentration, referred to the particle volume, mol/m³ of particle
 q_0 = adsorbed concentration, referred to the particle volume, in equilibrium with c_0 , mol/m³ of particle
 \bar{q} = average adsorbed concentration, referred to the particle volume, mol/m³ of particle
 q' = adsorbed concentration, referred to the solid volume, mol/m³ of solid
 q_s = maximum adsorbed concentration, referred to the solid volume, mol/m³ of solid
 r = radial coordinate in the particle, m
 r_i = core radius, m
 R_0 = particle radius, m

t = time, s

T = dimensionless throughput parameter $\{=[c_0(Ut - \varepsilon V)]/[(1 - \varepsilon)q_0V]\}$

u_0 = superficial velocity, m/s

u_i = interstitial velocity, m/s

w = concentration wave velocity, m/s

x = auxiliary variable, Eq. 15

y = dimensionless adsorbed phase concentration ($=q/q_0$)

\bar{y} = dimensionless average adsorbed phase concentration ($=\bar{q}/q_0$)

z = axial coordinate in the bed, m

Greek letters

α = dimensionless parameter in Eq. 14

β = dimensionless parameter in Eq. 14

γ = dimensionless parameter in Eq. 15 ($=1 + \alpha - \beta$)

ε = dimensionless bed porosity

ε_p = dimensionless particle porosity

ξ = capacity factor $\{=[(1 - \varepsilon)/\varepsilon](q_0/c_0)\}$

τ = space time, s

τ_p = time constant for intraparticle diffusion ($=R_0^2/D_{e_{pore}}$), s

Subscripts

Bp = breakthrough point

F = final (at saturation time)

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