Analytic solution of biparameter axial dispersion model

Shelly Arora\textsuperscript{1}, Vijay Kumar Kukreja\textsuperscript{2}, František Potúček\textsuperscript{3}

\textsuperscript{1}Department of Mathematics, Punjabi University, INDIA
aroshelly@gmail.com

\textsuperscript{2}Department of Mathematics, SLIET, INDIA
vkkukreja@gmail.com

\textsuperscript{3}Institute of Chemistry and Technology of Macromolecular Materials,
Faculty of Chemical Technology, University of Pardubice, Czech Republic
frantisek.potucek@upce.cz

Communicated by Giorgio Fotia

Abstract

A linear axial dispersion model involving two parameters, Peclet number (Pe) and retardation coefficient (R_d) has been presented. Model equations have been solved analytically, using Laplace transform. Solution has been obtained in terms of complementary error function. Two limiting cases of perfect mixing and perfect displacement have also been discussed. Verification of model is carried out by using the experimental data of a washing cell.

Keywords: Peclet number, retardation coefficient, Laplace transform, complementary error function.

AMS subject classification: 05A16, 65N38, 78M50.

1. Introduction.

Washing of porous, solid or semi solid particles in a porous bed with the aid of external fluid is of great importance in the field of chemical and process industries. During this process, the solute present in irregular void channels of bed diffuse out of particle pores when it comes in contact with the external fluid.

The models describing fluid mixing in chemical vessels are mainly based on diffusion like dispersion phenomenon. Mathematically, these models represent two point boundary value problems and are characterized as axial dispersion model. The parameter describing the ratio of convection to dis-
persion in the fluid is known as Peclet number \((Pe)\) whereas retardation coefficient is the rate of removal of solute adsorbed on particle surface and is always greater than 1. To solve these problems analytically, mathematical complexities are reduced by taking linear or finite rate isotherms. Washing process is highly dependent on orientation, geometry, packing and structure of particles. Therefore, present model has taken into account the displacement washing process of particles, which are highly compressible and having cylindrical geometry.


The basic material balance describing the flow of external fluid through the bed of particles, for any solute can be expressed as:

\[
\left( \text{Entering by flow} \right) + \left( \text{Entering by dispersion} \right) = \left( \text{Leaving by bulk flow} \right) + \left( \text{Leaving by dispersion} \right) + \left( \text{Accumulation on pulp fibers} \right)
\]

The dimensionless mass transport equation involving axial dispersion and mass transfer coefficients across the bed in one dimension can be written as:

\[
\frac{1}{Pe} \frac{\partial^2 C}{\partial \xi^2} = \frac{\partial C}{\partial \xi} + \frac{\partial C}{\partial \tau} + \left( \frac{1 - \epsilon}{\epsilon} \right) N_1 \frac{\partial N}{\partial \tau}
\]

Adsorption isotherm linking bulk fluid concentration and the concentration of solute adsorbed on fiber surface is taken to be linear:

\[
N = k_f C/N_1
\]

where \(k_f\) is the ratio of deposition rate constant to detachment rate constant. The deposition rate constant is in forward direction and detachment rate constant is in backward direction and both are of first order. Using equation (2) in equation (1), the latter takes the form:

\[
R_d \frac{\partial C}{\partial \tau} = \frac{1}{4Pe} \frac{\partial^2 C}{\partial \xi^2} - \frac{\partial C}{\partial \xi}
\]

where \(R_d = k_f(1 - \epsilon)/\epsilon\) is the retardation coefficient. Robins boundary conditions have been followed at creek and exit of the bed. No loss of solute is assumed at the initial point, while the concentration gradient is taken to be zero at the exit of the bed.

\[
C - \frac{1}{4Pe} \frac{\partial C}{\partial \xi} = 0, \text{ at } \xi = 0 \text{ and } \frac{\partial C}{\partial \xi} = 0, \text{ at } \xi = 1
\]
Initially, it is assumed that:

\[(5) \quad C = N = 1, \text{ at } \tau = 0\]

The analytic solution of a similar type of problem for fixed bed adsorbers has been given by [1,2].


Problems similar to equation (3) have been solved by using trigonometric functions by [2,3]

\[(6) \quad C_{e} = 2 \frac{Pe}{R_{d}}^{2} \exp \left(2 Pe - \frac{Pe \tau}{R_{d}} \right) \times \sum_{n=1}^{\infty} \frac{\lambda_{n}^{2}}{(\lambda_{n}^{2} + Pe^{2})[\lambda_{n}(1 + 2Pe)\sin(2\lambda_{n}) - (Pe^{2} - \lambda_{n}^{2} + Pe)\cos(2\lambda_{n})]}\]

These functions are complicated to compute and require number of approximations. To overcome this problem, the approximate solution is found by transforming the function into an exponential function. This method can be regarded as the generalized form of the method given by [4]. The concentration function \(C(\xi, \tau)\) is transformed into an exponential function using following transformation:

\[C(\xi, \tau) = y(\xi, \tau)\exp \left(2 Pe \xi - \frac{Pe}{R_{d}} \tau \right)\]

where \(y(\xi, \tau)\) is a continuously differentiable function with respect to \(\xi\). After transforming the concentration function \(C(\xi, \tau)\) into an exponential form and taking the Laplace transform of equation (3) and then solving using equation (4), following equations appears:

\[(7) \quad \bar{y} = \exp \left(-2 Pe \xi\right) + \frac{4Pe(\alpha + 2Pe)e^{-\alpha \xi}}{\alpha^{2} + 2Pe} \left(e^{2\alpha} + \alpha - 2Pe \right) \frac{1}{(p - (Pe/R_{d}))\left\{\alpha - 2Pe\right\}^{2} - (\alpha + 2Pe)^{2}e^{2\alpha}}\]

and \(\alpha = \sqrt{4PeR_{d}p}.\) It can be further simplified as:

\[(8) \quad \bar{y} = \frac{\exp(-2Pe \xi)}{p - \frac{Pe}{R_{d}}} - \frac{\exp(-\alpha \xi)}{p - \frac{Pe}{R_{d}}} + 4PeR_{d} \frac{\exp(-\alpha \xi)}{\left(\alpha + 2Pe\right)^{2}} - 16Pe^{2}R_{d} \frac{\exp(-\alpha(2 - \xi))}{\left(\alpha + 2Pe\right)^{3}}\]
Except the fourth term in equation (8), the inverse Laplace transform of other terms can be obtained from [5]. The inverse transform of fourth term of equation (8) is taken as:

\[
L^{-1}\left(\frac{16Pec^2Rd\exp(-\alpha(2 - \xi))}{(\alpha + 2Pec)^3}\right) = -4Pec^2Rd\frac{\partial}{\partial Pe}L^{-1}\left(\frac{\exp(-\alpha(2 - \xi))}{(\alpha + 2Pec)^2}\right)
\]

It is understood that \(\alpha\) should be treated as constant while differentiating with respect to \(Pe\), i.e., \(\alpha = \sqrt{4K'Rd}\) and carry \(K'\) as constant while performing inverse transformation and subsequent differentiation with respect to \(Pe\). After performing both operations set \(K' = Pe\), to get the following expression of \(C(\xi, \tau)\) [4]:

\[
C(\xi, \tau) = 1 - \frac{1}{2}\text{erfc}\left(\sqrt{\frac{PeRd}{\tau}}\xi - \sqrt{\frac{Pe\tau}{Rd}}\right)
+ 2e^{4Pe\xi}\text{erfc}\left(\sqrt{\frac{PeRd}{\tau}}\xi + \sqrt{\frac{Pe\tau}{Rd}}\right)\left(0.25 + Pe\xi + \frac{Pe\tau}{Rd}\right)
+ 2Pe e^{4Pe\xi}\text{erfc}\left(\sqrt{\frac{PeRd}{\tau}}(2 - \xi) + \sqrt{\frac{Pe\tau}{Rd}}\right)
\times \left(2 - \xi + \frac{2\tau}{Rd} + \left(1 + 2Pe(2 - \xi) + 2\frac{Pe\tau}{Rd}\right)\left(2 - \xi + \frac{\tau}{Rd}\right)\right)
- 2\sqrt{\frac{Pe\tau}{\pi Rd}}\exp\left(2Pe\xi - \frac{Pe\tau}{Rd}\right)
\times \left\{\exp\left(-\frac{PeRd\xi^2}{\tau}\right) + 2\left(1 + Pe(2 - \xi) + \frac{Pe\tau}{Rd}\right)\exp\left(-(2 - \xi)^2\frac{PeRd}{\tau}\right)\right\}
\]

Exit solute concentration is calculated by taking \(\xi=1\) as:

\[
C_e = 1 - \frac{1}{2}\text{erfc}\left(\sqrt{\frac{PeRd}{\tau}} - \sqrt{\frac{PeRd}{\tau}}\right)
+ \left(0.5 + 2Pe\left(3 + 4\frac{\tau}{Rd}\right) + \left(2Pe\left(1 + \frac{\tau}{Rd}\right)\right)^2\right)
\times e^{4Pe\xi}\text{erfc}\left(\sqrt{\frac{PeRd}{\tau}} + \sqrt{\frac{Pe\tau}{Rd}}\right)
- 2\sqrt{\frac{Pe\tau}{\pi Rd}}\left(2 + 2Pe\left(1 + \frac{\tau}{Rd}\right)\right)\exp\left(-\frac{Pe}{\tau Rd}(Rd - \tau)^2\right)
\]
Taking $\tau^* = \tau/(\tau + R_d)$ in equation (11), one gets:

$$
C_e = 1 - \frac{1}{2} \text{erfc} \left( \sqrt{\frac{Pe}{\tau R_d}}(R_d - \tau) \right)
+ \left( 0.5 + 2Pe \left( \frac{3}{1 - \tau^*} + \frac{\tau}{R_d} \right) + \frac{4Pe^2}{(1 - \tau^*)^2} \right)
\times e^{4Pe} \text{erfc} \left( \sqrt{\frac{Pe}{\tau R_d}}(R_d + \tau) \right)
- 2\sqrt{\frac{Pe}{\pi R_d}} \left( 3 + \frac{2Pe}{1 - \tau^*} \right) \exp \left( -\frac{Pe}{\tau R_d}(R_d - \tau)^2 \right)
$$

(12)

The asymptotic solution given by equation (12) involves exponential and complementary error functions. However, for $Pe \geq 20$ and $R_d < 1.5$, fluctuations are observed in equation (12) for large time period. To overcome this problem, the following asymptotic expression of complementary error function involving $\sqrt{Pe/\tau R_d}(R_d + \tau)$ has been considered, see e.g. [5]:

$$
\sqrt{\pi z^2} \exp(-z^2) \text{erfc}(z) = 1 + \sum_{m=1}^{\infty} (-1)^m \frac{1 \times 3 \times 5 \times \ldots \times (2m - 1)}{(2z^2)^m}
$$

(13)

The modified asymptotic expression for exit solute concentration can now be written as:

$$
C_e = 1 - \frac{1}{2} \text{erfc} \left( \sqrt{\frac{Pe}{\tau R_d}}(R_d - \tau) \right)
+ \sqrt{\tau^*(1 - \tau^*)} \frac{4\pi Pe}{\tau^*} \exp \left( -\frac{Pe}{\tau R_d}(R_d - \tau)^2 \right) \sum_{j=0}^{\infty} \phi_j(\tau^*)
$$

(14)

where $\phi_j(\tau^*) = (-1)^j \times (1 \times 3 \times 5 \times \ldots \times (2j + 1)) \times \left( \frac{1}{2j+1} - 6\tau^* + 4(j + 1)\tau^*^2 \right) \times \left( \frac{\tau^*(1-\tau^*)}{2Pe} \right)^j$.

4. Results and discussions.

4.1. Limiting cases.

Two types of limiting cases are discussed in the present study. These are also known as ideal cases of the flow pattern. Practically, flow through the packed bed lies between these two ideal limits, i.e., flow pattern is non
ideal.

**Perfect mixing**: $Pe$ is negligible, i.e., $Pe \to 0$. In this case the axial dispersion equation under consideration becomes singular. In this situation an equal volume of fluid is displaced from the bed as each differential element of solvent introduced into the bed instantaneously mixes with the contents of the bed. The dimensionless time becomes indefinitely large, i.e., $\tau \to \infty$, due to abrupt increase in axial dispersion coefficient.

**Perfect displacement**: $Pe$ is indefinitely large, i.e., $Pe \to \infty$ and the dispersion term approaches to zero. In this situation the initial contents of the bed are pushed out in a piston like manner by the displacing liquid as $\tau \to 0$. However, as $Pe$ increases, the effect of $\tau$ starts decreasing and flow term rapidly approaches to steady state condition. As $Pe \to \infty$, the complementary error function approaches to zero, the series on the right hand side of equation (14) being convergent, the effect of large $Pe$ is overcome by small $\tau$. As a result the flow term $C$ (at $\xi = 1$) approaches to steady state condition rapidly for small $\tau$ and $R_d$.

4.2. **Effect of Peclet number.**

With the change in $Pe$, dispersion term containing axial dispersion coefficient changes. Area under breakthrough curves increases with the increase in $Pe$ as dispersion term becomes stiffer as compared to time and space gradients. In Figure 1 the behavior of solution profiles is shown for $Pe$ varying from 0.5 to 15 and in Figure 2 for $Pe$ varying from 20 to 40. It is observed from Figure 1 that solution profiles takes a longer time to converge to steady state condition for $Pe$ varying from 0.5 to 15, whereas in Figure 2 the convergence of solution profiles to steady state condition is faster due to fall in axial dispersion coefficient. It increases the area under curve forcing the solution profiles to follow a Z-shaped curve. It is also observed that for $Pe$ varying from 20 to 40 the difference between solution profiles is comparatively small than Figure 1. In Figure 3 the solution profiles are plotted for $Pe$ varying from 50 to 150. This is the situation in which solution profiles converge to steady state condition for $\tau \leq 1.4$ and the difference between the solution profiles is very small and area under the curve is increases. It signifies the fact that the solute adsorbed on particle surface is removed rapidly because of small axial dispersion coefficient as compared to greater one shown in Figure 1. It also confirms the case of perfect displacement, which shows that with the increase in $Pe$, the time of washing decreases.
Figure 1. Behavior of solution profiles for $R_d=1.1$ and for $Pe$ varying from 1 to 15.

Figure 2. Behavior of solution profiles for $R_d=1.1$ and for $Pe$ varying from 20 to 40.

4.3. Effect of retardation coefficient.

In Figure 4 and Figure 5, effect of $R_d$ is shown on solution profiles for different ranges. It is observed from Figure 4 that for $R_d$ varying from 1.5 to 10, the solution profiles for $Pe=100$ becomes broaden and take a long
Figure 3. Behavior of solution profiles for $R_d=1.1$ and for $Pe$ varying from 50 to 150.

Figure 4. Behavior of solution profiles for $Pe=100$ and for $R_d$ varying from 1.5 to 10.

time to converge to steady state condition. For $R_d=10$ solution profiles converge to steady state condition for $\tau \geq 11$ as compared to $R_d=1.5$ where solution profiles converge to steady state condition for $\tau \leq 1.5$. Similarly in Figure 5, the solution profiles are plotted for $R_d$ varying from 15 to 30. It is observed from this figure that solution profiles follows a $Z$-shaped
curve and converge to steady state condition for $\tau > 15$. This is because of the reason that with the increase in $R_d$, the effect of time and space gradients increases on solution profiles as compared to that of dispersion term. Moreover, with the increase in $R_d$, the detachment rate constant and the bed porosity decreases, which ultimately reduce the removal rate of impurities adsorbed on particle surface. Therefore, more time is consumed by the flow term to converge to steady state condition.

5. Experimental study.

To check the applicability of the model equations, the same have been applied on a lab scale washing cell used for the displacement washing of unbleached, unkraft, softwood pulp fibers. The stimulus-response experiments, using a step input signal, have been carried out in the displacement washing cell consisting of a vertical glass cylinder 110 mm high, 36.4 mm inside diameter, and closed at the lower end by a permeable septum. Both the piston and the septum were made permeable by 64 holes, 1 mm in diameter. In order to prevent fibers of fine losses from bed, both piston and septum were covered with 45 mesh screen. During washing, direct observation of pulp bed was possible. The values of initial solute concentration, bed consistency, cake thickness and interstitial velocity have been calculated on the basis of experiments. These values have been followed to calculate the input parameters such as $Pe$ and $R_d$. Exit solute concentration has been
calculated at different intervals of time and then transformed into dimensionless form by dividing with the initial solute concentration. The values of input parameters are given in detail in [6]. In Table 1, the comparison between values calculated from equation (12) and experimental values is shown for $Pe=20.81$, $R_d=1.00002$. This comparison makes it clear that the values obtained from equation (12) are in good agreement with the experimental values obtained at different time intervals.

<table>
<thead>
<tr>
<th>Equation (12)</th>
<th>Experimental values</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.93575</td>
<td>0.93850</td>
<td>0.29302</td>
</tr>
<tr>
<td>0.81811</td>
<td>0.81690</td>
<td>0.14812</td>
</tr>
<tr>
<td>0.66844</td>
<td>0.67430</td>
<td>0.86905</td>
</tr>
<tr>
<td>0.53772</td>
<td>0.53350</td>
<td>0.79100</td>
</tr>
<tr>
<td>0.45446</td>
<td>0.45600</td>
<td>0.33772</td>
</tr>
<tr>
<td>0.35410</td>
<td>0.35560</td>
<td>0.42182</td>
</tr>
<tr>
<td>0.26905</td>
<td>0.26850</td>
<td>0.20484</td>
</tr>
<tr>
<td>0.18524</td>
<td>0.18490</td>
<td>0.18388</td>
</tr>
<tr>
<td>0.10948</td>
<td>0.10950</td>
<td>0.01827</td>
</tr>
<tr>
<td>0.043496</td>
<td>0.042940</td>
<td>1.29482</td>
</tr>
<tr>
<td>0.0054793</td>
<td>0.0054230</td>
<td>0.13817</td>
</tr>
<tr>
<td>0.0018856</td>
<td>0.0018750</td>
<td>0.56533</td>
</tr>
<tr>
<td>0.00096274</td>
<td>0.00095800</td>
<td>0.51577</td>
</tr>
</tbody>
</table>

6. Conclusions.

Analytic solution of a generalized reaction diffusion model involving $Pe$ and $R_d$ has been proposed using Laplace transforms. It can be concluded from the numerical results that both $Pe$ and $R_d$ effect the concentration profiles to a significant extent by influencing the dispersion term and time gradients. The solution is represented in terms of complementary error function which is quite simple and easy to compute. The verification of the model on a lab scale washing cell validates the applicability of proposed model for displacement washing process of compressible particles. However, the model equations can also be verified for non-compressible particles having high $Pe$ and small $R_d$.

Acknowledgements.

Dr. Shelly is thankful to UGC for providing financial assistance in the form of research grant F. No. 41-786/2012(SR). Authors are thankful to the reviewers for their valuable comments.
REFERENCES


