

Time and bed height dependent concentration vs. particle radius profiles in packed-bed adsorption columns:
Non-equilibrium model simulation studies
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Time and bed height dependent concentration vs. particle radius profiles in packed-bed adsorption columns: Non-equilibrium model simulation studies

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Abstract

A new mathematical model and a simulation program have been developed for the prediction of the intra-particle uptake profiles at packed-bed adsorption processes. This work introduces a systematic and theoretically sound approach to linear driving force (LDF) approximations by taking into account the non-equilibrium conditions prevailing in the column. It is shown that the methodology presented in this work allows quantitative investigations of solute adsorption dynamics within a single adsorbent particle of the packed-bed column, which adds a new tool to the available methods for characterizing and optimizing adsorption processes.

Keywords: intra-particle uptake, packed-bed adsorption, non-equilibrium modelling.

1. Introduction

This communication will demonstrate the application of a new methodology on the acquirement of time and bed height dependent intraparticle concentration vs. particle radius profiles in packed-bed adsorption columns, which brings a new perception on the analysis of particle internal and external mass transfer resistances to intraparticle concentration profiles. Usually the understanding of packed-bed adsorption and mathematical modelling approaches to describe intraparticle adsorption and transport of solutes are limited to data obtained from finite bath and packed-bed breakthrough studies, with the change of solute concentration in the fluid phase as the only source of information. This approach corresponds to the end result of the actual amount of adsorbed solutes overlaid within the adsorbent and has limited use for the development and verification of models describing intraparticle transport.

Frequently the nature of the adsorption isotherm becomes a decisive factor on the solution strategy of packed-bed adsorption column governing differential equations. Assumption of linear isotherm leads to a transport equation which can be solved

analytically (Lapidus and Amundsen, 1952). If the expression for the adsorption equilibrium isotherm that is used in a particular dynamic adsorption model is nonlinear, then the solution to that model is obtained numerically (Heeter and Liapis, 1997). In general, three models are used for the diffusion of solute molecules relevant to adsorption processes that are the pore, surface and homogeneous (solid) diffusion (Chang and Lenhoff, 1998; Carta and Cincotti, 1998; Chen et al., 2002; Hunter and Carta, 2000). Because of mathematical and numerical difficulties associated with these models, the use of simplified approximations is often desirable. A simple theoretical approach is to assume that local equilibrium (LE) exists between the bulk fluid and the solid phase. The LE model neglects all transient resistances, i.e. there is no concentration gradient within a particle or in the liquid film. Especially for nonlinear adsorption isotherms, local equilibrium based models usually become less effective in predicting experimentally observed distended breakthrough fronts and causes the predicted curves to be too sharp (Schork and Fair, 1998; Özdural et al., 2004). In this case, extended tailing and asymmetrical breakthrough curves which can be observed experimentally in packed-bed adsorption processes can only be explained as a result of dispersion and diffusion in the fluid phase (Guiochon et al. 1994; Worch, 2004; Rahman and Worch, 2005). However the validity of the assumption of local equilibrium (LE) conditions is uncertain in the dynamic state that exists in a packed-bed adsorption column (Skoog et al. 2003). Furthermore at the classical adsorption isotherm experiments, there would be no need to bring into contact and agitate the solid and liquid phases for prolonged times if the so called equilibrium conditions could instantly be attained between the liquid and solid phases under dynamic conditions.

The assessment presented above illustrates that in order to reach a factual packed-bed adsorption column dynamics portrait the inclusion of non-equilibrium constraints in the modelling studies, as separate identities, is essential at least for the case of larger, slowly diffusing molecules. The term non-equilibrium adsorption is used in the sense that the adsorption equilibrium is not established instantaneously during the transport process due to mass transfer restrictions, and it combines external film mass transfer and intra-particle transport. On the other hand, it is reasonable to assume that the interphase fluid concentration c_s^* is in equilibrium with the interphase solid concentration, q_s^* since adsorption itself (transfer of solute at the interphase to adsorbed state) is generally very fast (Foo and Rice, 1975). Fig. 1 illustrates the interphase equilibrium conditions. In this work, nonlinear fluid-solid interphase concentrations are related with Langmuir isotherm, where the following version of Langmuir adsorption isotherm expression holds for dynamic conditions. The q_m and K_L terms in Eq. (1) are the Langmuir constants.

$$q_s^*(x, t) = \frac{q_m K_L c_s^*(x, t)}{1 + K_L c_s^*(x, t)} \quad (1)$$

For mass transfer through the external film, the difference between the actual concentration in the bulk fluid phase, $c(x,t)$, and the concentration at the solid particle surface, $c_s^*(x,t)$, acts as a driving force. The mechanism of intraparticle diffusion is based on homogeneous (solid) diffusion. In this paper the consistency of the application of non-equilibrium model, proposed by Özdural et al. (2004) to the prediction of time and bed height dependent intraparticle concentration profiles will be explored by making use of the linear driving force (LDF).

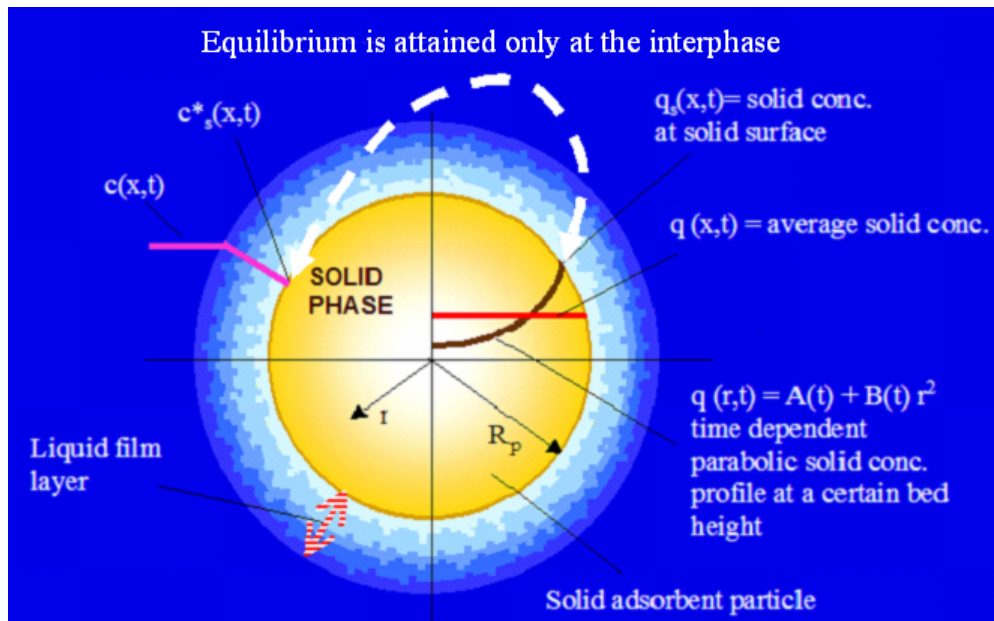


Figure 1. Visualization of non-equilibrium conditions between bulk liquid and adsorbent average concentrations where equilibrium is attained only at the interphase.

LDF model, which was originally proposed by Gleuckauf and Coates (1947) for adsorption chromatography, provides substantial simplifications in computations, and it has been widely employed in various problems that involve intraparticle diffusion (Basagaoglu et al. 2000). The original wording of the LDF approximation by Gleuckauf and Coates (1947) was as follows: "...the rate of diffusion into the grains is essentially proportional to the amount still required to produce equilibrium...". Eq. (1) gives LDF definition adapted for packed-bed columns, which is written in partial differential terms since volume average solute concentration in solid (mg/cm^3), $\bar{q}(x,t)$ is both packed-bed height, x and time, t dependent.

$$\frac{\partial \bar{q}(x,t)}{\partial t} \cong \xi [q^*(x,t) - \bar{q}(x,t)] \quad (2)$$

where $q^*(x,t)$ is the homogeneous solute concentration in solid (mg/cm^3) that would be in equilibrium with the bulk liquid phase concentration (mg/cm^3), $c(x,t)$. The proportionality constant ($1/\text{s}$), ξ is the effective LDF mass transfer coefficient at adsorbate loading, and t is the time (s).

It is generally agreed that the employment of parabolic intraparticle concentration profile for short contact times leads to unrealistic concentrations and even the concentration profile becomes negative at the inner regions of the adsorbent (Do and Rice, 1986; Do and Mayfield, 1987; Ching and Lu, 1988; Li and Yang, 1999; Hsuen, 2000; Sircar and Hufton, 2000). Do and Mayfield (1987) used an intraparticle concentration profile and in dimensional terms it is equal to:

$$q = a_0 + a_n r^n \quad (3)$$

where a_0 , a_n and n are all functions of time, and they further concluded that n value should decrease to zero from a large initial value.

The significance of this work is threefold. First, it delineates the importance of the contributions of mass transfer resistances on the intraparticle concentration profiles. Second, shows the unrealistically predicted negative intraparticle concentrations that were reported in the literature for short contact times via employment of parabolic concentration profiles might be attributed to the use of LE assumption, since no such incidences observed in the present case, where non-equilibrium methodology is introduced. Finally, use of this new technique allows us to suggest protocols for new system operations and/or scale-up processes of packed-bed adsorption systems.

2. Theoretical

The change of interstitial velocity of the liquid stream, v (cm/s), and the liquid concentration gradients in the radial direction of the adsorption column are considered to be negligible. The mathematical model used in this work considers that single component adsorption takes place. It is assumed that the adsorbent phase is composed of spherical particles (radius = r_p cm), it operates under isothermal conditions, the non-linear equilibrium data can be represented by Langmuir equation, and non-equilibrium conditions exist between the adsorbent particle average concentration and the liquid in the void fraction of the annulus. The model is based on a dual resistance model combining external mass transfer and intraparticle transport by homogeneous (solid) diffusion model and a constant homogeneous solid diffusivity, D_s (cm^2/s) is used throughout the analysis. Eq. (4) gives the intra-particle parabolic profile expression where $q(r,x,t)$ is the x (bed height), r (radial position within the particle), and t (time) dependent solid concentration.

$$q(r, x, t) = a_0(x, t) + a_2(x, t)r^2 \quad (4)$$

Equation (5) shows packed-bed column version of the well known expression derived for batch uptake systems (Yao and Tien, 1992). It gives the relationship between adsorbent average concentration, $\bar{q}(x, t)$ and adsorbent surface concentration, $q_s^*(x, t)$. This equation can be obtained by parabolic concentration profile assumption within a particle, and as explained in the introduction section, is equivalent to the employment of LDF model, where Bi is the Biot number.

$$q_s^*(x, t) = \bar{q}(x, t) + \frac{Bi}{5} [c(x, t) - c_s^*(x, t)] \quad (5)$$

$$Bi = \frac{k_f r_p}{D_s} \quad (6)$$

Eq. (7) gives the mass conservation equation for one-dimensional solute transport (Quinones et al., 2000), which is also called convection-dispersion adsorption equation, where D_a is the axial dispersion coefficient (cm²/s) and ε is the packed-bed voidage.

$$\frac{\partial c(x, t)}{\partial t} + v \frac{\partial c(x, t)}{\partial x} + \beta [c(x, t) - c_s^*(x, t)] = D_a \frac{\partial^2 [c(x, t)]}{\partial x^2} \quad (7)$$

$$\beta = \frac{3(1 - \varepsilon)}{\varepsilon r_p} k_f \quad (8)$$

Özdural et al. (2004) showed that for packed-bed adsorption columns with nonlinear adsorption isotherms, along with solid average and bulk fluid concentrations, the prediction of time and bed height dependent interphase concentrations i.e. $c_s^*(x, t)$ and $q_s^*(x, t)$ are possible via the introduction of non-equilibrium methodology during the numerical solution of Eq. (7).

Let's try to express the time and bed height dependent coefficients of parabolic intraparticle profile expression given by Eq. (4), namely $a_0(x, t)$ and $a_2(x, t)$, in terms of (i) time and bed height dependent driving force, i.e. the difference between bulk liquid concentration and interphase liquid concentration which is equal to $[c(x, t) - c_s^*(x, t)]$, and (ii) time and bed height dependent adsorbent surface concentration, $q_s^*(x, t)$. Thus, once $a_0(x, t)$ and $a_2(x, t)$ values are known, then it is possible to evaluate the intraparticle concentration, $q(r, x, t)$ through Eq. (4).

For a certain bed height ($x = x$), boundary conditions at the interface between the solid and the liquid phase are,

$$q(r, x, t)|_{r=r_p} = q_s^*(x, t) \quad (9)$$

$$D_s \frac{\partial q(r, x, t)}{\partial r} \Big|_{r=r_p} = k_f [c(x, t) - c_s^*(x, t)] \quad (10)$$

From Eq. (4),

$$\frac{\partial q(r, x, t)}{\partial r} \Big|_{r=r_p} = 2a_2(x, t)r_p \quad (11)$$

Combining Eqs. (10) and (11) gives

$$a_2(x, t) = \frac{k_f}{2r_p D_s} [c(x, t) - c_s^*(x, t)] \quad (12)$$

At $x = x$, the time dependent volume average solute concentration in spherical adsorbent particle, $\bar{q}(x, t)$ is,

$$\bar{q}(x, t) = \frac{\int_0^{r_p} 4\pi r^2 q(r, x, t) dr}{\frac{4}{3}\pi r_p^3} \quad (13)$$

substituting Eq. (4) into Eq. (13) gives,

$$\bar{q}(x, t) = a_0(x, t) + \frac{3}{5} a_2(x, t) r_p^2 \quad (14)$$

If Eq. (4) is written for the particle surface

$$a_0(x, t) = q_s^*(t) - a_2(t) r_p^2 \quad (15)$$

Eqs. (12) and (15) gives $a_2(x,t)$ and $a_0(x,t)$ values respectively. It is now possible to determine the change of intraparticle concentration with radial direction, r at a specified bed height, x and time, t through Eq. (4). For this purpose one needs to know $[c(x,t) - c_s^*(x,t)]$ and $q_s^*(x,t)$ values. The methodology of non-equilibrium modeling of packed-bed adsorption with non-linear adsorption isotherms, which was introduced by Özdural et al. (2004) allows collecting such information. They showed that $c_s^*(x,t)$ can be expressed as following.

$$c_s^*(x,t) = \frac{-M + \sqrt{M^2 + \frac{4}{K_L} \left[c(x,t) + \frac{5\bar{q}(x,t)}{Bi} \right]}}{2} \quad (16)$$

$$M = \frac{5q_m}{Bi} - \frac{5\bar{q}(x,t)}{Bi} + \frac{1}{K_L} - c(x,t) \quad (17)$$

Regarding the mass transfer resistances, Eq. (7) contains the k_f term only, but as shown in Eqs. (6), (16) and (17) solid internal resistance is inherently included in the $c_s^*(x,t)$ term. Once Eq. (16) is substituted into Eq. (7) then $c_s^*(x,t)$ term disappears but a new dependant variable, namely adsorbent particle average concentration $\bar{q}(x,t)$ appears. During the numerical solution procedure, the $\bar{q}(x,t)$ value at $j+1$ time panel is evaluated from the c and $\bar{q}(x,t)$ values at j time panel. Özdural et al. (2004) presented the resulting equation that gives the $\bar{q}(x,t)$ value at $j+1$ time panel as shown in Eq. (18) where Δt , the time step is k and Δx , the increment in bed height is h .

$$\bar{q}_{i,j} = \bar{q}_{i,j-1} + \frac{\varepsilon k}{2(1-\varepsilon)h} \left[v(c_{i-1,j} - c_{i+1,j}) - 2h \frac{\partial c(x,t)}{\partial t} + \frac{D_a(c_{i-1,j} - 2c_{j,i} + c_{i+1,j})}{h} \right] \quad (18)$$

3. Numerical solution strategies for predicting the change of intraparticle concentration with particle radial direction in packed-bed adsorption columns.

The purpose of this section is to explain the numerical solution algorithm that is employed for predicting particle radial direction, bed height and time dependent intraparticle concentration, $q(r,x,t)$ in packed-bed adsorption. For the numerical solution finite differences technique has been employed. Since explicit schemes may

suffer from stability limits finite differences with implicit schemes method is used. $\partial c/\partial x$ and $\partial^2 c/\partial x^2$ terms are evaluated by central difference approximation, and $\partial c/\partial t$ term is approximated by forward difference with reference to the grid network shown in Fig. 2.

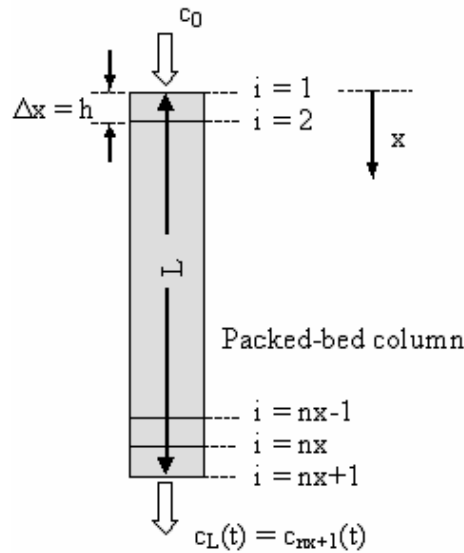


Figure 2. Schematic representation of a packed-bed adsorption column

| | | | |
|--------|-------------|-------------------------------|-----------------------------------|
| I.C. | $t = 0$ | for all x in the packed-bed | $c(x, t) = 0$ |
| B.C. 1 | for $t > 0$ | $x = 0$ | $c(x, t) = c_0$ |
| B.C. 2 | for $t > 0$ | $x = L$ | $\partial c(x, t)/\partial x = 0$ |

The above given B.C. 2 at $x = L$, i.e. at $nx+1$, is approximated by linear extrapolation of $c(x, t)$ values at $i = nx-1$ and $i = nx$. If there is a grid of $n+1$ spatial points for x direction, then at time $j+1$ there are $n+1$ unknown nodal values. We can assemble the set of $n+1$ equations. By solving this equation system, we determine c_1, c_2, \dots, c_{n+1} at time step $j+1$ from c_1, c_2, \dots, c_{n+1} at time step j . After discretizing the transport equation the set of $n+1$ algebraic equations to be solved simultaneously are as follows.

$i = 1$ (packed-bed inlet)

$$c_{i,j+1} = c_{i,j} = c_0 \quad (19)$$

$1 < i < nx+1$

$$-(\alpha + \gamma)c_{i-1,j+1} + (1 + 2\gamma)c_{i,j+1} + (\alpha - \gamma)c_{i+1,j+1} = (1 - \beta k)c_{i,j} + \frac{\beta k}{2} \left[\sqrt{M^2 + \frac{4}{K_L} \left(c_{i,j} + \frac{5\bar{q}_{i,j}}{Bi} \right)} - M \right] \quad (20)$$

$$\alpha = \frac{kv}{2h} \quad (21)$$

$$\gamma = \frac{kD_a}{h^2} \quad (22)$$

$i = nx+1$ (packed-bed outlet)

$$c_{nx-1,j+1} - 2c_{nx,j+1} + c_{nx+1,j+1} = 0 \quad (23)$$

The acquirement of $c(x,t)$, $c_s^*(x,t)$, $\bar{q}(x,t)$, $q_s^*(x,t)$ values via the proper inclusion of Eqs (1), (16) and (18) into the above mentioned algorithm, and thereby predicting $q(r,x,t)$ vs r values through Eq.(4) is now possible.

It might be interesting to note that the present approach of the solution of convection-diffusion adsorption equation obviates the solely trailed complicated procedure described in the literature (Liapis and Rippin,1978; Kaczmarski et al., 1997; Xiu et al., 2003), where solution of “coupled” partial differential equation (PDE) systems is required. The present methodology employs a single PDE by crediting the particle phase concentration at a specified bed height and time through the use of mass balance expressions which concurrently takes into account the accumulation and axial dispersion effects.

4. Simulation results

The influence of the parameters on the model output was studied for a single component adsorption. The algorithm presented is found to be very fast and easily converges within 2 seconds when it is run on a PC having an Intel Pentium® D 935 processor. Table 1 summarizes the adsorbate, adsorbent and column properties to be used in the prediction of intraparticle concentration profiles, which were taken from McCue et al. (2003). Employing this data, Özdural et al. (2004) calculated the film mass transfer coefficient, ($k_f = 1.54 \times 10^{-3}$ cm/s) and axial dispersion coefficient ($D_a = 6.50 \times 10^{-3}$ cm²/s) values for the superficial velocity 500 cm/h. The packed-bed inlet concentration is chosen as $c_0 = 1$ mg/cm³ and the homogeneous diffusivity of adsorbate hIgG in adsorbent PG 700 is taken as $D_s = 0.42 \times 10^{-9}$ cm²/s. The above mentioned system parameters and operating conditions are employed as pivot values.

Fig. 3 illustrates the break through curves of various simulation studies where pivot parameter values are used unless otherwise indicated on the figure.

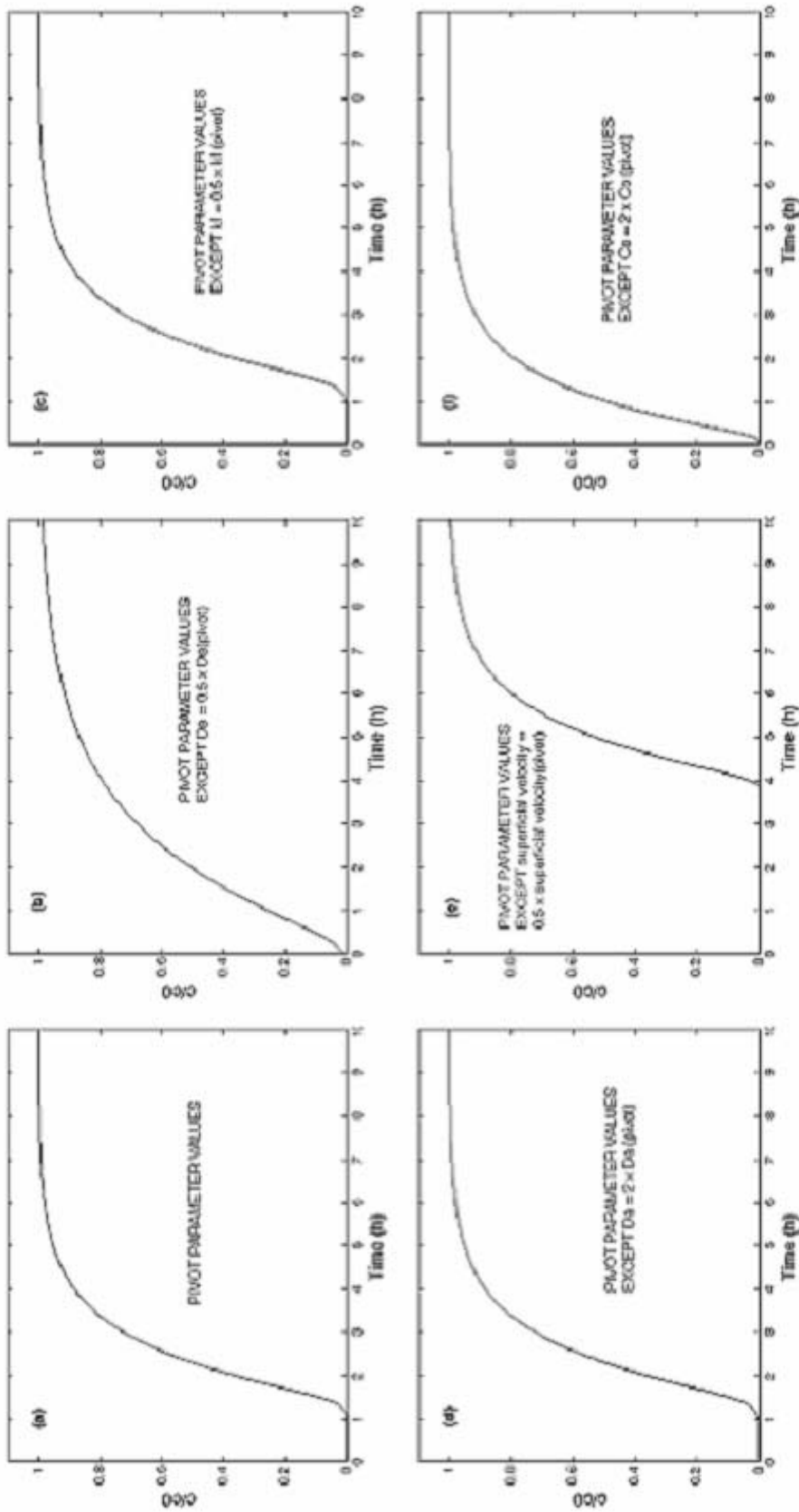


Figure 3. Break through curves of various simulation studies where pivot parameter values are used unless otherwise indicated on the figure

Along with the pivot parameters, in order to visualize the effect of homogeneous diffusivity, D_s external film mass transfer coefficient, k_f axial dispersion coefficient, D_a superficial velocity, u and packed-bed inlet concentration, c_0 on non-equilibrium model predicted break through curves, Figs 3 (a) to (f) are prepared.

Table 1

Data regarding adsorbate (hIgG), adsorbent (porous glass, PG 700) and column properties to be used in the prediction of intraparticle concentration is taken from McCue et al. (2003).

| Properties | PG 700 |
|---|--------|
| Bulk density (g/cm^3) | 0.39 |
| Particle porosity (-) | 0.68 |
| Average particle diameter (μm) | 100 |
| Bed voidage (-) | 0.43 |
| Bed height (cm) | 20.0 |
| Column I.D. (cm) | 0.66 |
| Langmuir isotherm q_m value (mg/cm^3 media) | 121 |
| Langmuir isotherm K_L value (cm^3/mg) | 18.9 |

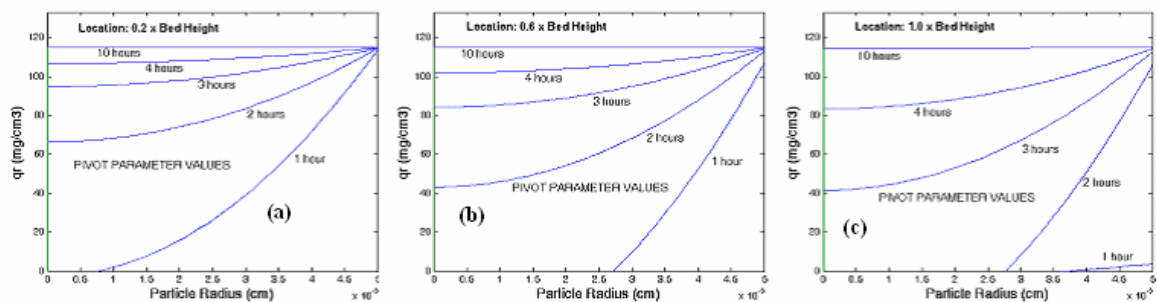


Figure 4. Change of non-equilibrium model predicted intraparticle concentration profiles with time at different packed-bed adsorption column locations – pivot parameters.

Fig. 4 illustrates the change of non-equilibrium model predicted intraparticle concentration profiles for the case of pivot parameters. Figs 4 (a) to (c) clearly visualize that at a certain bed location particle uptake increases with time. On the other hand, as expected from the breakthrough curve corresponding to this case i.e.

Fig. 3 (a), for a specified time particle loading decreases with the increase of bed length since the particles come across with less concentrated solutions. However for extended perfusion times, such as 10 hours, intraparticle concentration profiles flatten and the solid concentration reaches to $q = q_m$ value, regardless of the particle radial position.

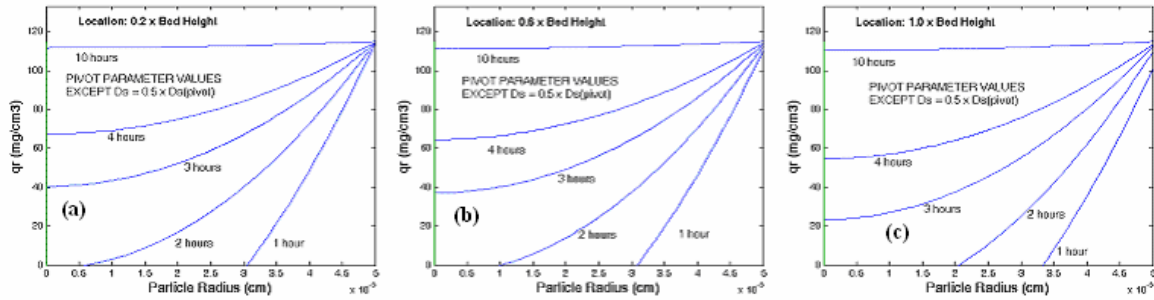


Figure 5. Change of non-equilibrium model predicted intraparticle concentration profiles with time at different packed-bed adsorption column locations – pivot parameters except: $D_s = 0.5 \times D_s(pivot)$

Fig. 5 shows the change of non-equilibrium model predicted intraparticle concentration profiles for the case of pivot parameters except the particle internal resistance is increased where $D_s = 0.5 \times D_s(pivot)$ is employed. The same comments regarding the effect of bed height and time on the particle uptake explained in Fig. 4 holds for this case too. Furthermore comparison of Fig 4 and Fig 5 illustrates that, keeping all other parameters constant, when particle internal resistance increases this reflects as a lesser amount of solute uptake by the particles which are in consistent with the corresponding breakthrough curve given by Fig. 3 (b).

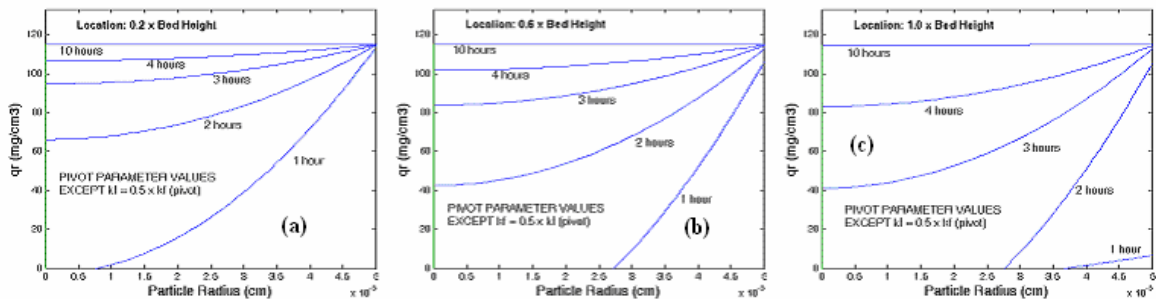


Figure 6. Change of non-equilibrium model predicted intraparticle concentration profiles with time at different packed-bed adsorption column locations – pivot parameters except: $k_f = 0.5 \times k_f(pivot)$

Fig. 6 shows the change of non-equilibrium model predicted intraparticle concentration profiles for the case of pivot parameters except the external film resistance is increased where $k_f = 0.5xk_f(pivot)$ is employed. The same comments regarding the effect of bed height and time on the particle uptake explained in Fig. 4 holds for this case too. Furthermore comparison of Fig 4 and Fig 6 illustrates that, keeping all other parameters constant, when particle external film resistance increases this reflects as a lesser amount of solute uptake by the particles which are in consistent with the corresponding breakthrough curve given by Fig. 3 (c). However it might worth to indicate that the effect of external film resistance is not as noticeable as that of internal particle resistance.

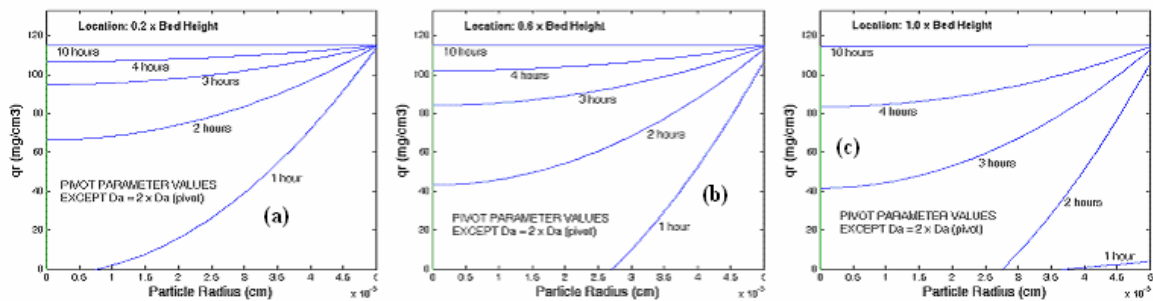


Figure 7. Change of non-equilibrium model predicted intraparticle concentration profiles with time at different packed-bed adsorption column locations – pivot parameters except: $D_a = 2.0xD_a(pivot)$

Fig. 7 shows the change of non-equilibrium model predicted intraparticle concentration profiles for the case of pivot parameters except the effect of axial diffusion is increased by a factor of two where $D_a = 2.0xD_a(pivot)$ is employed. The reason of increasing the value of axial diffusion is due to its almost indistinguishable outcome on the intraparticle concentration profiles when smaller values are used. The same comments regarding the effect of bed height and time on the particle uptake explained in Fig. 4 holds for this case too. Furthermore comparison of Fig 4 and Fig 7 illustrates that, keeping all other parameters constant, when axial diffusion increases it only reflects as a slightly higher amount of solute uptake by the particles. This effect is relatively more pronounceable for short times, and it fades out as time increases.

Fig. 8 shows the change of non-equilibrium model predicted intraparticle concentration profiles for the case of pivot parameters except the superficial velocity is decreased to half of its pivot value where $u = 0.5xu(pivot)$ is employed. The same comments regarding the effect of bed height and time on the particle uptake explained in Fig. 4 holds for this case too, but the outcome of the change of superficial velocity

on intraparticle concentration profiles is very significant. When superficial velocity decreases, as shown in the corresponding breakthrough curve given by Fig. 3 (e), the column outlet concentration becomes negligible almost up to four hours. This clearly explains why the intraparticle concentration profile of 1 hour after the start of perfusion is not observable at the 60 per cent bed height, and so does the intraparticle concentration profiles of less than four hours at the packed-bed outlet.

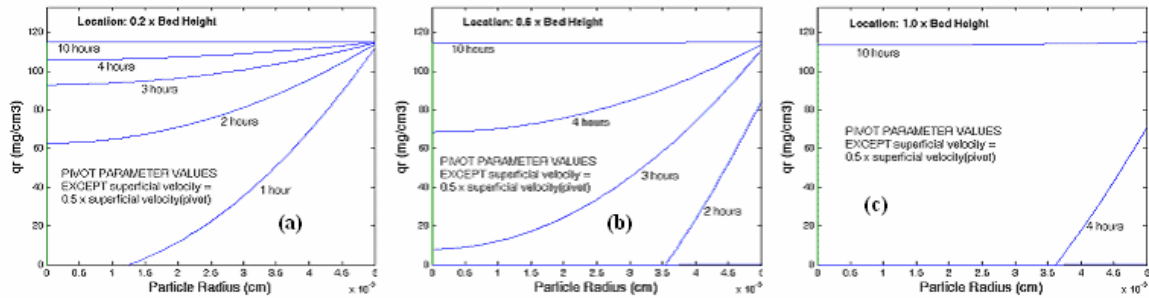


Figure 8. Change of non-equilibrium model predicted intraparticle concentration profiles with time at different packed-bed adsorption column locations – pivot parameters except: $u = 0.5 \times u(pivot)$

Fig. 9 shows the change of non-equilibrium model predicted intraparticle concentration profiles for the case of pivot parameters except the packed-bed inlet concentration is increased by a factor of two. The same comments regarding the effect of bed height and time on the particle uptake explained in Fig. 4 holds for this case too. Furthermore comparison of Fig 4 and Fig 9 illustrates that, keeping all other parameters constant, when inlet concentration increases this reflects as higher amount of solute uptake by the particles, which is of course an expected behaviour, since they are exposed to more concentrated liquid phase.

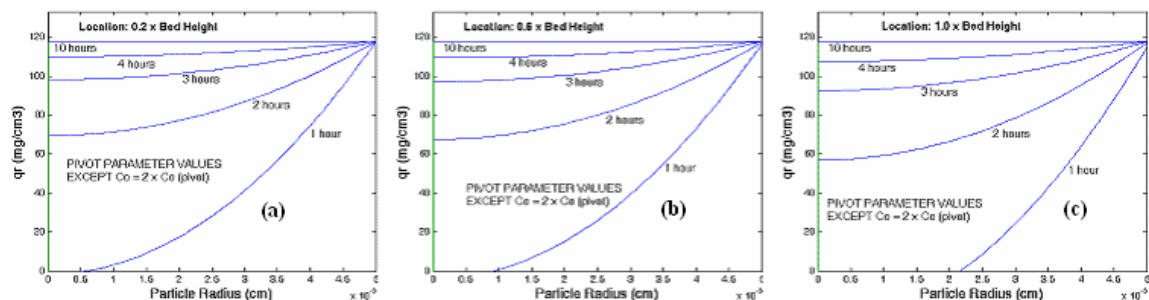


Figure 9. Change of non-equilibrium model predicted intraparticle concentration profiles with time at different packed-bed adsorption column locations – pivot parameters except: $c_0 = 2.0 \times c_0(pivot)$

5. Conclusion

A theoretical study has been presented for the prediction of time and bed height dependent intraparticle concentration vs. particle radius profiles in packed-bed adsorption columns by taking the advantage of non-linear non-equilibrium modelling of packed-bed adsorption columns. In the literature, the neglect of mass transfer resistances by local equilibrium (LE) approach considered the theoretical optimum which could be achieved for the simulation studies. In reality, however, mass transfer effects could not be eliminated from the separation process. It is shown that the methodology presented in this work allows quantitative investigations of solute adsorption dynamics within a single adsorbent particle of the packed-bed column,

The significance of this work is threefold. First, it delineates the importance of the contributions of mass transfer resistances on the intraparticle concentration profiles. Second, shows the unrealistically predicted negative intraparticle concentrations that were reported in the literature for short contact times via employment of parabolic concentration profiles might be attributed to the use of LE assumption, since no such incidences observed in the present case, where non-equilibrium methodology is introduced. Finally, use of this new technique allows us to suggest protocols for new system operations and/or scale-up processes of packed-bed adsorption systems.

6. Nomenclature

a_0 = parameter in Eq. (3) and (4)

a_2 = parameter in Eq. (4)

a_n = parameter in Eq.(3)

Bi = Biot number, $k_f r_p/D_s$

c = liquid concentration in the void fraction of packed-bed adsorption column, mg/cm^3

c_0 = liquid concentration at the packed-bed inlet, mg/cm^3

c_s^* = interphase liquid concentration, mg/cm^3

D_a = axial dispersion coefficient, cm^2/s

D_s = homogeneous (solid) diffusivity, cm^2/s

h = increment in distance, cm

i = x panel index used in numerical solution

j = t panel index used in numerical solution

K_L = constant in Langmuir isotherm, cm^3/mg

L = packed-bed height, cm

k = increment in time, s

k_f = film mass transfer coefficient, cm/s

q = radial position dependent particle concentration, mg/cm^3 solid

\bar{q} = adsorbent particle average concentration, mg/cm^3 solid

q_m = Langmuir isotherm maximum adsorption capacity, mg/cm^3 solid

q^* = particle homogeneous solute concentration that would be in equilibrium with the bulk liquid phase concentration, mg/cm^3 solid

q_s^* = solid concentration at the adsorbent surface, mg/cm^3 solid

r = adsorbent particle radial coordinate, cm

r_p = adsorbent particle average radius, cm

t = time, s

u = superficial velocity, cm/s

x = packed-bed axial distance, cm

v = interstitial velocity, cm/s

Greek Letters

α = parameter equal to $kv/(2h)$

β = parameter equal to $3(1-\varepsilon)k_f/(\varepsilon r_p)$

ε = void fraction in packed-bed adsorber

γ = parameter equal to kD_a/h^2

ξ = effective LDF mass transfer coefficient, 1/s

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