

Dispersion of a chemically reacting solute in a three – dimensional Newtonian fluid flow through a Darcy - Brinkman porous medium

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Abstract

In this paper, the dispersion of a chemically active solute in a sparsely packed porous medium is studied. The aim of this work is to study the effects permeability of the porous medium and a homogeneous chemical reaction on the dispersion coefficient. A mathematical model is obtained using the Gill – Sankarasubramanian(1970) approach for the three-dimensional flow of a Newtonian liquid. The velocity profile is obtained using Darcy – Brinkmann momentum equation. The effect of the chemical reaction rate parameter on the convection coefficient and dispersion coefficient is discussed. The mean concentration distribution is also computed for various values of the Darcy number and reaction rate parameter and the results are represented graphically. This problem finds its applications in the fields of waste water management, chemical engineering, and biomechanical problems.

Keywords: Dispersion, Newtonian liquid, Chemical reaction, Porous Medium, Darcy number, Brinkman number.

Introduction

The topic of fluid flow in porous medium has drawn the interest of fluid mechanics community for a long time. This due to the availability of porous materials

in most of the useful phenomena such as filtering and storage of water, cogeneration systems etc. Further, Dispersion in porous medium is one of the very useful studies in this respect. Early literature in this field have been found in the works of Taylor (1953) who studied small time dispersion, and Aris (1956) who studied long time dispersion. But a more generalized approach was later proposed by Gill and Sanakarasubramanian (1970). Soundalgekar and Gupta (1977) extended Taylor's approach to electrically conducting walls. Shivakumar et al. (1987) studied dispersion porous channel flows to obtain the closed form solution. Later, Pal (1998) extended the same approach to study the effect of first order chemical reaction on such a flow. Recently, Madie et al, (2022) studied dispersion in porous medium with varying dispersion coefficients.

The above mentioned works have considered two - dimensional flow of fluids. One can note that, an abundant literature is available with respect to three - dimensional flows in this regard too. It was Doshi et al (1978) who initially conducted such a research for studying the effect of the walls on the three - dimensional flow of the Newtonian liquids. Recently, Manjunath and Siddheshwar (2011) considered the couple stress effect on the three - dimensional laminar dispersion in the rectangular channel flows. In the present work, the unsteady dispersion is studied for a fully developed flow of the Newtonian liquid through the rectangular Darcy - Brinkman porous channel, and thereby the effects of the first order homogeneous chemical reaction on the dispersion coefficient and on the mean concentration profile are discussed.

1 Mathematical Formulation of the Problem

Figure 1 shows a physical system consisting of an infinitely sparsely packed porous medium with a cross section of breadth $2b$ and height $2l$. It is assumed that the flow is unidirectional and influenced by the porous matrix. The drag force is neglected. Under these conditions a fully developed flow can be governed by the following momentum equation.

$$\mu' \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) - \frac{\mu}{k} w = \frac{dp}{dz} \quad (1.1)$$

The equation (1.1) is called the Darcy - Brinkmann momentum equation. In this equation, ρ is the density of the fluid, w represents the filter velocity, μ is dynamic viscosity, μ' is the effective viscosity, k is the permeability of the porous medium.

The no - slip boundary condition to solve the equation (1.1) is as follows:

$$w = 0 \quad \text{at} \quad x = \pm b \quad \text{and} \quad w = 0 \quad \text{at} \quad y = \pm h \quad (1.2)$$

In the equation (1.2), we have assumed the no-slip boundary condition at both horizontal and vertical walls. In order to obtain the dimensionless form of the equation (1.1), we apply the following definitions:

$$X = \frac{x}{b}, Y = \frac{y}{h}, W = \frac{w}{w^* \left(-\frac{dp}{dz} \right)}, P = \frac{p}{p^*}, Z = \frac{z}{hPe} \quad (1.3)$$

where w^* and p^* are some reference velocity and reference pressure respectively, $Pe = (w^*h)/D$ and D is the solutal diffusivity. Using (1.3), the equation (1.1) takes the form:

$$\frac{1}{\alpha^2} \frac{\partial^2 W}{\partial X^2} + \frac{\partial^2 W}{\partial Y^2} - AW = -\Lambda \tag{1.4}$$

where $a = \frac{b}{h}$ is the aspect ratio, $Da = \frac{h}{\sqrt{K}}$, $Re = \frac{\rho u h}{\mu} (-\frac{dp}{dz})$, $A = \Lambda Da^2$, $\Lambda = \frac{\mu}{\mu'}$. Here, Λ is the Brinkman number, Da is the Darcy number and Re is the Reynolds number.

The equation (1.2) in non - dimensional form is given by

$$\begin{aligned} W = 0 \quad \text{at} \quad X = \pm 1, \quad -1 < Y < 1 \\ W = 0 \quad \text{at} \quad Y = \pm 1, \quad -1 < X < 1 \end{aligned} \tag{1.5}$$

Due to the symmetry of W about X and Y , the equation (1.5) can be replaced by:

$$\begin{aligned} W(X, 1) = 0, \quad 0 \leq X \leq 1 \\ W(1, Y) = 0, \quad 0 \leq Y \leq 1 \end{aligned} \tag{1.6}$$

$$\frac{\partial W}{\partial Y}(X, 0) = 0 \tag{1.7}$$

$$\frac{\partial W}{\partial X}(0, Y) = 0 \tag{1.8}$$

We also consider centre-line distribution along the X and Y directions as:

$$W(X, 0) = \eta(1 - X^2), \quad W(0, Y) = \eta(1 - Y^2) \tag{1.9}$$

where η to be determined later. Let us assume the Maclaurin series solution of the equation (1.4) in the following form:

$$W(X, Y) = \sum_{k=0}^{\infty} \sum_{h=0}^{\infty} S(k, h) X^k Y^h \tag{1.10}$$

On using the equation (1.10) in the equation (1.4) we get,

$$\begin{aligned} \frac{1}{\eta^2} (k+1)(k+2)S(k+2, h) + (h+1)(h+2)S(k, h+2) - A.S(k, h) \\ = -\Lambda \delta(k-0, h-0) \end{aligned} \tag{1.11}$$

along with certain specific coefficients as follows:

$$S(k, 1) = 0, \quad S(1, h) = 0 \tag{1.12}$$

A four - term solution of this equation is given by

$$W(X, Y) = \eta - \eta X^2 - \eta Y^2 - BX^2 Y^2 \tag{1.13}$$

where

$$B = \frac{a^2}{2} [A\eta + \Lambda]$$

For a fully developed flow which satisfies the above equation, an initial concentration is introduced to the source at $z = 0$ and assuming the solute undergoes first order homogeneous chemical reaction, the corresponding mass - balance equation is given by

$$\frac{\partial C}{\partial t} + w \frac{\partial c}{\partial z} = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right) - R_1 C \quad (1.14)$$

where D is the solutal diffusion coefficient and R_1 is the reaction rate constant.

To solve the equation (1.15), we use the following initial and boundary conditions:

$$C(x, y, z, 0) = \phi(x, y) \cdot \delta(z) \quad (1.15)$$

$$\left(\frac{\partial C}{\partial x} \right)_{x=0, b} = 0 \quad (1.16)$$

$$\left(\frac{\partial C}{\partial y} \right)_{y=0, h} = 0 \quad (1.17)$$

$$\lim_{z \rightarrow \infty} C = \lim_{z \rightarrow \infty} \left(\frac{\partial C}{\partial z} \right) = 0 \quad (1.18)$$

In the equation (1.16), $\delta(z)$ is the Dirac delta function. The strength of the initial slug input is given by the following equation.

$$\phi(x, y) = \begin{cases} C_0, & \text{for } \frac{-y_s}{2} \leq y \leq \frac{y_s}{2}, \frac{-x_s}{2} \leq x \leq \frac{x_s}{2}. \\ 0, & \text{otherwise.} \end{cases} \quad (1.19)$$

2 The Solute Dispersion Model

A dispersion model for the concentration involving the cross - sectional variations in terms the derivatives of concentraion was proposed by Taylor (1953). Aris (1956), then introduced the model in which the dispersion is asymptotically valid for small values of time. But, at large times after the release of the slug input, we have $C - C_m$ directly proportional to $\left(\frac{\partial C_m}{\partial z} \right)$. From such a postulate, Gill - Sankarasubramanian (1970) proposed a generalised dispersion model given by $C - C_m = \sum_{n=1}^{\infty} f_n(x, y, t) \frac{\partial^n C_m}{\partial z^n}$. Hence, let us assume the dispersion model to be

$$C(x, y, z, t) = C_m f_0(x, y, t) + \sum_{n=1}^{\infty} f_n(x, y, t) \frac{\partial^n C_m}{\partial z^n} \quad (2.1)$$

where

$$C_m = \frac{1}{bh} \int_0^h \int_0^b C dx dy \quad (2.2)$$

Equation (2.2) represents the mean concentration.

Integrating the equation (1.14) with respect to x and y as required by the equation (2.2) and applying the boundary conditions (1.16) and (1.17), we get

$$\frac{\partial C_m}{\partial t} + \frac{1}{bh} \frac{\partial}{\partial z} \int_0^h \int_0^b w C dx dy = D \frac{\partial^2 C_m}{\partial z^2} - R_1 C_m. \quad (2.3)$$

By using the equation (2.1) in the equation (2.3) we get,

$$\frac{\partial C_m}{\partial t} = K_1(t) \frac{\partial C_m}{\partial z} + K_2(t) \frac{\partial^2 C_m}{\partial z^2} + K_3(t) \frac{\partial^3 C_m}{\partial z^3} + \dots - R_1 C_m \quad (2.4)$$

where

$$K_n(t) = -\frac{1}{bh} \int_0^h \int_0^b w f_{n-1} dx dy + \delta_{n2} D \quad (2.5)$$

and δ_{n2} is Kronecker delta.

By substituting the equation (2.1) in the equation (1.14) and by equating the coefficients of each of $(\frac{\partial^n z}{\partial z^n})$ terms to zero and by simplifying we get the following equations for f_n

$$\frac{\partial f_0}{\partial t} = D \nabla^2 f_0 - R_1 f_0 \quad (2.6)$$

$$\frac{\partial f_1}{\partial t} = D \nabla^2 f_1 - (w + K_1) f_0 - R_1 f_1 \quad (2.7)$$

$$\frac{\partial f_n}{\partial t} = D \nabla^2 f_n - w f_{n-1} + D f_{n-2} - \sum_{i=1}^{\infty} K_i f_{n-i} - R_1 f_n \quad (2.8)$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$.

On solving the equation (2.4) with suitable boundary conditions and expressing it in its dimensionless form we get,

$$f_0 = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} A_{mn} \cos(m\pi Y) \cos(n\pi X) \exp[-(m^2 + \frac{n^2}{a^2})\pi^2 \tau] \exp[-\alpha^2 \tau] \quad (2.9)$$

where $\tau = \frac{tD}{h^2}$, $w^* = \frac{\mu P e}{h\rho}$, $\alpha^2 = \frac{h^2 R_1}{D}$ and A_{mn} are given by

$$A_{mn} = \frac{16}{\pi^2 mn Y_s X_s} \sin(\frac{\pi m Y_s}{2}) \sin(\frac{\pi n X_s}{2}). \quad (2.10)$$

Similarly on solving the equation (2.5) we get its solution in dimensionless form as follows:

$$f_1(X, Y, \tau) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} B'_{mn} \cos(m\pi Y) \cos(n\pi X) [1 - \exp[-(m^2 + \frac{n^2}{a^2})\pi^2 \tau - \alpha^2 \tau]] \quad (2.11)$$

Here, B'_{mn} are given by the following equation:

$$B'_{mn} = \frac{(-1)^{m+n} a^2}{(a^2 m^2 + n^4)} \left[\frac{16 a^2}{n^2 m^2 \pi^6} (\Lambda D a^2 \eta + 2 F \eta^2 + \Lambda), \forall m, n \in N. \quad (2.12) \right]$$

Now, by putting $n = 1$ in the equation (2.5) and non dimensionalizing it with suitable dimensionless ratios we get

$$K_1(\tau) = \int_0^1 \int_0^1 W f_0(X, Y, \tau) dX dY \tag{2.13}$$

where $K_1(\tau) = -\frac{K_1(t)}{w^*}$.

Now using the equations (1.13) and (2.9) in the equation (2.13) we obtain the expression for the dimensionless convection coefficient as follows:

$$K_1(\tau) = \frac{2a^2}{m^2 n^2 \pi^2} [\Lambda(Da)^2 \eta + \Lambda] \times \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} A_{mn} \cos(m\pi) \cos(n\pi) \exp[-(m^2 + \frac{n^2}{a^2})\pi^2 - \alpha^2] \tau. \tag{2.14}$$

Similarly by putting $n = 2$ in the equation (2.5) and simplifying it to express in its dimensionless form we obtain the following equation:

$$K_2(\tau) = - \int_0^1 \int_0^1 W f_1(X, Y, \tau) dX dY + \frac{1}{Pe^2}, \tag{2.15}$$

where

$$K_2(\tau) = -\frac{K_2(t)}{w^* . h . Pe}$$

On using the equation (2.11) in the equation (2.15) and simplifying, we get

$$K_2(\tau) = \frac{4B}{\pi^4} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{B'_{mn}}{m^2 n^2} \cos(m\pi) \cos(n\pi) [1 - \exp[-(m^2 + \frac{n^2}{a^2})\pi^2 \tau - \alpha^2 \tau]] + \frac{1}{Pe^2} \tag{2.16}$$

where B'_{mn} 's are given by the equation (2.12).

To find the mean concentration

We observe that $K_3, K_4...$ have numerically too small magnitude to be neglected. Hence the truncated form of the equation (2.4) is given by:

$$\frac{\partial C_m}{\partial t} = K_1(t) \frac{\partial C_m}{\partial z} + K_2(t) \frac{\partial^2 C_m}{\partial z^2} - R_1 C_m \tag{2.17}$$

Equation (2.17) can be further reduced to get the unsteady diffusion equation by using the following transformations.

$$z_1 = z + t \overline{K_1(t)}, \tag{2.18}$$

$$t_1 = \frac{t \overline{K_2(t)}}{D}, \tag{2.19}$$

where

$$\overline{K_i(t)} = \frac{1}{t} \int_0^t K_i(\gamma) d\gamma \quad (i = 1, 2, 3, \dots) \quad (2.20)$$

By solving the equation (2.17) using the method of infinite Fourier transforms and by applying the suitable initial and boundary conditions we obtained the solution in its simplified, dimensionless form as follows:

$$\theta_m = \frac{e^{-\alpha^2 \tau}}{\sqrt{4\pi\tau K_2(\tau)}} \exp\left[-\frac{(Z + \tau \overline{K_1(\tau)})^2}{4\tau \overline{K_2(\tau)}}\right] \quad (2.21)$$

3 Results and Discussions

In the present research, we have studied the three – dimensional unsteady convective diffusion of a solute that undergoes a first - order homogeneous chemical reaction in a porous medium using the generalized miscible theory of dispersion of Gill – Sankarasubramanian (1970) and Doshi et al. (1978).

From the figure 2, we note that the filter velocity is symmetric about the two axes of X and Y. To see the symmetry more clearly, we have plotted the figures 3 and 4. From this, it is evident that the velocity does have symmetry about y axis. Similarly, one can see its symmetry about the x axis. We also observe that as there is an increase in Brinkman number there is an increase in the velocity. This is due to the increase in the viscous dissipation causing the rise in the temperature. However, increase in the Darcy number is creating a quite opposite effect. This is due to an increase in the permeability of porous medium.

Figures 5 - 7 shows that the dimensionless convection coefficient grows exponentially with the value of the aspect ratio a . We have taken three different values of the Darcy number, $Da = 3, 4, 5...$ in the figure. As there is a decrease in the value of Da , there is an increase in the value of $K_1(\tau)$. Similarly, we note that the value of $K_1(\tau)$ increases in the same fashion with the increase in the value of a for the chemical reaction rate, $\alpha = 0.4, 0.8, 1.2$. The increase of $K_1(\tau)$ with a is steep for large values of both α and Da . This shows that the chemical reaction reduces the convection coefficient. This result holds true for a uniform source and when the reaction at the sidewalls is ignored.

Figures 8 and 9 shows that the dispersion coefficient increases with increase in dimensionless time for small values of time and levels off later. On this occasion too, we observe that the Darcy number and Brinkman number are creating opposite effects on the dispersion. we also observed from calculations that the difference in chemical reaction rate does not make a huge difference in the values of the dispersion coefficient.

Figure 10 clearly indicates that the increase in the chemical reaction causes the increase in the dispersion and hence resulting in the decrease in the mean concentration. Figure 11 shows that the differences in Darcy number causes no huge difference in attaining the peak of the mean concentration. Figure 12, obviously indicate the same effect as in figure 10, but the value of the

concentration is more as the point close to the axis. Figures 13 and 14 shows the Gaussian nature of the mean concentration against the axial distance which clearly indicates that the concentration distribution on either sides of the axis is similar. Apart from that, the effects of other parameters remains the same.

Figures

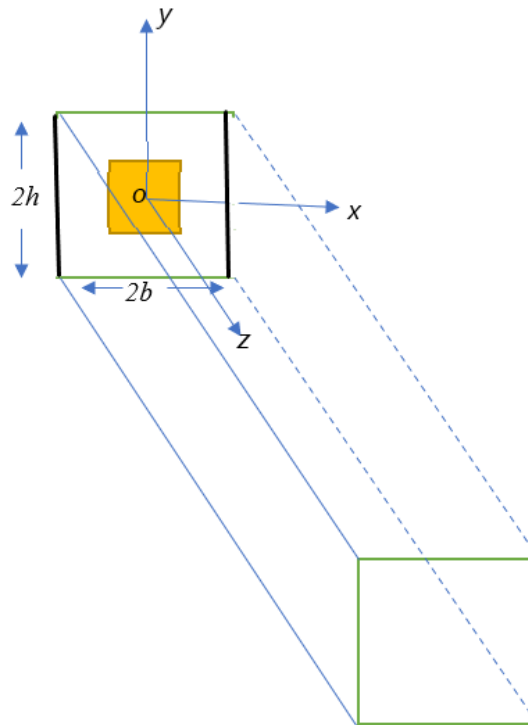


Figure 1: Representation of the rectangular duct and the slug input

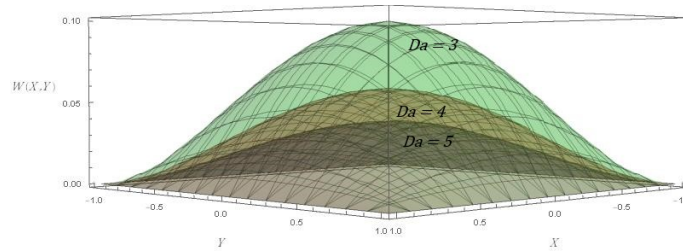


Figure 2: Three - Dimensional plots of the filter velocity distribution, $W(X, Y)$ for various values of the Darcy number Da , with the Brinkmann number $\Lambda = 2$, and the Aspect ratio $a = 1$.

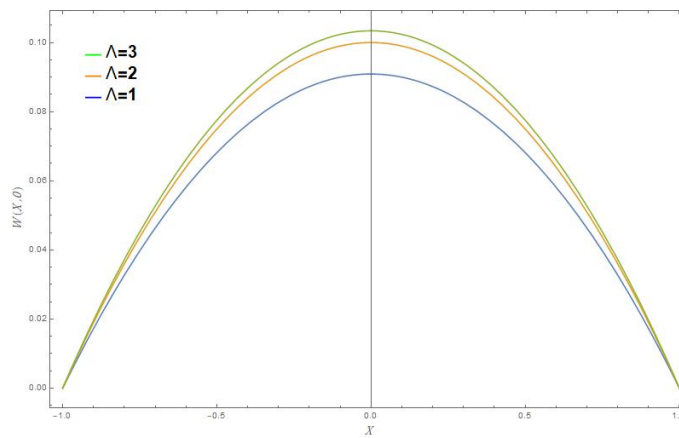


Figure 3: Plots of the mid-plane filter velocity, $W(X, 0)$, for various values of Λ with $Da = 3, a = 1$.

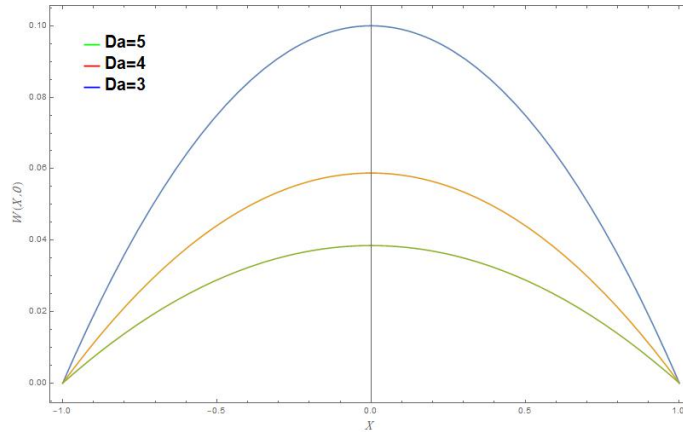


Figure 4: Plots of the dimensionless convection coefficient, $K_1(\tau)$ vs a , for various values of Da with $\Lambda = 2, a = 1$. and the chemical reaction rate parameter, $\alpha = 0.8$.

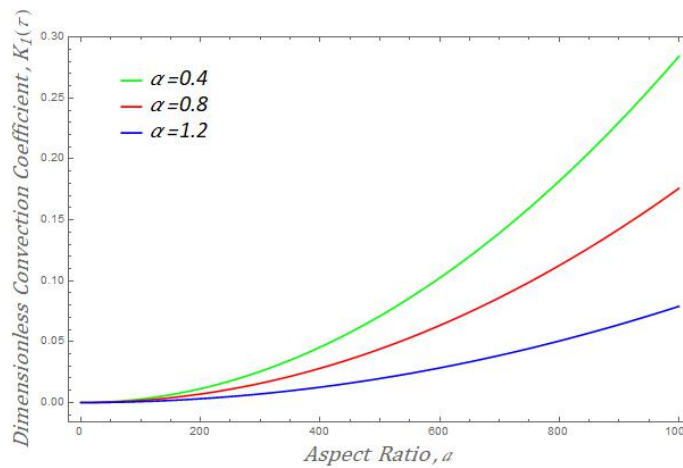


Figure 5: Plots of $K_1(\tau)$ vs a , for various values of α with $\Lambda = 2, a = 1$ and $Da = 3$

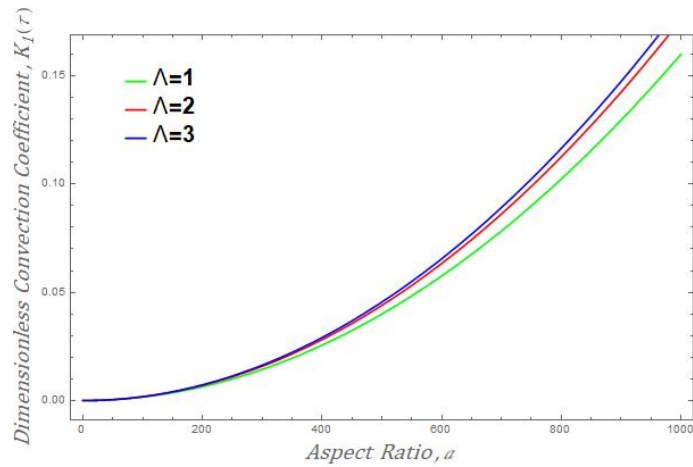


Figure 6: Plots of $K_1(\tau)$ vs a , for various values of λ with $\alpha = 0.8, a = 1$ and $Da = 3$.

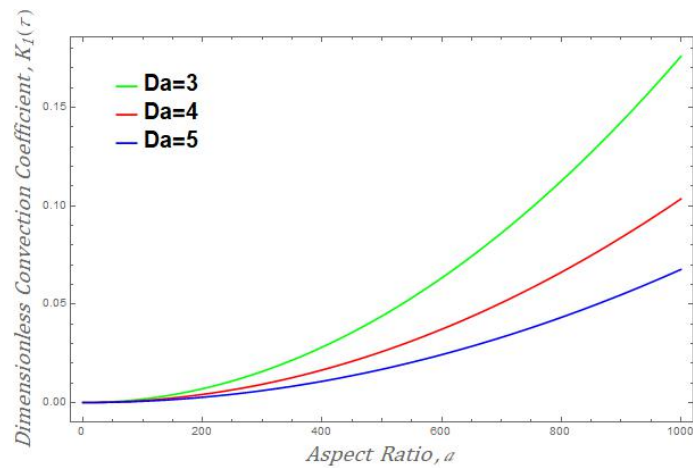


Figure 7: Plots of $K_1(\tau)$ vs a , for various values of Da with $\Lambda = 2, a = 1$ and $\alpha = 0.8$

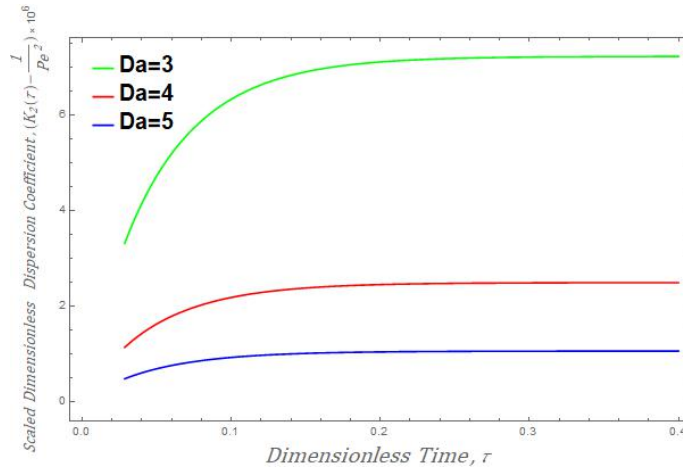


Figure 8: Plots of the scaled dispersion coefficient, $(K_2(\tau) - \frac{1}{Pe^2}) \times 10^6$, vs the dimensionless time, τ , for various values of Da with $\alpha = 0.8$, $\Lambda = 2$, $a = 1$.

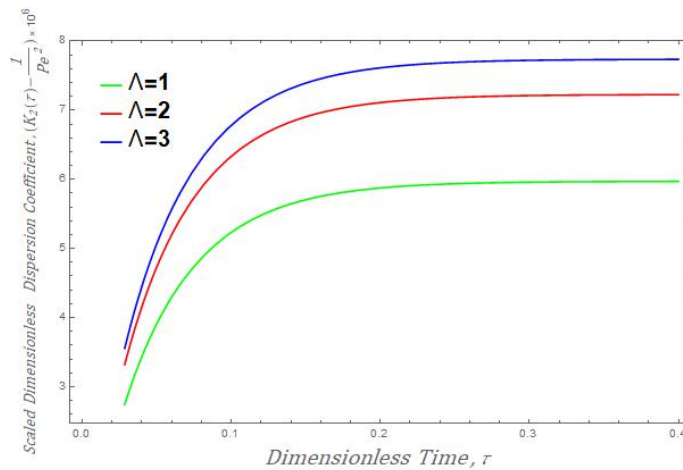


Figure 9: Plots of $(K_2(\tau) - \frac{1}{Pe^2}) \times 10^6$, vs τ for various values of Λ , $Da = 3$, $a = 1$ and $\alpha = 0.8$.

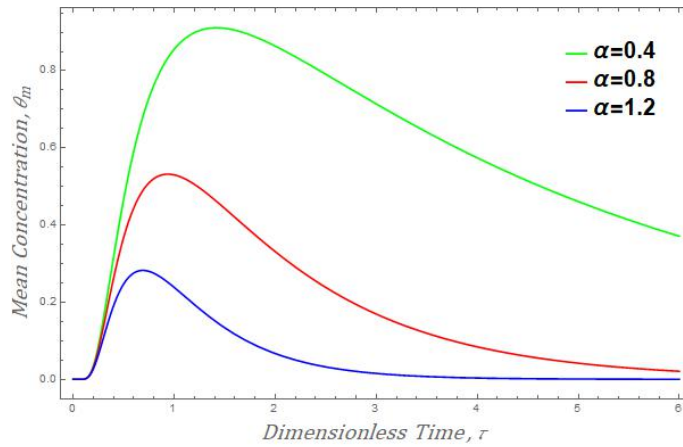


Figure 10: Plots of mean concentration θ_m vs τ at axial distance $Z = 0.2$ for various values of α with $\Lambda = 2, F = 2, a = 1$ and $Da = 3$

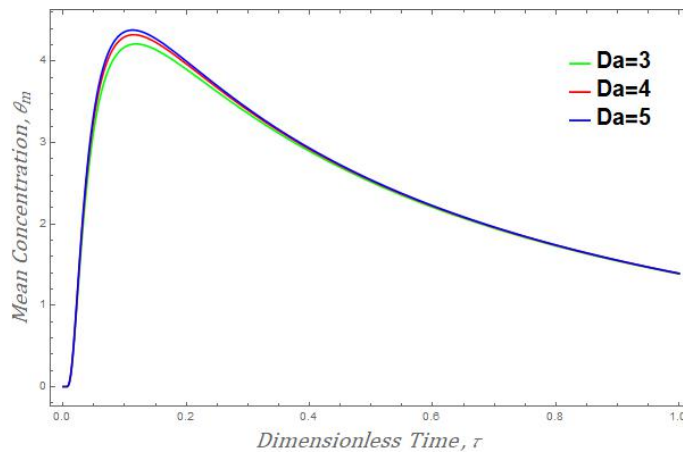


Figure 11: Plots of θ_m vs τ at $Z = 0.05$ for various values of Da with $\Lambda = 2, a = 1$ and $\alpha = 0.8$.

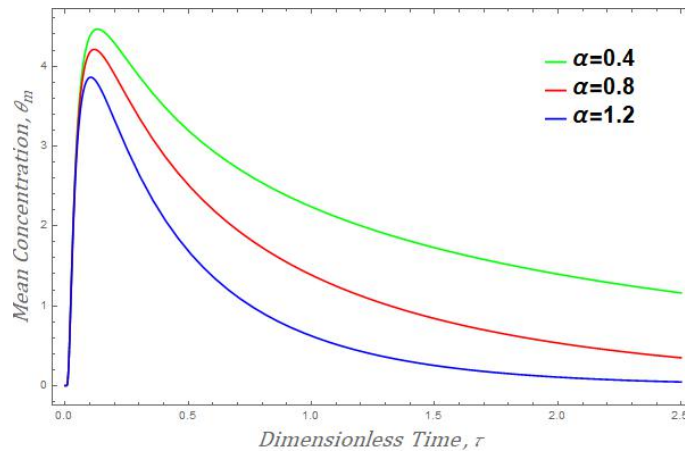


Figure 12: Plots of θ_m vs τ at $Z = 0.05$ for various values of α with $\Lambda = 2, a = 1$ and $Da = 3$.

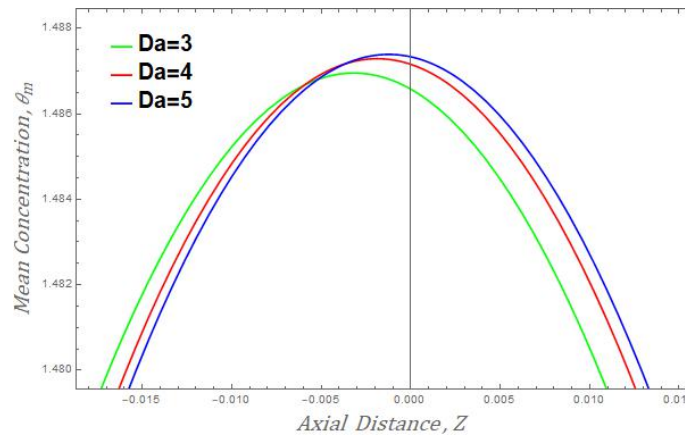


Figure 13: Plots of θ_m vs Z , for various values of Da with $\Lambda = 2, \tau = 1, a = 1$ and $\alpha = 0.8$

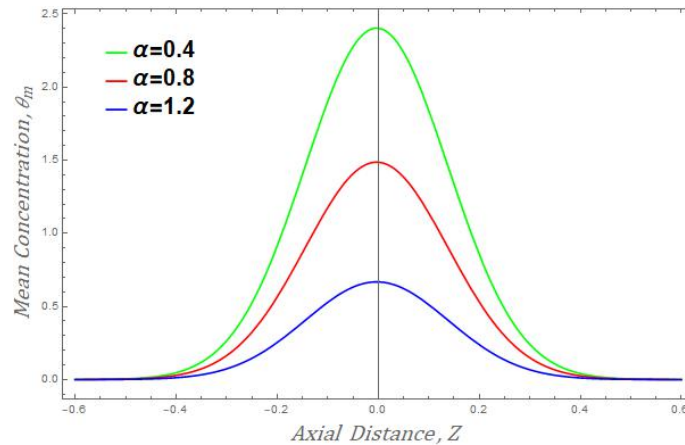


Figure 14: Plots of θ_m vs Z , for various values of α with $\Lambda = 2$, $\tau = 1a = 1$ and $Da = 3$

Nomenclature

$w(x, y)$ - Axial Filter Velocity

μ - Dynamic Viscosity

μ' - Effective Viscosity

\bar{w} - Average Fluid Velocity

$\Lambda = \frac{\mu}{\mu'^2}$ - Brinkman number

$Da = \frac{h}{\sqrt{K}}$ - Darcy number

Re - Reynolds number

W - Dimensionless filter velocity

Z - Dimensionless axial distance

τ - Dimensionless time

$\phi(x, y)$ - Strength and location of slug input

C - Local concentration

C_m - Mean Concentration

θ_m - Dimensionless mean concentration

a - Aspect Ratio

α - Chemical reaction rate coefficient

Pe - Peclet number

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