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Dispersion of Contaminants in Groundwater with Chemical Reaction

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Abstract. A mathematical model presented in this paper describes the dispersion and concentration of contaminants (fine and coarse) in porous medium with the effect of chemical reaction. Solute transport in porous media is discussed by means of advection-dispersion equation. The effect of particle mass parameter and reaction rate parameter on the dispersion coefficient and mean concentration of a chemical solute is studied by introducing a slug of finite length. Analytical solutions are obtained by varying the dimensionless time, axial distance and length of the solute. The results are depicted using graphs.

Index to information contained in this paper

1. Introduction

Contamination of groundwater is an issue of major concern in residential areas which may occur as a result of landfills, spillages of hazardous chemicals, dumping of toxic wastes, waste water or industrial discharges[7]. Groundwater quality varies due to the chemical, geochemical and biochemical reactions of the pollutants in the subsurface flow systems[3]. Concern about contamination of the subsurface environment has greatly stimulated research of solute transport phenomena in porous

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media[8]. Large number of cases of groundwater pollution at landfills and the substantial resources spent in remediation suggest that landfill leachate is a significant source of groundwater pollution.Landfills are supposed to have a protective bottom layer to prevent contaminants from getting into the water. However, if there is no layer, or it is cracked, contaminants from the landfill can make their way down into the groundwater.

The transport of landfill leachate in soil is subject to various physical, chemical and biological processes that affect the eventual concentration of pollutants in soil and groundwater. Contamination transport is generally described with the advection-dispersion equation (ADE) which is derived from mass balance principles. Leakage of inorganic and organic pollutants from landfills over time can influence the groundwater quality and cause serious threat to drinking water resources. Leachate is described as a water based solution of compounds from the waste. Landfill leachate is generated by excess rainwater percolating through the waste layers[6].

The literature on solute transport in porous medium is voluminous. Abriola and Pinder[1] developed a general model that addressed the multiphase flow problem and the transport of organic species. Notodarmojo et al.[12] presented a numerical model for phosphorous transport in soils and groundwater with two consecutive reactions. Li et al.[9] developed a numerical model to simulate contaminant transport through soils taking into account the influence of mechanisms of the miscible contaminant transport including advection, mechanical dispersion , molecular diffusion and adsorption.

Shivakumar et al.[16] have obtained a closed form of solution for unsteady convection diffusion in a fluid-saturated of sparsely packed porous medium. Chen and Liu[4] derived analytical solutions for one-dimensional advective- dispersive transport in finite spatial domain with three simple time dependent inlet conditions including constant, exponentially decaying and sinusoidally periodic input function and demonstrate th applicability of solution. Valsamy and Nirmala P.Ratchagar[17] developed a mathematical model to study the unsteady transport of bacteria and virus in groundwater. The generalized dispersion theory developed can be extended to consider the dispersion phenomena for a wide variety of flows which are too complex to solve analytically [10,11,13,14].

The objective of the present paper is to study the unsteady dispersion of a solute with chemical reaction following the generalized dispersion model of Gill and Sankarasubramanian[6]. They showed that an exact solution of the unsteady convection diffusion equation valid for all time can be developed by using the series expansion originally proposed by Gill[5]. The fluid is assumed to be viscous, incompressible and contaminated (fine and coarse).

2. Mathematical Formulation

The continuity and momentum equation of the motion of unsteady, viscous, incompressible fluid with uniform distribution of contaminated particles are given by :
   For fluid phase ,

$$\nabla.\vec{u} = 0 \tag{1}$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}.\nabla)\vec{u} = -\frac{\nabla p}{\rho} + \nu\nabla^2\vec{u} + \frac{RN}{\rho}(\vec{v} - \vec{u}) - \frac{\nu}{k}\vec{u} \tag{2}$$

For contaminated phase ,

$$\nabla.\vec{v} = 0 \tag{3}$$

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v}.\nabla)\vec{v} = \frac{R}{m}(\vec{u} - \vec{v}) \tag{4}$$

where,

u = velocity of the fluid phase (LT^{-1}),
v = velocity of the contaminated phase (LT^{-1}),
ρ = density of the fluid (ML^{-3}),
p = pressure of the fluid $(ML^{-1}T^{-2})$,
N = number density of contaminated particle (M^{-3}),
ν = kinematic viscosity (L^2T^{-1}),
$R = 6\pi a\mu$ = stoke's resistance (drag coefficient), dimensionless,
a = spherical radius of the contaminated particle (L^2),
m = mass of the contaminated particle (M),
μ = coefficient of viscosity of fluid particle $(ML^{-1}T^{-1})$,
k = permeability of porous medium (L^2),
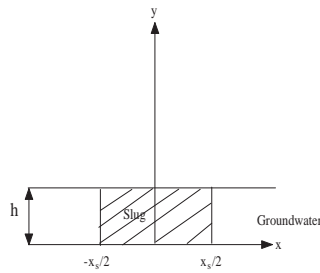t = time (T).

Figure 1. **Physical Configuration**

In the present case, we have assumed that the flow is unidirectional and parallel to layers due to constant pressure gradient in that direction.

Hence the momentum equation for fluid phase and contaminated phase in equations (2) and (3) take the form

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\frac{\partial^2 u}{\partial y^2} + \frac{RN}{\rho}(v - u) - \frac{\nu}{k}u \tag{5}$$

$$\frac{\partial v}{\partial t} = \frac{K}{m}(u - v) \tag{6}$$

Equations (5) and (6) are solved subject to the following initial and boundary conditions;

Initial condition : $u=0$, $v=0$ at $t=0$
Boundary condition: $u=0$ at $y = 0$ and $y = h$ for $t > 0$

We make these equations dimensionless using

$$u^* = \frac{uL}{\nu}; \quad v^* = \frac{vL}{\nu}; \quad t^* = \frac{t\nu^2}{L}; \quad x^* = \frac{x}{L}; \quad y^* = \frac{y}{L}; \quad p^* = \frac{p}{\rho\nu^2} \tag{7}$$

The asterisks(∗) denote the dimensionless quantities.
Substituting equation (7) into equation (5) and (6) and for simplicity neglecting the asterisks we get,

$$\frac{\partial u}{\partial t} = -\frac{\partial p}{\partial x} + \frac{\partial^2 u}{\partial y^2} + S(v - u) - Xu \tag{8}$$

$$\frac{\partial v}{\partial t} = \frac{1}{G}(u - v) \tag{9}$$

where,

$$S = \frac{RNL^2}{\nu\rho}; \quad X = \frac{\rho L^2}{k}; \quad G = \frac{m\nu}{RL^2}; - \text{ particle mass parameter}$$

Since the applied pressure gradient is constant for $t>0$, then

$$-\frac{\partial p}{\partial x} = c_0 \tag{10}$$

Hence the equation (8) and (9) becomes

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial y^2} + S(v - u) - Xu + c_0 \tag{11}$$

$$\frac{\partial v}{\partial t} = \frac{1}{G}(u - v) \tag{12}$$

The initial and boundary condition becomes,
    $u=0$, $v=0$ at $t=0$
    $u=0$ at $y = 0$ and $y = 1$ for $t >0$

3. Method of Solution

The Laplace transformations on U and V are defined as
        $U = \int_0^\infty e^{-st} u \, dt$ and $V = \int_0^\infty e^{-st} v \, dt$
    Applying the above Laplace transformations in equations (11) and (12) and using the initial and boundary conditions, we get

$$sU = \frac{\partial^2 u}{\partial y^2} + S(V - U) - XU + \frac{c_0}{s} \tag{13}$$

$$V = \frac{U}{1 + Gs} \tag{14}$$

Eliminating V from (13) and (14) we get the following equation

$$\frac{\partial^2 U}{\partial y^2} - \frac{(Gs^2 + (SG + XG + 1)s + X)U}{1 + GS} = -\frac{c_0}{s}$$

$$\frac{\partial^2 u}{\partial y^2} - Q^2 U = -\frac{c_0}{s} \tag{15}$$

where, $Q^2 = \frac{(Gs^2 + (SG + XG + 1)s + X)}{1 + GS}$

The velocities of fluid and contaminated particle (fine and coarse) are obtained by solving the equation (15), with the boundary conditions

$$U = 0 \quad at \quad y = 0 \tag{16}$$
$$U = 0 \quad at \quad y = 1$$

follows,

$$U = \frac{c_0}{Q^2 s}[\frac{SinhQ(y-1) - SinhQy}{SinhQ} + 1] \tag{17}$$

$$V = \frac{c_0}{Q^2 s(1 + Gs)}[\frac{SinhQ(y-1) - SinhQy}{SinhQ} + 1] \tag{18}$$

By taking inverse Laplace transforms of equations (17) and (18) and using Cauchy's Residue Theorem and Jordan's Lemma,we get

$u = \frac{1}{2\pi i} \int_{r-iw}^{r+iw} e^{st} U dt = $ sum of the residues of $e^{st}U$ at its poles

$v = \frac{1}{2\pi i} \int_{r-iw}^{r+iw} e^{st} V dt = $ sum of the residues of $e^{st}V$ at its poles Residue of u

(at $s = 0$) $= \frac{c_0}{X} \left[\frac{\sinh[\sqrt{X}(y-1)] - \sinh[\sqrt{X}y]}{\sinh[\sqrt{X}]} + 1 \right]$

Residue of u (at $s = y_1$) $= 0$

Residue of u (at $s = y_2$) $= 0$

Residue of u (at $s = x_1$) $= \frac{4c_0}{\Pi} \sum\limits_{n=1}^{\infty} \frac{1}{2n+1} \sin(2n + 1)\Pi y \frac{(1 + Gx_1)^2 e^{x_1 t}}{x_1(1 + Gx_1)^2 + SG}$

Residue of u (at $s = x_2$) $= \frac{4c_0}{\Pi} \sum\limits_{n=1}^{\infty} \frac{1}{2n+1} \sin(2n + 1)\Pi y \frac{(1 + Gx_1)^2 e^{x_1 t}}{x_1(1 + Gx_1)^2 + SG}$

$u = $ sum of the residues of $e^{st}U$ at its poles

$$u = \frac{c_0}{X} \left[\frac{\sinh[\sqrt{X}(y-1)] - \sinh[\sqrt{X}y]}{\sinh[\sqrt{X}]} + 1 \right]$$
$$+ \frac{4c_0}{\Pi} \sum_{n=1}^{\infty} \frac{1}{2n+1} \sin(2n + 1)\Pi y \frac{(1 + Gx_1)^2 e^{x_1 t}}{x_1(1 + Gx_1)^2 + SG} + \frac{(1 + Gx_2)^2 e^{x_2 t}}{x_2(1 + Gx_2)^2 + SG} \tag{19}$$

Similarly, $v =$ Sum of the residues of $e^{st}V$ at its poles

$$v = \frac{c_0}{X}\left[\frac{\sinh[\sqrt{X}(y-1)] - \sinh[\sqrt{X}y]}{\sinh[\sqrt{X}]} + 1\right]$$

$$+ \frac{4c_0}{\Pi}\sum_{n=1}^{\infty}\frac{1}{2n+1}\sin(2n+1)\Pi y \frac{(1+Gx_1)e^{x_1t}}{x_1(1+Gx_1)^2 + SG} + \frac{(1+Gx_2)e^{x_2t}}{x_2(1+Gx_2)^2 + SG} \tag{20}$$

where, $y_1 = -\frac{1}{2G}(xG + SG + 1) + \frac{1}{2G}\sqrt{(xG + SG + 1)^2 - 4Gx}$

$y_2 = -\frac{1}{2G}(xG + SG + 1) - \frac{1}{2G}\sqrt{(xG + SG + 1)^2 - 4Gx}$

$x_1 = -\frac{1}{2G}(xG + SG + Gn^2\pi^2 + 1) + \frac{1}{2G}\sqrt{(xG + SG + Gn^2\pi^2 + 1)^2 - 4G(n^2\pi^2 + x)}$

$x_2 = -\frac{1}{2G}(xG + SG + Gn^2\pi^2 + 1) - \frac{1}{2G}\sqrt{(xG + SG + Gn^2\pi^2 + 1)^2 - 4G(n^2\pi^2 + x)}$

The average velocity, is given by

$$\bar{u} = \int_0^1 u\,dy = \frac{c_0}{X\sin h\sqrt{X}}\left[\frac{2 - 2\cos h\sqrt{X} + \sqrt{X}\sin h\sqrt{X}}{\sqrt{X}}\right]$$

$$+ \frac{8c_0}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{(2n+1)^2}\left[\frac{(1+Gx_1)^2 e_1^x t}{x_1(1+Gx_1)^2 + SG} + \frac{(1+Gx_1)^2 e_1^x t}{x_1(1+Gx_1)^2 + SG}\right]$$

4.   Generalized Dispersion

The concentration of contaminants in the groundwater which diffuse in a fully developed flow, is given by

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) - \alpha c \tag{21}$$

The initial and boundary conditions for equation (21) are

$$(i)\ \ C(0, x, y) = \begin{cases} C_0, |x| \leqslant \dfrac{x_s}{2} \\ 0, |x| > \dfrac{x_s}{2} \end{cases}$$

$$(ii)\ \ \frac{\partial C}{\partial y}(t, x, 0) = \frac{\partial C}{\partial y}(t, x, h) = 0$$

$$(iii)\ \ C(t, \infty, y) = \frac{\partial C}{\partial x}(t, \infty, y) = 0 \tag{22}$$

where, α is the reaction rate parameter, D is the mass diffusivity, C_0 is the initial concentration, x_s is the solute slug length.

Introducing non-dimensional variables,

$$\theta = \frac{C}{C_0}; \quad X = \frac{Dx}{h^2\bar{u}}; \quad X_s = \frac{Dx_s}{h^2\bar{u}}; \quad Y = \frac{y}{h}; \quad \tau = \frac{Dt}{h^2}; \quad u_f^* = \frac{u_f}{\bar{u}_f}; \quad Pe = \frac{h\bar{u}}{D};$$

the equation (21) becomes,

$$\frac{\partial\theta}{\partial\tau} + u^*\frac{\partial\theta}{\partial X_1} = \frac{1}{Pe^2}\frac{\partial^2\theta}{\partial X_1^2} + \frac{\partial^2\theta}{\partial Y^2} - K\theta \tag{23}$$

where, $K = \dfrac{\alpha h^2}{D}$ is the Damkohler parameter.

Axial coordinate moving with the average velocity of flow is defined as
$x_1 = x - \bar{u}t$ which in dimensionless form is given by
$X_1 = X - \tau$ where, $X_1 = \dfrac{Dx_1}{h^2\bar{u}_f}$
Then equation(23) becomes,

$$\frac{\partial\theta}{\partial\tau} + U\frac{\partial\theta}{\partial X_1} = \frac{1}{Pe^2}\frac{\partial^2\theta}{\partial X_1^2} + \frac{\partial^2\theta}{\partial Y^2} - K\theta \tag{24}$$

with $U = \dfrac{u - \bar{u}}{\bar{u}}$
The non-dimensional initial and boundary conditions of (22) takes the form

$$(i) \quad \theta(0, X_1, Y) = \begin{cases} 1, |X_1| \leqslant \frac{X_s}{2} \\ 0, |X_1| > \frac{X_s}{2} \end{cases}$$

$$(ii) \quad \frac{\partial\theta}{\partial Y}(\tau, X_1, 0) = \frac{\partial\theta}{\partial Y}(\tau, X_1, 1) = 0$$

$$(iii) \quad \theta(\tau, \infty, Y) = \frac{\partial\theta}{\partial X_1}(\tau, \infty, Y) = 0 \tag{25}$$

Following Gill and Sankarasubramanian(1970), the solution to equation (24) can be written as a series expansion in the form

$$\theta(\tau, X_1, Y) = \theta_m(\tau, X_1) + \sum_{k=1}^{\infty} f_k(\tau, Y)\frac{\partial^k\theta_m}{\partial X_1^k} \tag{26}$$

where, θ_m is the dimensionless cross sectional average concentration, given by

$$\theta_m(\tau, X_1) = \int_0^1 \theta(\tau, X_1, Y)dY \tag{27}$$

Integrating equation (24) with respect to y in $[0, 1]$ and substituting for θ_m we get,

$$\frac{\partial \theta_m}{\partial \tau} = \frac{1}{Pe^2} \frac{\partial^2 \theta_m}{\partial X_1^2} - \frac{\partial}{\partial X_1} \int_0^1 U \; \theta \; dY - K\theta_m \qquad (28)$$

The generalized dispersion model with time dependent dispersion coefficient can be written as

$$\frac{\partial \theta_m}{\partial \tau} = K_1 \frac{\partial \theta_m}{\partial X_1} + K_2 \frac{\partial^2 \theta_m}{\partial X_1^2} + K_3 \frac{\partial^3 \theta_m}{\partial X_1^3} + ... \qquad (29)$$

Introducing equations (29) in (28) and making use of the boundary condition (ii) of (25) gives

$$K_1 \frac{\partial \theta_m}{\partial X_1} + K_2 \frac{\partial^2 \theta_m}{\partial X_1^2} + K_3 \frac{\partial^3 \theta_m}{\partial X_1^3} + ...$$

$$= \frac{1}{Pe^2} \frac{\partial^2 \theta_m}{\partial X_1^2} - \frac{\partial}{\partial X_1} \int_0^1 U \left(\theta_m (\tau, X_1) + f_1 (\tau, Y) \frac{\partial \theta_m}{\partial X_1} + f_2 (\tau, Y) \frac{\partial^2 \theta_m}{\partial X_1^2} ... \right) dY - K\theta_m \qquad (30)$$

Comparing the coefficient of $\dfrac{\partial^k \theta_m}{\partial X_1^k}$ $(k = 1, 2, 3, ...)$, we get

$$K_1(\tau) = - \int_0^1 U dY \qquad (31)$$

$$K_2(\tau) = \frac{1}{Pe^2} - \int_0^1 U f_1(\tau, Y) dY \qquad (32)$$

$$K_3(\tau) = - \int_0^1 U f_2(\tau, Y) dY, \quad ... \qquad (33)$$

Substituting equation (26) in (24),we get

$$\frac{\partial (\theta_m(\tau, X_1)}{\partial \tau} + f_1(\tau, Y) \frac{\partial \theta_m}{\partial X_1}(\tau, X_1) + f_2(\tau, Y) \frac{\partial^2 \theta_m}{\partial X_1^2}(\tau, X_1) + ...)$$

$$+ U \frac{\partial (\theta_m(\tau, X_1)}{\partial \tau} + f_1(\tau, Y) \frac{\partial \theta_m}{\partial X_1}(\tau, X_1) + f_2(\tau, Y) \frac{\partial^2 \theta_m}{\partial X_1^2}(\tau, X_1) + ...)$$

$$= \frac{1}{Pe^2} \frac{\partial^2 (\theta_m(\tau, X_1)}{\partial X_1} + f_1(\tau, Y) \frac{\partial \theta_m}{\partial X_1}(\tau, X_1) + f_2(\tau, Y) \frac{\partial^2 \theta_m}{\partial X_1^2}(\tau, X_1) + ...)$$

$$+\frac{\partial^2(\theta_m(\tau,X_1)}{\partial Y^2}+f_1(\tau,y)\frac{\partial\theta_m}{\partial X_1}(\tau,X_1)+f_2(\tau,Y)\frac{\partial^2\theta_m}{\partial X_1^2}(\tau,X_1)+.....)$$

$$-K(\theta_m(\tau,X_1)\partial Y^2+f_1(\tau,Y)\frac{\partial\theta_m}{\partial X_1}(\tau,X_1)+f_2(\tau,Y)\frac{\partial^2\theta_m}{\partial X_1^2}(\tau,X_1)+..... \qquad (34)$$

Following Gill and Sankarasubramanian(1970) we have,

$$\frac{\partial^{k+1}\theta_m}{\partial\tau\partial X_1^k}=\sum_{i=1}^{\infty}K_i(\tau)\frac{\partial^{k+i}\theta_m}{\partial X_1^{k+i}}\quad\text{for k=1,2,3,\dots}$$

we get,

$$K\theta_m+\left[\frac{\partial f_1}{\partial\tau}-\frac{\partial^2 f_1}{\partial Y^2}+U+k_1(\tau)+f_1K\right]\frac{\partial\theta_m}{\partial X_1}+$$

$$\left[\frac{\partial f_2}{\partial\tau}-\frac{\partial^2 f_2}{\partial Y^2}+Uf_1+k_1(\tau)f_1+k_2(\tau)-\frac{1}{P_e^2}+f_2K\right]\frac{\partial^2\theta_m}{\partial X_1^2}$$

$$+\sum_{k=1}^{\infty}\left[\frac{\partial f_{k+2}}{\partial\tau}-\frac{\partial^2 f_{k+2}}{\partial Y^2}+Kf_{k+2}+Uf_{k+1}+k_1(\tau)f_{k+1}+\left(k_2(\tau)-\frac{1}{P_e^2}\right)f_k\right.$$

$$\left.+\sum_{i=3}^{k+2}k_if_{k+2-i}\right]\frac{\partial^{k+2}\theta_m}{\partial X_1^{k+2}}=0(35)$$

with $f_0=1$. Equating the coefficients of $\dfrac{\partial^k\theta_m}{\partial X_1^k}$ $(k=1,2,3,\dots)$ to zero, a set of differential equations are obtained:

$$\frac{\partial f_1}{\partial\tau}=\frac{\partial^2 f_1}{\partial Y^2}-U-K_1(\tau)-f_1K \qquad (36)$$

$$\frac{\partial f_2}{\partial\tau}=\frac{\partial^2 f_2}{\partial Y^2}-Uf_1-K_1(\tau)f_1-K_2(\tau)+\frac{1}{Pe^2}-f_2K \qquad (37)$$

$$\frac{\partial f_{k+2}}{\partial\tau}=\frac{\partial^2 f_{k+2}}{\partial Y^2}-Uf_{k+1}-K_1(\tau)f_{K+1}-\left(K_2(\tau)-\frac{1}{Pe^2}\right)f_k-Kf_{k+2}-\sum_{i=3}^{k+2}K_if_{k}(38)$$

To evaluate K_i's we should know f_k's and its corresponding initial and boundary conditions are,

$$(i)f_k(0,Y)=0 \qquad (39)$$

$$(ii)\frac{\partial f_k}{\partial Y}(\tau,0)=0 \qquad (40)$$

$$(iii)\frac{\partial f_k}{\partial Y}(\tau,1)=0 \qquad (41)$$

$$(iv)\int_0^1 f_k(\tau,Y)dY=0,\quad\text{for k=1,2,3,\dots} \qquad (42)$$

From equation (31), we get K_1 as

$$K_1(\tau) = 0 \tag{43}$$

Equation (32) implies

$$K_2(\tau) = \frac{1}{Pe^2} - \int_0^1 U f_1 dY$$

Let

$$f_1 = f_{10}(y) + f_{11}(\tau, y) \tag{44}$$

where, $f_{10}(y)$ corresponds to an infinitely wide slug which is independent of τ satisfies

$$(i) f_{11} = -f_{10}(Y) \ at \ \tau = 0$$

$$(ii) \ \frac{\partial f_{11}}{\partial Y} = 0 \ \ at \ \ Y = 0$$

$$(iii) \ \frac{\partial f_{11}}{\partial Y} = 0 \ \ at \ \ Y = 1 \ \ \ and$$

$$(iv) \int_0^1 f_{11} dY = 0 \tag{45}$$

Substituting (44) in (36) gives

$$\frac{d^2 f_{10}(Y)}{dY^2} + f_{10} K = U(Y) \ \ \ \ and$$

$$\frac{\partial f_{11}}{\partial \tau} = \frac{\partial^2 f_{11}}{\partial Y^2} - f_{10} K$$

which is solved by separation of variables.

Hence the solution of f_1 is given by

$$
\begin{aligned}
f_1 = {} & Ae^{\sqrt{K}Y} + Be^{-\sqrt{K}Y} + \frac{1}{K}\left(\frac{c_0}{X \sinh \sqrt{X}}\left[\frac{1}{X - K}\right.\right. \\
& \left(\frac{1}{2}e^{\sqrt{X}Y}(\cos h\sqrt{X} - \sin h\sqrt{X} - 1) - \frac{1}{2}e^{-\sqrt{X}Y}(\cos h\sqrt{X} + \sin h\sqrt{X} - 1)\right) \\
& \left.\left. - \frac{1}{K}\sin h\sqrt{X}\right] + \frac{4c_0}{\pi}\sum_{n=1}^{\infty}\frac{A_1}{2n+1}\frac{\sin(2n+1)\pi Y}{(2n+1)^2\pi^2 - K} - \frac{K}{K}\right) \\
& + \sum_{m=1}^{\infty} A_m e^{-(m^2\pi^2 - K)\tau}\cos(m\pi Y)
\end{aligned} \tag{46}
$$

where,

$$A_1 = \frac{(1+Gx_1)^2 e^{x_1 t}}{x_1(1+Gx_1)^2 + SG} + \frac{(1+Gx_2)^2 e^{x_2 t}}{x_2(1+Gx_2)^2 + SG}$$

$$E = \frac{c_0}{X \sin h\sqrt{X}} \left[\frac{2 - 2\cosh\sqrt{X} + \sqrt{X}\sin h\sqrt{X}}{\sqrt{X}} + \frac{8c_0}{\pi^2} \sum_{m=1}^{\infty} \frac{A_1}{(2n+1)^2} \right]$$

$$A = -\frac{1}{\sqrt{K}} \left(\frac{\sqrt{K}}{e^{\sqrt{K}} - e^{-\sqrt{K}} - 2} \left(\frac{e^{\sqrt{K}}}{\sqrt{K}} - \frac{1}{\sqrt{K}} \right) \left(\frac{\sqrt{X}\sin h\sqrt{X}}{X - K} - \frac{4c_0}{\pi^2} \sum_{n=1}^{4} \frac{A_1}{(2n+1)^2 - K} \right. \right.$$

$$\left. \left. -\sqrt{K}\sin h\sqrt{X} \left(\frac{1}{\sqrt{X}(X-K)} - \frac{1}{K} \right) + \frac{K\sqrt{K}}{K} + \frac{8c_0\sqrt{K}}{\pi^3} \sum_{n=1}^{\infty} \left(\frac{A}{(2n+1)^2 - K} \frac{1}{2n+1} \right) \right) \right)$$

$$B = -\left(\frac{1}{e^{\sqrt{K}} - e^{\sqrt{-K}} - 2} \left(\frac{e^{\sqrt{K}}}{\sqrt{K}} - \frac{1}{\sqrt{K}} \right) \left(\frac{\sqrt{X}\sin h\sqrt{X}}{X-K} - \frac{4c_0}{\pi^2} \sum_{n=1}^{\infty} \frac{A_1}{(2n+1)^2 - K} \right) \right.$$

$$\left. -\sqrt{K}\sin h\sqrt{X} \left(\frac{1}{\sqrt{X}(X-K)} \right) + \frac{E\sqrt{K}}{K} + \frac{8c_0\sqrt{K}}{\pi^3} \sum_{n=1}^{\infty} \left(\frac{A_1}{(2n+1)^2 - K} \frac{1}{2n+1} \right) \right)$$

$$A_m = 2\left(\sqrt{K} \left(Ae^{\sqrt{K}} - Be^{\sqrt{-K}} \right) + \frac{1}{E} \left(\frac{c_0}{X\sinh\sqrt{X}} \left(\frac{1}{X-K} \left(\sqrt{X} \left(1 - \cosh\sqrt{X} \right) \right) \right) \right.$$

$$\left. -4c_0 \sum_{n=1}^{\infty} \left(\frac{A_1}{(2n+1)^2\pi^2 - K} \right) \left(\frac{-(-1)^m}{m^2\pi^2} \right) \right) + \left(\sqrt{K}(A - B) + \right.$$

$$\frac{1}{E} \left(\frac{c_0}{X\sinh\sqrt{X}} \left(\frac{1}{X-K} \left(\sqrt{X}(\cosh\sqrt{X} - 1) \right) \right) \right.$$

$$\left. +4c_0 \sum_{n=1}^{\infty} \left(\frac{A_1}{(2n+1)^2\pi^2 - K} \right) \right) \left(\frac{1}{m^2\pi^2} \right) + \left(K\sqrt{K} \left(Ae^{\sqrt{K}} - Be^{\sqrt{-K}} \right) \right.$$

$$\left. +\frac{1}{E} \left(\frac{c_0}{X\sin h\sqrt{X}} \left(\frac{1}{X-K} \left(X\sqrt{X}(1 - \cos h\sqrt{X}) \right) \right) \right) +$$

$$4c_0 \sum_{n=1}^{\infty} \left(\frac{A_1(2n+1)^2\pi^2}{(2n+1)^2\pi^2 - K} \right) \right) \left(\frac{(-1)^m}{m^4\pi^4} \right)$$

$$+\left(K\sqrt{K}(A - B) + \frac{1}{E} \left(\frac{c_0}{X\sinh\sqrt{X}} \left(\frac{1}{X-K} \left(X\sqrt{X}(\cos h\sqrt{X} - 1) \right) \right) \right.$$

$$\left. -4c_0 \sum_{n=1}^{\infty} \left(\frac{A_1(2n+1)^2\pi^2}{(2n+1)^2\pi^2 - K} \right) \right) \left(\frac{1}{m^4\pi^4} \right)$$

and $\lambda_m = m\pi$

Therefore substituting f_1 in equation (32) gives the solution of K_2 for u velocity, which is for fluid phase.

Neglecting $K_i(\tau)$, i >2, as the values are small compared to $K_2(\tau)$, the dispersion model (29) takes the form

$$\frac{\partial \theta_{m_f}}{\partial \tau} = K_2 \frac{\partial^2 \theta_{m_f}}{\partial X_1^2} \tag{47}$$

5. Mean Concentration

The solution to equation (47) can be solved with the initial and boundary conditions

$$\theta_m(0, X_1) = \begin{cases} 1, |X_1| \leqslant \frac{X_s}{2} \\ 0, |X_1| > \frac{X_s}{2} \end{cases} \qquad (48)$$

can be obtained using Fourier Transform (Sankara Rao,1995) as

$$\theta_m(\tau, X_1) = \frac{1}{2}\left[erf\left(\frac{\frac{X_s}{2} + X_1}{2\sqrt{T}}\right) + erf\left(\frac{\frac{X_s}{2} - X_1}{2\sqrt{T}}\right)\right] \qquad (49)$$

where, $T = \int_0^\tau K_2(y)dy$ and $erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-z^2}dz$.

6. Coefficient of Skin Friction

The shear stress at any point in the fluid is given by

$$\tau_y = \mu\frac{du}{dy}$$

where, μ is the dynamic viscosity of the fluid. From the point of view of applications in technology, it is of interest to know the coefficient of skin friction C_f at both the walls.

$$C_f = \frac{2}{Re}\frac{du}{dy} \ ,$$

defines the non-dimensional form of coefficient of skin friction for fluid phase.

   This gives the dispersion coefficient, mean concentration and coefficient of skin friction for fluid phase.

   In a similar manner we apply generalized dispersion method to find the dispersion coefficient, mean concentration and coefficient of skin friction for the contaminant phase.

7. Results and Discussion

In this paper, an attempt has been made to study the dispersion of contaminants in the groundwater consisting a mixture of fluid phase and solid phase (fine and coarse particle) with the effect of chemical reaction rate parameter.

   The velocity and the dominant dispersion coefficient is obtained analytically and they are numerically computed using MATHEMATICA 8.0 and the results are depicted graphically. Figures 2 and 3 which represent the velocity profiles of fluid and solid particles [fine($G < 1$) and coarse particle($G > 1$)] are parabolic in nature. Figures 4 and 5 show the velocity profile for different porous parameter k at a given instant of time. It is seen that u and v decreases with an increase in porous parameter k. This shows that the velocity profile in the porous media deviates as the permeability of the porous media increases.

Figures 6,7 and 8 represent the coefficient of skin friction on the lower surface $y = 0$ and upper surface $y = 1$ for different values of porous parameter. Figure 6 reveals coefficient of skin friction increases at both the walls $y = 0$ and $y = 1$ for fluid phase. For the contaminant phase,when$(G < 1)$ coefficient of skin friction decreases at the wall $y = 1$ and increases at the wall $y = 0$ which is displayed through figure 7. For $G > 1$ (coarse), coefficient of skin friction increases at both the walls, but the values at the wall $y = 1$ are greater when compared with the values at the wall $y = 0$ is revealed through figure 8. The negative values show that flow arises reversal within the boundary layer[2].

The time-dependent dispersion coefficient is evaluated using the generalized dispersion model which is valid for all time. The dominant dispersion coefficient is computed for different values of chemical reaction rate parameter and the effect of chemical reaction rate parameter is discussed through figures 9 to 11. It is observed from the figure that the dispersion coefficient decreases with increase in chemical reaction rate parameter. Also the figures reveal that the dispersion coefficient is greater for coarse particle when compared with the fine particle. For larger values of the reaction rate parameter K, the normalized solute distribution is almost flat. The flatness of K shows that the pore fluid is well mixed, with the contaminants.

Figure 12 to 14 depict the plot of mean concentration distribution θ_m versus axial distance X for fixed time τ, and different values of chemical reaction rate parameter, K. The peak value represents that the mean concentration decreases, when chemical reaction rate parameter K increases. The curves are bell shaped and perfectly symmetrical about the origin.

The effect of chemical reaction rate parameter, K, on mean concentration, inside $(X_1 = 0.005)$ the slug at $Xs = 0.02$ is studied through figures 15 to 17. In general, we observe a gradual decrease in θ_m for increasing time,τ inside the slug. Also the figure reveals that there is a marked variation of concentration with the axial distance and the dimensionless time and it is clear that, the mean concentration is greater for coarse particle compared with fine contaminant. Also for very smaller values of τ, the concentration inside the slug shows a rapid decrease.
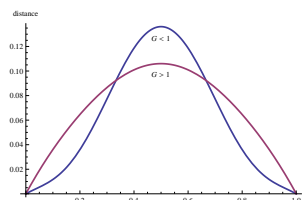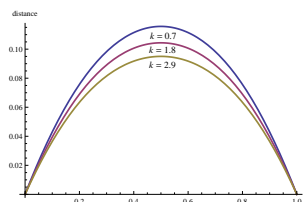

Figure 2. velocity profile for solid phase

Figure 3. Effects of porous parameter on velocity profile for fluid
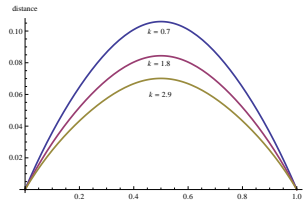
Figure 4. Effects of porous parameter on velocity profile for fine contaminant
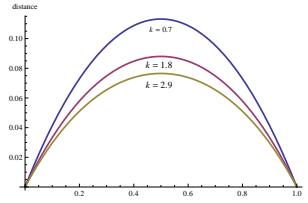

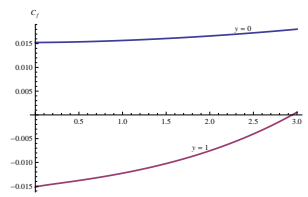Figure 5. Effects of porous parameter on velocity profile for coarse contaminant

Figure 6. coefficient of skin friction versus k for fluid phase
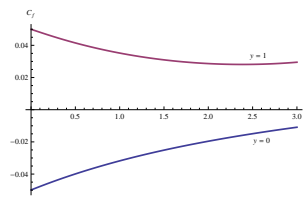

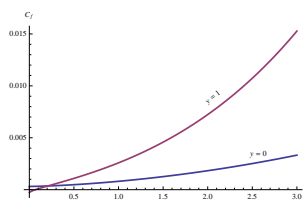Figure 7. coefficient of skin friction versus k for fine contaminants

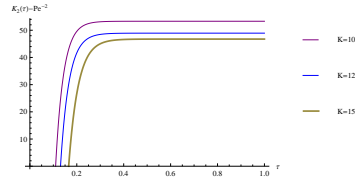Figure 8. coefficient of skin friction versus k for coarse contaminants

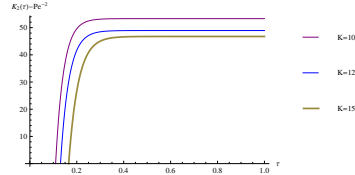Figure 9. Dispersion coefficient varying with dimensionless time for fluid for different reaction parameter

Figure 10. Dispersion coefficient varying with dimensionless time for fine contaminants for different reaction parameter
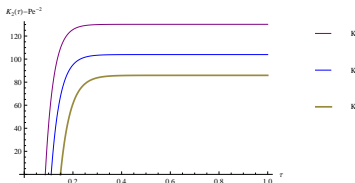

Figure 11. Dispersion coefficient varying with dimensionless time for coarse contaminants for different reaction parameter
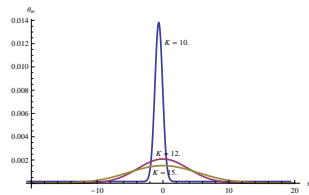

Figure 12. Mean concentration varying with axial distance for fluid for different reaction rate parameter
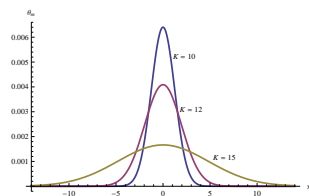

Figure 13. Mean concentration varying with axial distance for fine contaminants for different reaction rate parameter
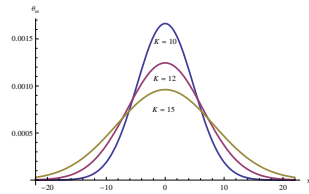
Figure 14.   Mean concentration varying with axial distance for coarse contaminants for different reaction rate parameter
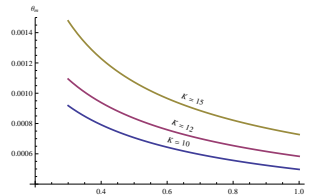

Figure 15. Mean concentration varying with dimensionless time τ for fluid at $X_1=0.005$ with $X_s=0.02$
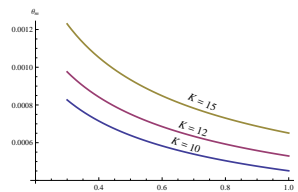

Figure 16.   Mean concentration varying with dimensionless time τ for fine contaminants at $X_1=0.005$ with $X_s=0.02$
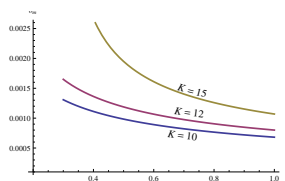

Figure 17.   Mean concentration varying with dimensionless time τ for coarse contaminants at $X_1=0.005$ with $X_s=0.02$

8.   Conclusion

Groundwater contamination has long been recognized as a serious hazard to human health. Chemicals are often added in groundwater remediation for a variety of different reasons and purposes. One of the most challenging problems in modeling of the solute transport in groundwater is how to effectively characterize and quantify the effects of chemical reactions on the transport purposes. To be effective for their intended purpose, the chemicals generally need to be added in the appropriate amounts and concentrations, and mixed in a suitable manner to have the desired effect.

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