INFLUENCE OF ZERO-ORDER SOURCE AND DECAY COEFFICIENTS ON THE CONCENTRATION OF CONTAMINANTS IN TWO-DIMENSIONAL CONTAMINANT FLOW

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Abstract

In this article, an eigenfunctions expansion method is used in studying the behavior of two-dimensional contaminant flow problem with non-zero initial concentration. The mathematical model describing the contaminant flow is described by advection, dispersion, adsorption, first order decay and zero-order source. It is assumed that the adsorption term is modeled by Freudlich isotherm. Before the application of the eigenfunctions method, the parameter expanding method is applied on the model and the boundary conditions are transformed to the homogeneous type. Thereafter, the approximate solution of the resulting initial value problem was obtained successively. The results obtained are expressed graphically to show the effect of change in the zero-order source and decay coefficients on the concentration of the contaminants. From the analysis of the results, it was discovered that the contaminant concentration decreases with increase in the distance from the origin as the zero-order source and decay coefficient increases.

Keywords: Advection, adsorption, contaminant, dispersion, eigenfunctions.

1. Introduction

The problem of contaminant transport in soil, groundwater and surface water has been a research of great concern in hydro-geology for many years. This is largely due to immense contamination of groundwater and surface water by industrial and human activities such as agricultural chemicals, accidental spills, landfills and buried hazardous materials. Though, agricultural chemicals could generally be useful in the surface of the soil, their penetration into the saturated and unsaturated zone of groundwater could contaminate groundwater.

Groundwater in its natural state is generally of excellent quality because the physical structure and mineral constituents of rock have facility for purifying water. Before the coming of industries and factories, the major threats to groundwater are viruses and bacteria. The presence of these microbiological contaminants like bacteria, viruses and parasites in groundwater may pose some threat to our community health.

The transport equation which models the movement of contaminants through groundwater and surface water environments was reported by (Bear, 1997). They are often advection-dominated and require a lot of care when solved numerically. In order to predict the contaminant migration in the geological formation more accurately, a tasking job emerges for scientists. The involves defining the flow lines of groundwater of the aquifers, the travel time of water along the flow lines and to predict the chemical reaction and zero order source coefficient which alter the concentration during transport.

2. **Literature Review**

Most researchers are of the view that the flow in the solute transport or contaminant flow model is predominantly horizontal as found in (Bear, 1997). Further research by (Brainard and Gelhar, 1991) discovered that appreciable vertical flow components do occur in the domain of vertically penetrating wells and streams.

In an effort to provide solutions to the contaminant flow problems, a lot of successes were achieved by some researchers but mostly on one-dimensional cases with various initial and boundary conditions. (Okedayo and Aiyesimi, 2005) came out with the influence of retardation factor on the nonlinear contaminant flow problem. (Okedayo *et al*. 2011) studied on the 1-Dimensional nonlinear contaminant transport equation with an initial and instantaneous point source. Their investigation revealed that the contaminant concentration decreases with increase in the distance from the origin. On the dispersion of solute, (Ramakanta and Mehta, 2010) explored the effect of longitudinal dispersion of miscible fluid flow through porous media.

The analytical solution to temporally dependent dispersion through semi-infinite homogeneous porous media by Laplace transform technique (LTT) was provided by (Yadav *et al.* 2011). On the effect of reactive and non-reactive contaminant on the flow, (Aiyesimi and Jimoh, 2012,2013) embarked on computational analysis of 1-dimensional non-linear contaminant flow problem with an initial continuous point source using homotopy perturbation method. They discovered that the concentration decreases with increase in time and distance from the origin for the non-reactive case.

In order to understand the movement of contaminants in a flow, several models were formulated. i.e., Bear (1972), Cherry *et al.* (1979), Yadav *et al.* (2011), Yadav and Jaiswal (2011), etc. In their formulations, assumptions were made. Bear (1972) assumed that flow takes place only in the horizontal direction. Yadav et al. (2011), Chen *et al.* (2006), Singh *et al*. (2014) and Yadav and Jaiswal (2011) believed that both advection and dispersion happen in the horizontal and vertical direction but did not anticipate that there could be any reaction between the contaminants in the flow.

In this paper, the two-dimensional contaminant flow problem incorporating flow in both horizontal and vertical direction in addition to first-order decay and zero order sources is studied using the combination of parameter expanding method (PEM) and eigenfunctions method.

3. **Methodology**

3.1 Formulation of the Model

We consider an incompressible fluid flow through a semi-infinite homogeneous porous media with non-zero initial concentration in the transport domain. We assume that the flow is two-dimensional and in the direction of x and y-axis. The source concentration is assumed at the origin (i.e. at $x = 0$ and $y = 0$). The contaminant concentration is a function of space and time.

Following (Bear, 1997), (Yadav, *et al.* 2011), (Freezer and Cherry, 1979), Batu (2006), Ujile (2013), Singh (2013) and Singh *et al*. (2015), the two dimensional partial differential equation describing hydrodynamic dispersion in adsorbing, homogeneous and isotropic porous medium can be written as

$$\frac{\partial C}{\partial t}+\frac{\partial S}{\partial t}=D_{xx}\frac{\partial^2 C}{\partial x^2}+D_{yy}\frac{\partial^2 C}{\partial y^2}-u(t)\frac{\partial C}{\partial x}-v(t)\frac{\partial C}{\partial y}-\gamma(t)C+\mu(t) \qquad (1)$$

Where,

$$\left.\begin{aligned} D_{xx} &= \frac{\alpha_L u^2}{\sqrt{u^2+v^2}}+\frac{\alpha_T v^2}{\sqrt{u^2+v^2}} \\ D_{yy} &= \frac{\alpha_L v^2}{\sqrt{u^2+v^2}}+\frac{\alpha_T u^2}{\sqrt{u^2+v^2}} \end{aligned}\right\} \qquad (2)$$

as used in Batu (2006). This is an extension of the advection-diffusion equations. The concentration of adsorbed contaminant in the medium is directly proportional to that of the dissolved contaminant iin the flow (Schiedegger, 1961). i.e., $S=K_d C$ where C is the concentration of the dissolved contaminant and S is the concentration of the adsorbed contaminant.

$$\frac{\partial S}{\partial t}=K_d\frac{\partial C}{\partial t} \qquad (3)$$

Hence, equation (3.3) yields

$$R\frac{\partial C}{\partial t}=D_{xx}\frac{\partial^2 C}{\partial x^2}+D_{yy}\frac{\partial^2 C}{\partial y^2}-u(t)\frac{\partial C}{\partial x}-v(t)\frac{\partial C}{\partial y}-\gamma(t)C+\mu(t) \qquad (4)$$

where,

$R=1+K_d$, is the retardation coefficient, accounting for equilibrium linear sorption process

K_d is the distribution coefficient which is defined as the ratio of the adsorbed contaminant to the dissolved contaminants

D_{xx} is the longitudinal dispersivity

D_{yy} is the transverse dispersivity

t is the time

x is the distance measured from the origin in the longitudinal direction

y is the distance measured from the origin in the transverse direction

$\gamma(t)$ is a first order decay term

$\mu(t)$ is the zero order source term.

As initial and boundary conditions, we choose

$$\left.\begin{array}{l} C(x,y,t)=c_i; x\ge 0, y\ge 0, t=0 \\ C(x,y,t)=C_0(1+\exp(-qt)); x=0, y=0, t>0 \\ C(x,y,t)=c_p; x\to l, y\to l, t\ge 0 \end{array}\right\} \quad (5)$$

where C_0 is the solute concentration and q is the parameter like flow resistance coefficient.

We let

$$\left.\begin{array}{l} v(t)=v_0 f(t) \\ u(t)=u_0 f(t) \\ D_{xx}=D_{x0} f(t) \\ D_{yy}=D_{y0} f(t) \\ \gamma(t)=\gamma_0 f(t) \\ \mu(t)=\mu_0 f(t) \end{array}\right\} \quad (6)$$

where $f(t)$ is arbitrary function of time. By substituting equation (6) into (4), we obtain

$$\frac{R}{f(t)}\frac{\partial C}{\partial t}=D_{x0}\frac{\partial^2 C}{\partial x^2}+D_{y0}\frac{\partial^2 C}{\partial y^2}-u_0\frac{\partial C}{\partial x}-v_0\frac{\partial C}{\partial y}-\gamma_0 C+\mu_0 \quad (7)$$

where

$$D_{x0} f(t)=\frac{\alpha_L u_0{}^2+\alpha_T v_0{}^2}{\sqrt{u_0{}^2+v_0{}^2}} \quad (8)$$

$$D_{y0} f(t)=\frac{\alpha_L v_0{}^2+\alpha_T u_0{}^2}{\sqrt{u_0{}^2+v_0{}^2}} \quad (9)$$

as cited in Batu (2006) and $f(t)$ is the arbitrary function of time.

D_{x0} is the initial dispersion coefficient in x direction

D_{y_0} is the initial dispersion in the y direction

u_0 is the initial velocity component in the x-direction

v_0 is the initial velocity component in the y-direction

γ_0 is the initial first order decay term

μ_0 is the initial zero-order source term.

A new time variable is introduced as in Crank (1975) and Olayiwola *et al*. (2013)

$$\tau = \frac{1}{R}\int_0^t f(t)dt \tag{10}$$

and

$$f(t) = \mathrm{Re}^{-qt} \tag{11}$$

such that from equation (10),

$$\frac{d\tau}{dt} = \frac{f(t)}{R} \text{ and } \frac{dt}{d\tau} = \frac{R}{f(t)} \tag{12}$$

By substituting equations (10), (11) and (12) in equations (5) and (7), we obtain

$$\left.\begin{array}{l} \dfrac{\partial C}{\partial \tau} = D_{x0}\dfrac{\partial^2 C}{\partial x^2} + D_{y0}\dfrac{\partial^2 C}{\partial y^2} - u_0\dfrac{\partial C}{\partial x} - v_0\dfrac{\partial C}{\partial y} - \gamma_0 C + \mu_0 \\ C(x,y,\tau) = c_i; x \geq 0, y \geq 0, \tau = 0 \\ C(x,y,\tau) = C_0(2 - q\tau); x = 0, y = 0, \tau < 0 \\ C(x,y,\tau) = c_p; x \to l, y \to l, \tau \geq 0 \end{array}\right\} \tag{13}$$

3.2 Solutions of the Model

We introduce a new space variable as found in Yadav *et al.* (2011), Mahato *et al*. (2015) and Yadav *and* Jaiswal (2011) as follows:

$$\eta = x + y\sqrt{\frac{D_{y0}}{D_{x0}}} \tag{14}$$

into equation (13) and obtain

$$\frac{\partial C}{\partial \tau} = D\frac{\partial^2 C}{\partial \eta^2} - U\frac{\partial C}{\partial \eta} - \gamma_0 C + \mu_0 \tag{15}$$

with the corresponding initial and boundary conditions

$$\left.\begin{array}{l} C(\eta,\tau) = c_i; \eta \geq 0, \tau = 0 \\ C(\eta,\tau) = C_0(2 - q\tau); \eta = 0, \tau > 0 \\ C(\eta,\tau) = c_p; \eta \to l, \tau \geq 0 \end{array}\right\} \quad .(16)$$

where,

$$D = D_{x0}\left(1 + \left(\frac{D_{y0}}{D_{x0}}\right)^2\right) \tag{17}$$

$$U = \left(u_0 + v_0 \sqrt{\frac{D_{y0}}{D_{x0}}} \right) \tag{18}$$

3.3 Non-Dimensionalization

The following dimensionless variables are used to non-dimensionalize the equation (15)

$$\left.\begin{aligned} \tau &= \frac{L}{U}\tau' \\ \eta &= \eta' L \\ C &= C_0 C' \\ \partial\tau &= \frac{L}{U}\partial\tau' \\ \partial\eta &= L\eta' \end{aligned}\right\} \tag{16}$$

and we obtain

$$\Rightarrow \frac{\partial C}{\partial \tau} = D_1 \frac{\partial^2 C}{\partial \eta^2} - \frac{\partial C}{\partial \eta} - \gamma_0 C + \mu_0 \tag{17}$$

where ,

$$D_1 = \frac{D}{LU} \tag{18}$$

The non-dimensionalized equation together with the initial and boundary conditions is

$$\left.\begin{aligned} &\frac{\partial C}{\partial \tau} = D_1 \frac{\partial^2 C}{\partial \eta^2} - \frac{\partial C}{\partial \eta} - \gamma_0 C + \mu_0 \\ &C(\eta,0) = \frac{c_i}{c_0} \\ &C(0,\tau) = 2 - q\tau,\ \tau \geq 0 \\ &C(1,\tau) = \frac{c_p}{c_0},\ \tau \geq 0 \end{aligned}\right\} \tag{19}$$

3.4 Parameters Expanding Method (PEM)

The above initial boundary value problem is solved for when the initial spatial concentration c_i is non-zero. By using parameter expanding method and let $1 = a\gamma_0$ in the advection term of equation (19) and

$$C(\eta,\tau) = C_0(\eta,\tau) + \gamma_0 C_1(\eta,\tau) \tag{20}$$

as used by Olayiwola *et al*. (2013), He (2006) and Sweilam and Khader (2010), Equation (19) becomes

$$
\begin{aligned}
&\frac{\partial}{\partial \tau}(C_0(\eta,\tau)+\gamma_0 C_1(\eta,\tau)+\gamma_0{}^2 C_2(\eta,\tau)+...)\\
&= D_1\frac{\partial^2}{\partial \eta^2}(C_0(\eta,\tau)+\gamma_0 C_1(\eta,\tau)+\gamma_0{}^2 C_2(\eta,\tau)+...)\\
&- a\gamma_0\frac{\partial}{\partial \eta}(C_0(\eta,\tau)+\gamma_0 C_1(\eta,\tau)+\gamma_0{}^2 C_2(\eta,\tau)+...)\\
&- \gamma_0(C_0(\eta,\tau)+\gamma_0 C_1(\eta,\tau)+\gamma_0{}^2 C_2(\eta,\tau)+...)+\mu_0
\end{aligned} \tag{21}
$$

Equating corresponding coefficients on both sides of equation (21), we obtain the following initial boundary problems:

$$
\left.\begin{aligned}
&\frac{\partial C_0}{\partial \tau} = D_1\frac{\partial^2 C_0}{\partial \eta^2}+\mu_0\\
&C_0(\eta,0)=\frac{c_i}{c_0}\\
&C_0(0,\tau)=2-q\tau\\
&C_0(1,\tau)=\frac{c_p}{c_0}
\end{aligned}\right\} \tag{22}
$$

$$
\left.\begin{aligned}
&\frac{\partial C_1(\eta,\tau)}{\partial \tau} = D_1\frac{\partial^2 C_1}{\partial \eta^2}-a\frac{\partial C_0}{\partial \eta}-C_0\\
&C_0(\eta,0)=0\\
&C_0(0,\tau)=0\\
&C_0(1,\tau)=0
\end{aligned}\right\} \tag{23}
$$

We transform equations (22) and (23) to homogeneous boundary conditions problem as follows:

From (22), let

$$w_0(\tau)=\alpha(\tau)+\frac{\eta}{l}(\beta(\tau)-\alpha(\tau)), \quad l=1 \tag{24}$$

where $\alpha(\tau)=2-q\tau$ and $\beta(\tau)=\frac{c_p}{c_0}$,

$$C_0(\eta,\tau)=v_0(\eta,\tau)+w_0(\tau) \tag{25}$$

i.e.,

$$C_0(\eta,\tau)=v_0(\eta,\tau)+(2-q\tau)+\eta\left(\frac{c_p}{c_0}-(2-q\tau)\right) \tag{26}$$

We transform equation (23) and (23) using equation (26) and obtained the following equations

$$\left.\begin{aligned}&\frac{\partial v_0}{\partial \tau} = D_1 \frac{\partial^2 v_0}{\partial \eta^2} + \mu_0 - (\eta - 1)q \\ &v_0(0,\tau) = 0 \\ &v_0(1,\tau) = 0 \\ &v_0(\eta,0) = \frac{c_i}{c_0} - 2(\eta - 1) - \eta \frac{c_p}{c_0}\end{aligned}\right\} \tag{27}$$

$$\left.\begin{aligned}&\frac{\partial v_1(\eta,\tau)}{\partial \tau} = D_1 \frac{\partial^2 v_1}{\partial \eta^2} - a \frac{\partial v_0}{\partial \eta} - v_0 \\ &v_0(\eta,0) = 0 \\ &v_0(0,\tau) = 0 \\ &v_0(1,\tau) = 0\end{aligned}\right\} \tag{28}$$

The initial boundary value problem (27) is solved by eigenfunctions expansion technique

From (27), we have

$$F(\eta,\tau) = \mu_0 - (\eta - 1)q \tag{29}$$

$$F(\eta) = \frac{c_i}{c_0} + 2(\eta - 1) - \eta \frac{c_p}{c_0} \tag{30}$$

In Fourier series expansion,

$$b_n = 2\int_0^1 F(\eta)\sin(n\pi)\eta d\eta \tag{31}$$

$$b_n = 2\int_0^1 \left(\frac{c_i}{c_0} + 2(\eta - 1) - \eta \frac{c_p}{c_0}\right)\sin(n\pi)\eta d\eta \tag{32}$$

$$b_n = -\frac{2c_i}{n\pi c_0}(\cos(n\pi) - 1) - \frac{4}{n\pi} + \frac{2c_p}{n\pi c_0}\cos n\pi \tag{33}$$

$$F_n(\tau) = 2\int_0^1 (\mu - (\eta - 1)q)\sin(n\pi\eta d\eta) \tag{34}$$

$$F_n(\tau) = -\frac{2\mu_0}{n\pi}(\cos(n\pi) - 1) + \frac{2q}{n\pi} \tag{35}$$

$$C_n(\tau) = \int_0^\tau e^{\left(\alpha - k(n\pi)^2(\tau - t)\right)} F_n(t)dt + b_n e^{\left(\alpha - k(n\pi)^2 \tau\right)} \tag{36}$$

Therefore,

$$C_n(\tau)=\frac{2}{D_1(n\pi)^3}\left(q-\mu_0(\cos(n\pi)-1)\right)\left(1-e^{\left(-D_1(n\pi)^2\tau\right)}\right)+\begin{pmatrix}-\dfrac{2c_i}{n\pi c_0}(\cos(n\pi)-1)\\ -\dfrac{4}{n\pi}+\dfrac{2c_p}{n\pi c_0}\cos n\pi\end{pmatrix}e^{\left(-D_1(n\pi)^2\tau\right)} \quad (37)$$

$$C_0(\eta,\tau)=v_0(\eta,\tau)+w_0(\tau) \quad (38)$$

i.e.,

$$C_0(\eta,\tau)=w_0(\tau)+\sum_{n=1}^{\infty}C_n(\tau)\sin(n\pi\eta) \quad (39)$$

$$\begin{aligned}C_0(\eta,\tau)&=(2-q\tau)(1-\eta)+\eta c_p\\&+\sum_{n=1}^{\infty}\left(\begin{array}{l}\dfrac{2}{D_1(n\pi)^3}\left(q-\mu_0(\cos(n\pi)-1)\right)\left(1-e^{\left(-D_1(n\pi)^2\tau\right)}\right)\\ +\begin{pmatrix}-\dfrac{2c_i}{n\pi c_0}(\cos(n\pi)-1)-\dfrac{4}{n\pi}\\ +\dfrac{2c_p}{n\pi c_0}\cos n\pi\end{pmatrix}e^{\left(-D_1(n\pi)^2\tau\right)}\end{array}\right)\sin(n\pi\eta)\end{aligned} \quad (40)$$

Similarly, the solution of equation (27) is substituted in equation (28) and solved using the eigenfunctions method and obtained the following results.

$$C_1(\eta,\tau)=-\sum_{n=1}^{\infty}\left(\begin{array}{l}\left(\sum_{n=1}^{\infty}\dfrac{2}{D_1(n\pi)^3}\left(q-\mu_0(\cos(n\pi)-1)\right)\left(\begin{array}{l}\dfrac{1}{D_1(n\pi)^2}-\tau e^{\left(-D_1(n\pi)^2\tau\right)}\\ -\dfrac{e^{\left(-D_1(n\pi)^2\tau\right)}}{D_1(n\pi)^2}\end{array}\right)\right)\sin(n\pi\eta)\\ -\sum_{n=1}^{\infty}\left(\sum_{n=1}^{\infty}\begin{pmatrix}-\dfrac{2c_i}{n\pi c_0}(\cos(n\pi)-1)-\dfrac{4}{n\pi}\\ +\dfrac{2c_p}{n\pi c_0}\cos n\pi\end{pmatrix}e^{\left(-D_1(n\pi)^2\tau\right)}\tau\right)\sin(n\pi\eta)\end{array}\right) \quad (41)$$

The solution of the contaminant flow problem (13) when $c_i \neq 0$ is therefore

$$C(\eta,\tau)=C_0(\eta,\tau)+\gamma_0 C_1(\eta,\tau) \quad (42)$$

Where $C_0(\eta,\tau)$ and $C_1(\eta,\tau)$ are as given in (40) and (41).

4. **Results and Discussion**

The analytical solution obtained in equation (42) is used to study the behavior of the contaminant concentration in the flow for values of $C_i = 2,\ C_0 = 1,\ q = 3,\ \gamma = 0.1,\ \mu = 0.3,\ D_{x0} = 1,\ u_0 = 0.1,\ v_0 = 0.1$ with D_{y0} varying as 1.5, 1.6, 1.7 and the graph presented in figure 1. Similarly, with μ_0 varying as 0.3, 0.6, 0.9, we obtained the graphs in figure 2 and 3. Figure 4 is obtained by varying the first order decay coefficient γ as 0.1, 0.5 and 0.9.

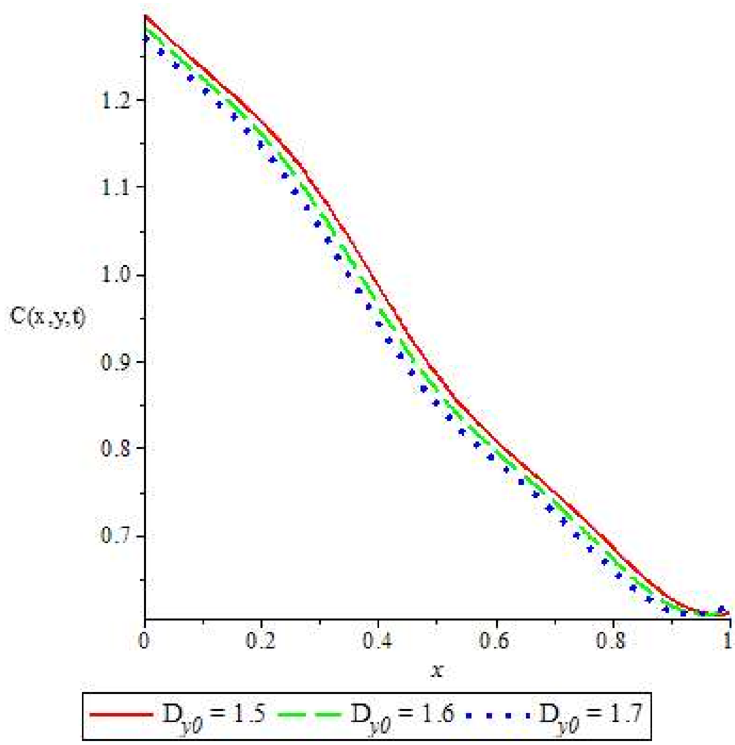

Figure 1: Contaminant Concentration profile for $D_{y0} = 1.5$, $D_{y0} = 1.6$, $D_{y0} = 1.7$ when $c_0 = 1$, $c_p = 1$, $q = 3$, $\gamma_0 = 0.1$, $\mu_0 = 0.3$, $D_{x0} = 1$, $u_0 = 0.1$, $v_0 = 0.1$ with y and t fixed as 0.5.

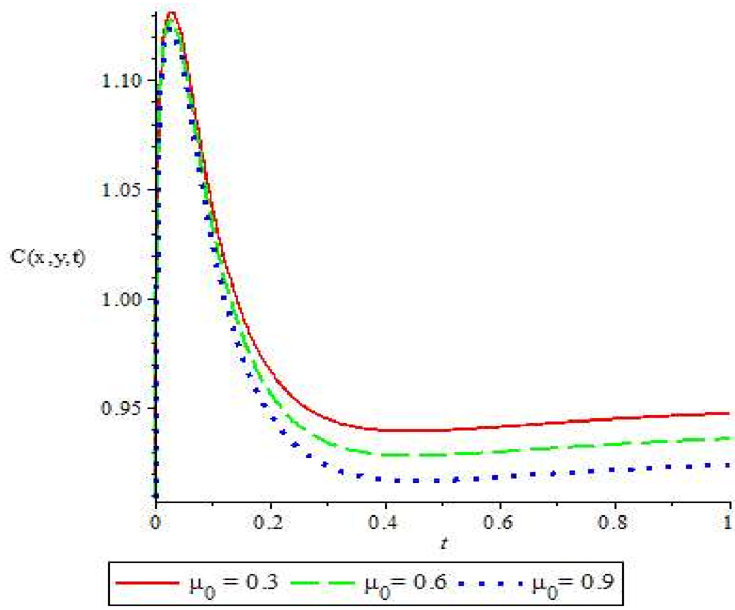

Figure 2: Contaminant Concentration profile for $\mu_0 = 0.3, \mu_0 = 0.6$, $\mu_0 = 0.9$ when $c_0 = 1, c_p = 1$, $q = 3$, $\gamma_0 = 0.1$, $D_{x0} = 1$, $D_{y0} = 1.5$, $u_0 = 0.1, v_0 = 0.1$ with y and x fixed as 0.5.

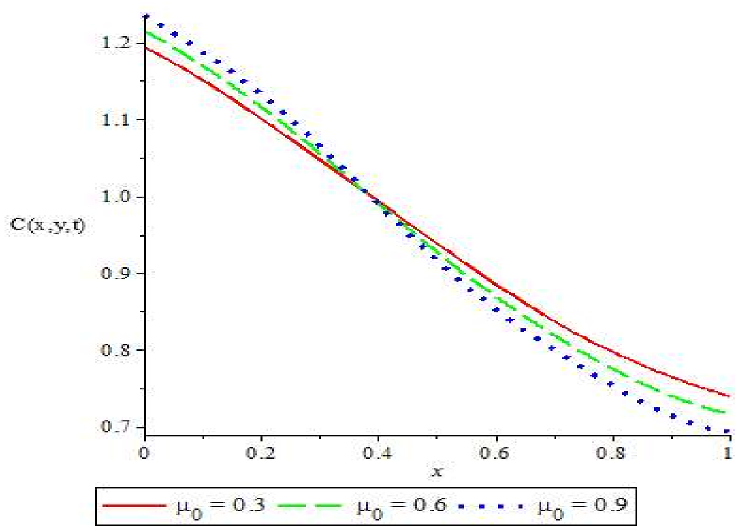

Figure 3: Contaminant Concentration profile for $\mu_0 = 0.3, \mu_0 = 0.6$, $\mu_0 = 0.9$ when $c_0 = 1, c_p = 1$, $q = 3$, $\gamma_0 = 0.1$, $D_{xo} = 1$, $D_{y0} = 1.5$, $u_0 = 0.1, v_0 = 0.1$ with y and t fixed as 0.5.

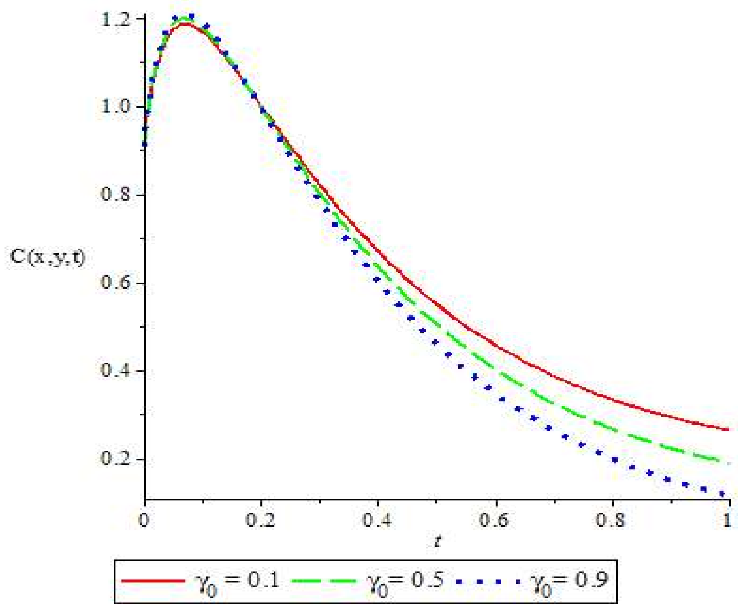

Figure 4: Contaminant Concentration profile for $\gamma_0 = 0.1, \gamma_0 = 0.5$, $\gamma_0 = 0.9$ when $c_0 = 1$, $\mu_0 = 0.3$, $c_p = 1$, $q = 3$, $D_{xo} = 1$, $D_{y0} = 1.5$, $u_0 = 0.1, v_0 = 0.1$ with y and x fixed as 0.5.

Figure 1 shows the contaminant concentration profile with distance x for varying vertical dispersion coefficient. The graph shows that the contaminant concentration decreases as the vertical dispersion coefficient increases. Figure 2 is the contaminant concentration profile with time for varying zero-order source coefficient. It shows that as the zero-order source coefficient increases, the contaminant concentration decreases with time. Figure 3, which is the graph of contaminant concentration against distance x shows that the contaminant concentration decreases with increase in distance as the zero-order source coefficient increases. Similarly, figure 4 also reveal that as the contaminant concentration decreases with time as the decay coefficient increases.

5. **Conclusion**

A two-dimensional contaminant flow model with non-zero initial concentration is solved to predict the effect of change in the zero-order source and decay coefficients on the contaminant concentration along transient groundwater in a finite homogeneous medium by eigenfunctions expansion method. The zero-order source and decay coefficient are varied to study the contaminant behavior along the flow. Our findings reveal that the contaminant concentration decreases along the spatial direction as the zero-order source and decay coefficient increases. This model, if properly implemented could help the geologist in locating the point at which the contaminant concentration is approximately zero.

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