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Behavior of Contaminant in a Flow due to Variations in the Cross-Flow dispersion under a Dirichlet Boundary Conditions.

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Abstract

The advection-dispersion equation (ADE) is mostly adopted in evaluating solute migration in a flow. This study presents the behavior of contaminant in a flow due to variations in the cross-flow dispersion under a Dirichlet boundary conditions. The analytical solution of a two-dimensional advection-dispersion equation for evaluating groundwater contamination in a homogeneous finite medium which is initially assumed not contaminant free was obtained. In deriving the model equation, it was assumed that there was a constant point-source concentration at the origin and a Dirichlet type boundary condition at the exit boundary. The cross-flow dispersion coefficients, velocities and decay terms are time-dependent. The modeled equation was transformed using some space and time variables and solved by parameter expanding and Eigen-functions expansion method. Graphs were plotted to study the behavior of the contaminant in the flow. The results showed that increase in the cross-flow coefficient decline the concentration of the contaminant with respect to increase in time, vertical distance and horizontal distance in different patterns.

Keyword: contaminant, cross-flow dispersion, advection, dispersion, decay parameter, Eigen- function, parameter expanding method.

INTRODUCTION

Groundwater is the water found below Earth's surface in cracks of rocks and spaces in soil. It is stored in and moves slowly through geologic formation of soil, sand and rocks called aquifers. The depth at which soil pore spaces or fractures and voids in rock become completely saturated with water is called water table. Usually, Groundwater is recharged from the surface; it may discharge from the surface naturally at springs and seeps. Groundwater, under most conditions, is safer and more reliable for use than surface water. Thus, groundwater serves as an essential source of drinking water and other domestic use in most part of the world. However, its pollution is one of the most typical hydro-geological and environmental problems. Groundwater contamination occurs when pollutants are released into the environment and make their way down into groundwater. In many parts of the world, groundwater resources are under increasing threat from growing demands, wasteful use and contamination. The movement of solute in soils and groundwater has long been a focus of experimental and theoretical research in subsurface hydrology. Once the groundwater is contaminated, it is extremely difficult and expensive to remove the contaminants from the groundwater (Gurganus, 1993).

Most of the groundwater contaminants are reactive in nature and they infiltrate through the vadoze zone, hit the water-table and continue to move in the direction of groundwater flow. Therefore, it is essential to understand the transport mechanism of contaminants through the subsurface porous media. Surface water is more readily exposed to contaminants from sources such as agricultural activities, indiscriminate disposal of all kinds of wastes, factories or traffic than groundwater. Thus, groundwater is an important source of water for domestic use. There are two major methods applied in examining contaminant transport with regard to reactions in porous media. These methods are classified as stochastic and deterministic (Flury *et al.*, 1998; Gao *et al.*, 2013). Stochastic methods deal with reaction coefficients and are considered to 'be stationary processes'. The quality of groundwater that passes through hydro chemical analyses was evaluated through samples taken from the canals, drains and groundwater (Ghorba *et al.*, 2013). Laboratory study and mathematical modeling were presented in their work, providing two numerical computer models by applying finite difference method to study the flow of water as a three-dimensional and unsteady state. A guide on planning of water resource projects

and estimation of the available water in aquifer plays an important role in groundwater modeling as contained in (Ghose *et al.*, 2013). The first step in the water availability estimation is the computation of runoff resulting from the precipitation on river catchments. A three-dimensional groundwater flow model to evaluate the groundwater potential and assess the effects of groundwater withdrawal on the regional water level and flow direction was developed in the central Beijing area (Seyf-Laye *et al.*, 2012). They estimated current contaminant fluxes to the central area and site streams via groundwater by developing a program of groundwater model.

The pollutant transport from a source through a medium of air or water is described by a partial differential equation of parabolic type derived on the principle of conservation of mass and is known as advection-diffusion equation (Singh, 2011). The analytical solution of solute concentration for space-time variation in unsteady flow via a homogeneous finite aquifer subjected to point source contamination under the sinusoidal form and exponentially decreasing flow velocity was obtained and analyzed (Singh *et al.*, 2009). The steady state flow condition of the contaminant in two dimensions where inorganic contaminants in aqueous waste solutions are disposed off at the land surface before it migrates through the vadoze zone to underground water was modeled in (Cole *et al.*, 2017). The solution of one-dimensional contaminant flow problem which is characterized by advection, dispersion and adsorption processes with constant initial and boundary conditions was developed using Bubnov-Galerkin weighted residual technique (Jimoh *et al.*, 2017). In order to evaluate the groundwater contaminant processes, a development of groundwater contamination processes frame work was carried out (Ujile, 2013). In contaminant transport, the effect of dispersion of solute is usually higher than that of advection. It was in this vein that contaminant's horizontal dispersion along and against sinusoidally varying velocity from pulse type source was examined (Singh *et al.* 2015).

Similarly, efforts made in understanding the movement and dispersion of solutes was boosted with a study on a two-dimensional model incorporating the cross-flow dispersion to account for off-diagonal dispersions with various initial and boundary conditions (Lee and Kim, 2012; Jimoh and Adebayo, 2021). The literature in Lee and Kim (2012) did not consider decay and reaction of the contaminant with the fluid and solid matrix. In the study, a decay or reaction term and a convective term are incorporated in order to see the behavior of the concentration under Dirichlet boundary condition.

Model Formulation

The transport of a contaminant through a homogeneous finite medium of length $x = L$ under transient state flow is formulated. It is assumed that at time $t = 0$, the flow is not clean. Let c_i be the initial contaminant concentration and $c(x, y, t)$ describe the distribution of the concentration at all points in the flow domain. A time dependent concentration is assumed at the boundary ($x = 0$) of the flow. The velocities of the flow in the horizontal and vertical direction are $u(t)$ and $v(t)$ respectively.

Following the work of Lee and Kim (2012); Jimoh and Shuaibu (2021); Olayiwola *et al.* (2013); Jimoh and Adebayo (2021); the cross-flow contaminant flow model can be formulated as follows:

$$\frac{\partial c}{\partial t} + \frac{\partial s}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = \frac{\partial}{\partial x} \left(D_L \frac{\partial c}{\partial x} + D_{LT} \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial y} \left(D_{TL} \frac{\partial c}{\partial x} + D_T \frac{\partial c}{\partial y} \right) - \alpha c \quad (1)$$

i.e;

$$(1 + kd) \frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} + D_T \frac{\partial^2 c}{\partial y^2} + 2D_{LT} \frac{\partial^2 c}{\partial x \partial y} - u \frac{\partial c}{\partial x} - v \frac{\partial c}{\partial y} - \alpha c \quad (2)$$

$$\text{Since } D_{LT} \frac{\partial^2 c}{\partial x \partial y} = D_{TL} \frac{\partial^2 c}{\partial y \partial x}$$

Where D_L is the Longitudinal dispersion coefficient, D_T the vertical dispersion coefficient, $D_{TL} = D_{LT}$ is cross-flow vertical dispersion coefficient, c – solute concentration in the liquid phase, v – seepage or average pure water velocity and u initial velocity.

By introducing a new time variable,

$$\tau = \frac{1}{R} \int f(t) dt \quad (3)$$

$$\text{where } f(t) = R e^{-qt} \quad (4)$$

and also introducing a space variable,

$$\eta = x + y \sqrt{\frac{D_{T0}}{D_{L0}}} \quad (5)$$

The use of the transformations (3), (4) and (5) in equation (2) result into the following:

$$\frac{\partial c}{\partial \tau} = D_{L_0} \frac{\partial^2 c}{\partial \eta^2} + D_{T_0} \frac{D_{T_0}^2}{D_{L_0}} \frac{\partial^2 c}{\partial \eta^2} + 2D_{LT_0} \frac{\partial^2 c}{\partial \eta^2} - u_0 \frac{\partial c}{\partial \eta} - v_0 \sqrt{\frac{D_{T_0}}{D_{L_0}}} \frac{\partial c}{\partial \eta} - \alpha_0 c \quad (6)$$

Further simplification of equation (6) leads to

$$\frac{\partial c}{\partial \tau} = \left(D_{L_0} + \frac{D_{T_0}^2}{D_{L_0}} + 2D_{LT_0} \sqrt{\frac{D_{T_0}}{D_{L_0}}} \right) \frac{\partial^2 c}{\partial \eta^2} - \left(u_0 + v_0 \sqrt{\frac{D_{T_0}}{D_{L_0}}} \right) \frac{\partial c}{\partial \eta} - \alpha_0 c \quad (7)$$

$$\text{By taking } D = D_{L_0} + \frac{D_{T_0}^2}{D_{L_0}} + 2D_{LT_0} \sqrt{\frac{D_{T_0}}{D_{L_0}}}, \text{ and } u = u_0 + v_0 \sqrt{\frac{D_{T_0}}{D_{L_0}}} \quad (8)$$

Equation (7) may be written as

$$\frac{\partial c}{\partial \tau} = D \frac{\partial^2 c}{\partial \eta^2} - u \frac{\partial c}{\partial \eta} - \alpha c \quad (9)$$

The associating initial and boundary conditions are as chosen below

$$c(\eta, 0) = c_i; \quad \tau = 0 \quad (10)$$

$$c(0, \tau) = c_0 (1 + e^{-q\tau}); \quad \eta = 0 \quad (11)$$

$$c(l, \tau) = 0, \quad \eta = l \quad (12)$$

By applying the new time variable in equation (3) on the boundary conditions, the initial boundary value problem becomes

$$\left. \begin{aligned} \frac{\partial c}{\partial \tau} &= D \frac{\partial^2 c}{\partial \eta^2} - u \frac{\partial c}{\partial \eta} - \alpha c \\ c(\eta, 0) &= c_i \\ c(0, \tau) &= c_0 (2 - q\tau) \\ c(l, \tau) &= 0 \end{aligned} \right\} \quad (13)$$

Non-dimensionalization

Equation (13) is non-dimensionalized with the aid of the dimensionless variables

$$\left. \begin{aligned} c^* &= \frac{c_i}{c_0} \\ \eta^* &= \frac{\eta}{l} \\ \tau^* &= \frac{\tau u}{l} \end{aligned} \right\} \quad (14)$$

The non-dimensionalized equation with the initial and boundary conditions (13) becomes

$$\left. \begin{aligned} \frac{\partial c^*}{\partial \tau^*} &= D^* \frac{\partial^2 c^*}{\partial \eta^{*2}} - \frac{\partial c^*}{\partial \eta^*} - \alpha^* c^* \\ c^*(\eta, 0) &= \frac{c_i}{c_0} \\ c^*(0, \tau) &= 2 - q\tau; \quad \tau \geq 0 \\ c^*(1, \tau) &= 0; \quad \eta = 1 \end{aligned} \right\} \quad (15)$$

The parameter expanding method is applied to the equation (15) as follows:

$$\text{Let } c^*(\eta, \tau) = c_0(\eta, \tau) + \alpha c_1(\eta, \tau) + \dots$$

and with the assumption $1 = b\alpha$ in the advection term of equation (15) as used in [16]. The following equation is obtained (15)

$$\left. \begin{aligned} \frac{\partial}{\partial \tau} (c_0(\eta, \tau) + \alpha c_1(\eta, \tau) + \alpha^2 c_2(\eta, \tau) + \dots) &= D^* \frac{\partial^2}{\partial \eta^2} (c_0(\eta, \tau) + \alpha c_1(\eta, \tau) + \alpha^2 c_2(\eta, \tau) + \dots) \\ &\quad - b\alpha \left(\frac{\partial}{\partial \eta} (c_0(\eta, \tau) + \alpha c_1(\eta, \tau) + \alpha^2 c_2(\eta, \tau) + \dots) \right) \\ &\quad - \alpha (c_0(\eta, \tau) + \alpha c_1(\eta, \tau) + \alpha^2 c_2(\eta, \tau) + \dots) \end{aligned} \right\} \quad (16)$$

From equation (16) the following equations are generated for order zero and order one:

$$\left. \begin{aligned} \frac{\partial c}{\partial \tau} &= D^* \frac{\partial^2}{\partial \eta^2} c_0(\eta, \tau) \\ c_0(\eta, 0) &= \frac{c_i}{c_0} \\ c(0, \tau) &= 2 - q\tau \\ c(1, \tau) &= 0 \end{aligned} \right\} \quad (17)$$

$$\left. \begin{aligned} \frac{\partial c_1}{\partial \tau} &= D^* \frac{\partial^2}{\partial \eta^2} c_1 - b \frac{\partial}{\partial \eta} c_0 - c_0 \\ c_1(\eta, 0) &= 0 \\ c_1(0, \tau) &= 0 \\ c_1(1, \tau) &= 0 \end{aligned} \right\} \quad (18)$$

The above equations (17) and (18) are transformed to satisfy the homogeneous boundary conditions. This is done by using a function $g_0(\eta, \tau)$ which satisfies the boundary conditions:

$$g_0(\eta, \tau) = \alpha(\tau) + \frac{\eta}{l}(\beta(\tau) - \alpha(\tau)) \quad (19)$$

where $\alpha(\tau) = 2 - q\tau$ and $\beta(\tau) = 0$

so that

$$c_0(\eta, \tau) = w_0(\eta, \tau) + g_0(\eta, \tau) \quad (20)$$

Substituting (20) into (17) and (18), the following initial boundary value problems are obtained:

$$\left. \begin{aligned} \frac{\partial w_0}{\partial \tau} &= D^* \frac{\partial^2 w_0}{\partial \eta^2} - q(\eta - 1) \\ w_0(\eta, 0) &= \frac{c_i}{c_0} + 2(\eta - 1) \\ w_0(0, \tau) &= 0 \\ w_0(1, \tau) &= 0 \end{aligned} \right\} \quad (21)$$

$$\left. \begin{aligned} \frac{\partial w_1}{\partial \tau} &= D^* \frac{\partial^2 w_1}{\partial \eta^2} - b \frac{\partial w_0}{\partial \eta} - w_0 \\ w_1(\eta, 0) &= 0 \\ w_1(0, \tau) &= 0 \\ w_1(1, \tau) &= 0 \end{aligned} \right\} \quad (22)$$

Then equations (21) and (22) are solved by Eigen-function expansion technique to obtain a solution of the form:

$$w_0(\eta, \tau) = \sum_{n=1}^{\infty} w_n(\tau) \sin n\pi\eta \quad (23)$$

as used by [16].

where

$$w_n(\tau) = \int_0^{\tau} e^{-D^* \left(\frac{n\pi}{l}\right)^2 (t-\tau)} \cdot F_n(t) dt + b_n e^{-D^* (n\pi)^2 \tau} \quad (24)$$

$$F_n(\tau) = \frac{2}{l} \int_0^l F(\eta, \tau) \sin n\pi\eta d\eta \quad (25)$$

$$b_n = \frac{2}{l} \int_0^l F(\eta) \sin n\pi\eta d\eta \quad (26)$$

The solution of the initial boundary value problem (21) and (22) are therefore given below:

$$c_0(\eta, \tau) = (2 - q\tau)(1 - \eta) + \sum_{n=1}^{\infty} \left(\frac{2q}{D^* (n\pi)^3} \left[1 - e^{-D^* (n\pi)^2 \tau} \right] - \frac{2}{n\pi} \left(\frac{c_i}{c_0} (\cos n\pi - 1) + 2 \right) e^{-D^* (n\pi)^2 \tau} \right) \sin n\pi\eta \quad (27)$$

$$c_1(\eta, \tau) = w_1(\eta, \tau) \quad (28)$$

$$c_1(\eta, \tau) = - \sum \left(\sum \frac{2q}{D^* (n\pi)^3} \left[\frac{1}{D^* (n\pi)^2} \left(1 - e^{-D^* (n\pi)^2 \tau} \right) - \tau e^{-D^* (n\pi)^2 \tau} \right] \right) \sin n\pi\eta + \sum \left(\sum \frac{2}{n\pi} \left[\frac{c_i}{c_0} (\cos n\pi - 1) + 2 \right] \tau e^{-D^* (n\pi)^2 \tau} \right) \sin n\pi\eta \quad (29)$$

Therefore, the solution of the cross-flow dispersion problem (2) is therefore

$$c(\eta, \tau) = c_0(\eta, \tau) + \alpha c_1(\eta, \tau) \quad (30)$$

where $b = \frac{1}{\alpha}$ (as approximated from the expansion perturbation parameter)

RESULTS AND DISCUSSIONS

In this section, the solution obtained for the cross-flow dispersion problem is expressed in graphical forms with the aid of the Mathematical software called MAPLE 16. The suitable initial values of the parameters used are $D_{L0} = 1.0$, $D_{T0} = 1.5$, $D_{LT0} = 4.0$, $q = 3.0$, $u_0 = 0.1$, $v_0 = 0.1$ and $\alpha = 0.1$.

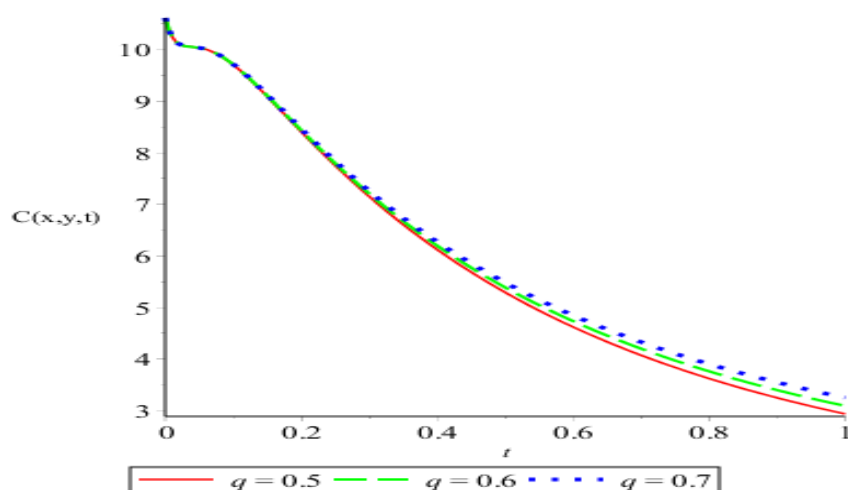


Figure 1: Concentration Profile of Contaminant Concentration with Time for Varying Flow Resistance Coefficient.

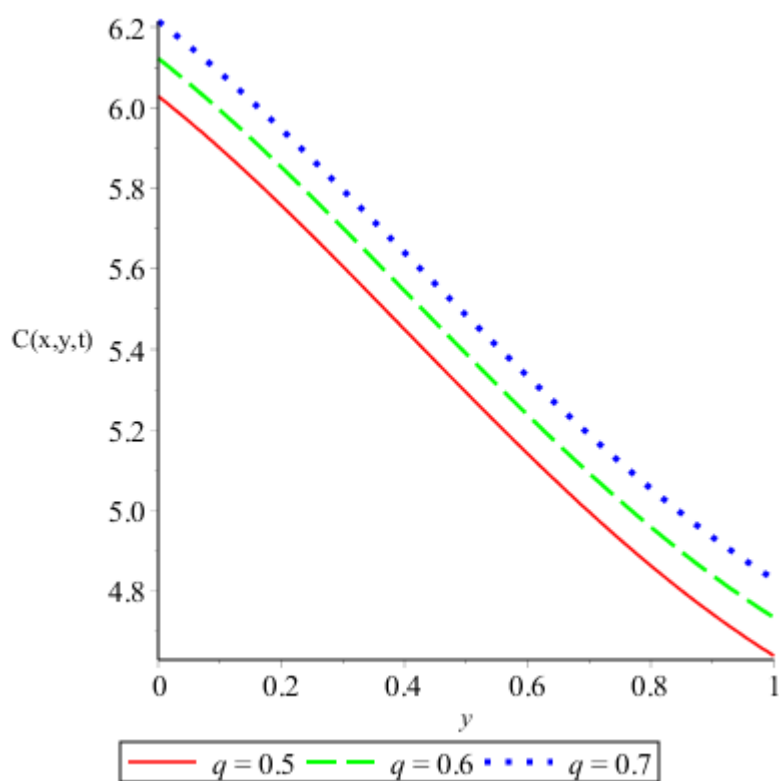


Figure 2: Concentration Profile of Contaminant Concentration with Vertical Distance y for Varying Flow Resistance Coefficient.

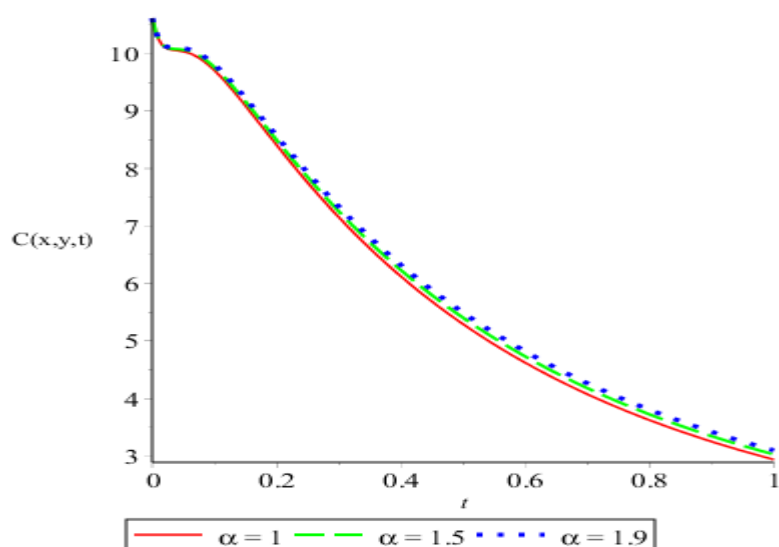


Figure 3: Concentration Profile of Contaminant Concentration with Time for Varying Decay Parameter.

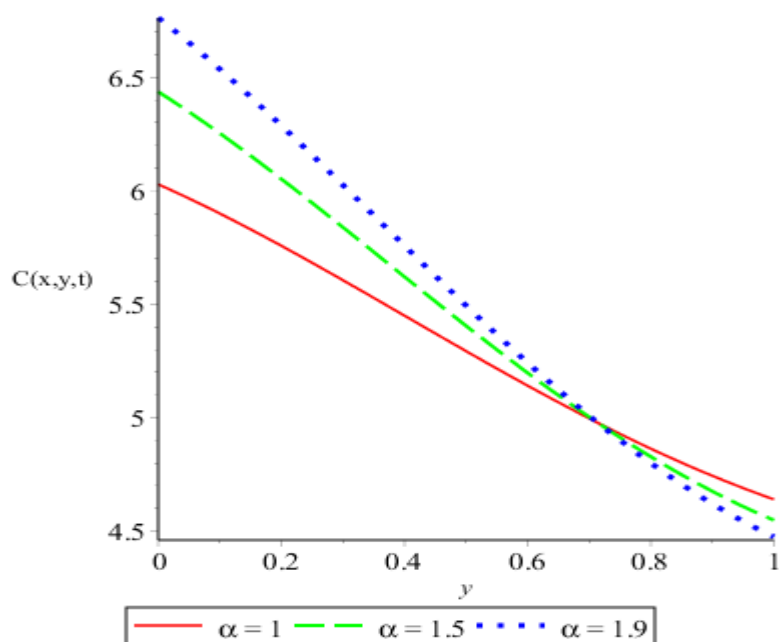


Figure 4: Concentration Profile of Contaminant Concentration with Horizontal Distance y for Varying Initial Decay Coefficient.

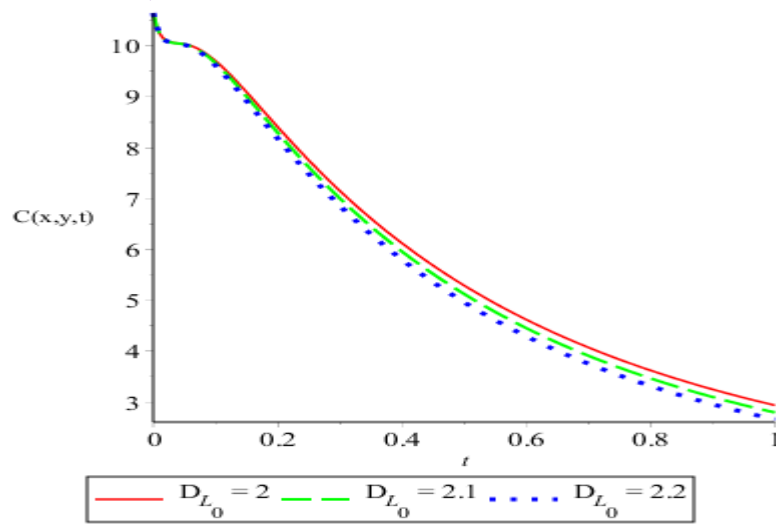


Figure 4: Concentration Profile of Contaminant Concentration with Time for Varying Longitudinal Dispersion Coefficient.

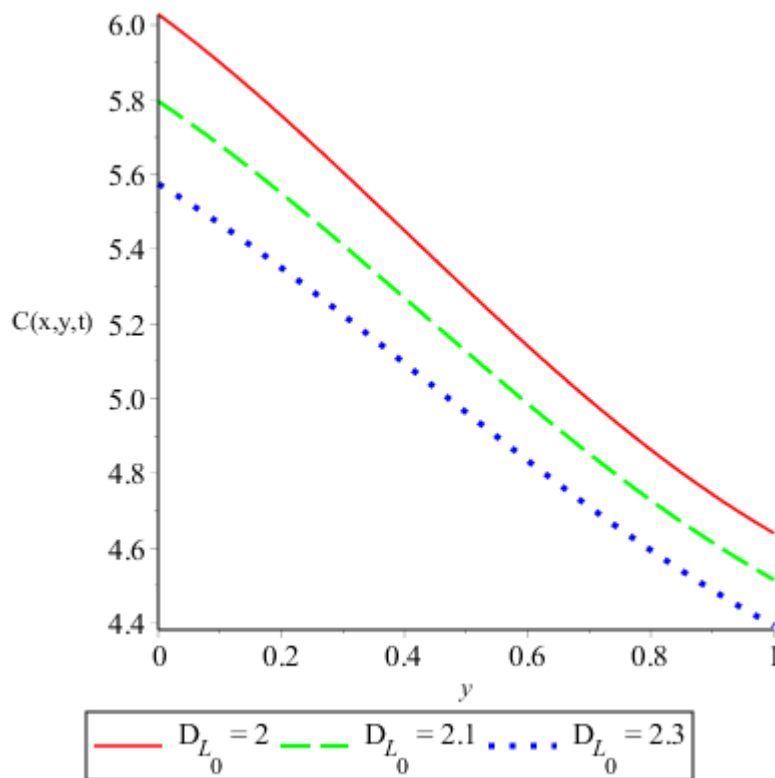


Figure 6: Concentration Profile of Contaminant Concentration with Vertical Distance y for Varying Initial Horizontal Dispersion Coefficient.

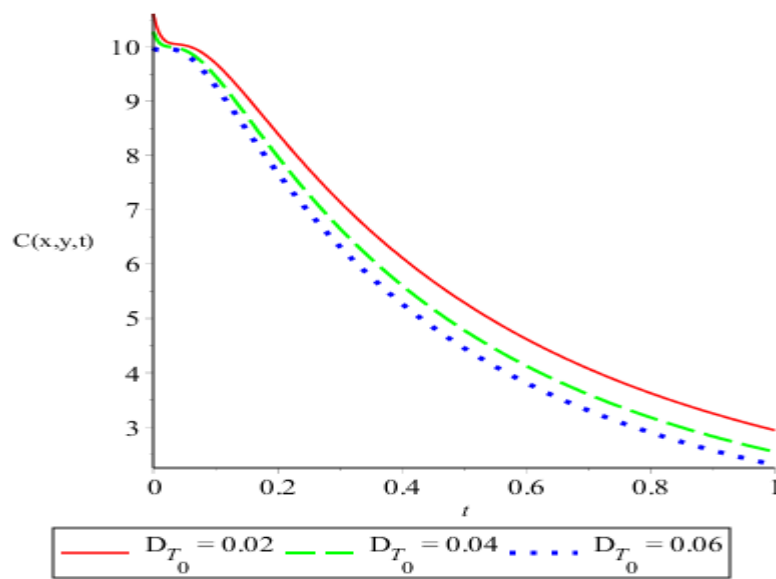


Figure 7: Concentration Profile of Contaminant Concentration with Time for Varying Vertical Dispersion Coefficient.

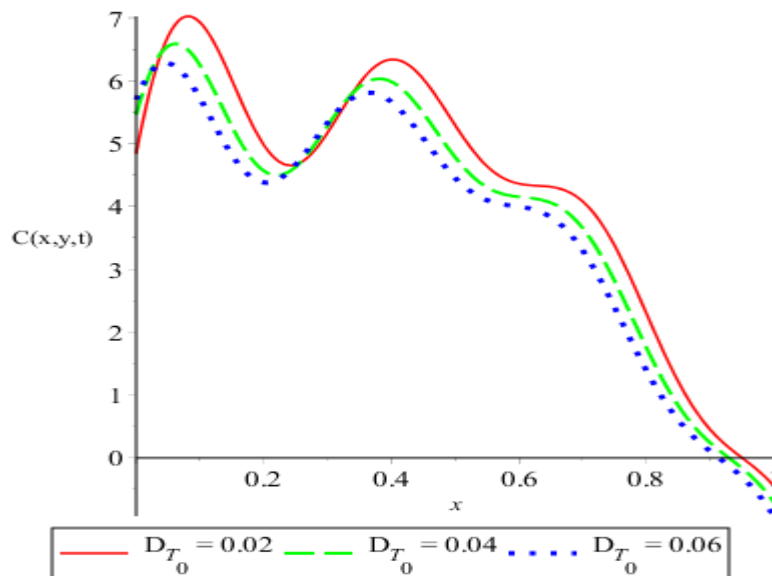


Figure 8: Concentration Profile of Contaminant Concentration with Horizontal Distance x for Varying Initial Vertical Dispersion Coefficient.

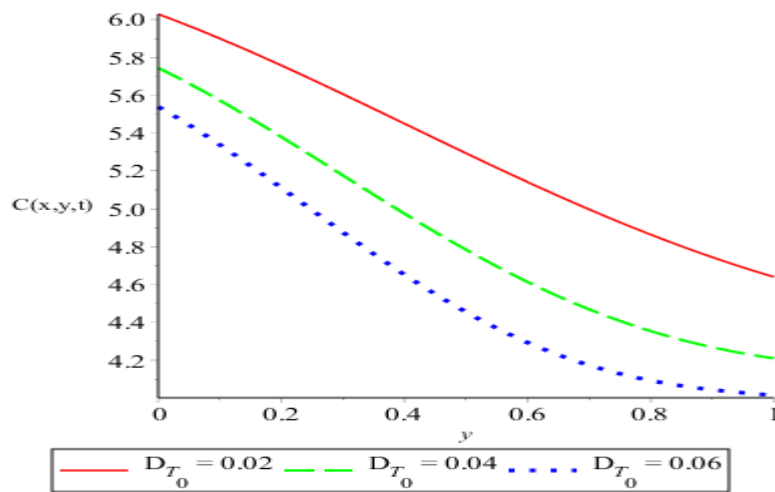


Figure 9: Concentration Profile of Contaminant Concentration with Vertical Distance y for Varying Initial Horizontal Dispersion Coefficient.

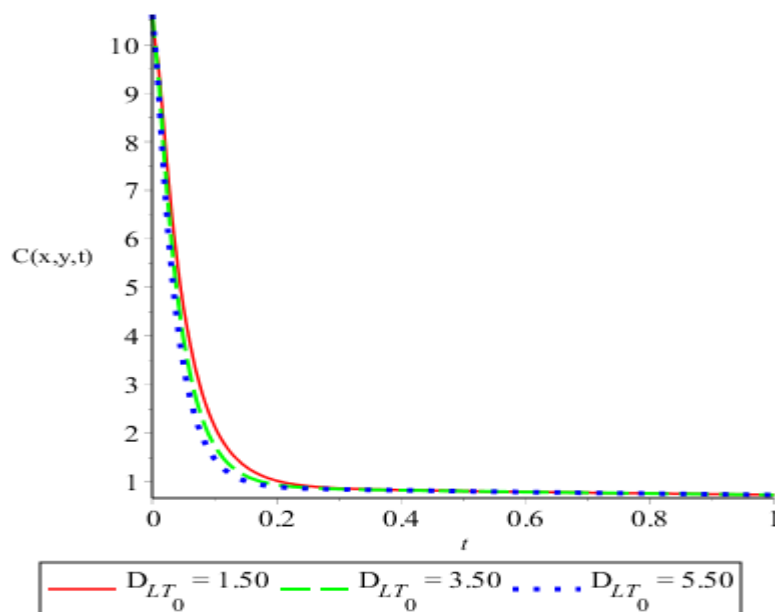


Figure 10: Concentration Profile of Contaminant Concentration with Time for Varying Cross-flow Dispersion Coefficient.

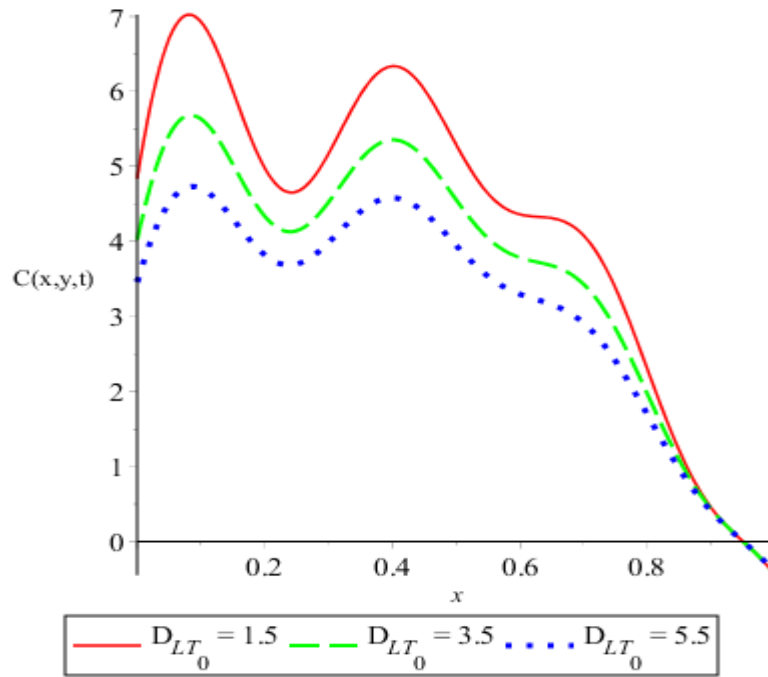


Figure 11: Concentration Profile of Contaminant Concentration with Horizontal Distance x for Varying Initial Cross-flow Dispersion Coefficient.

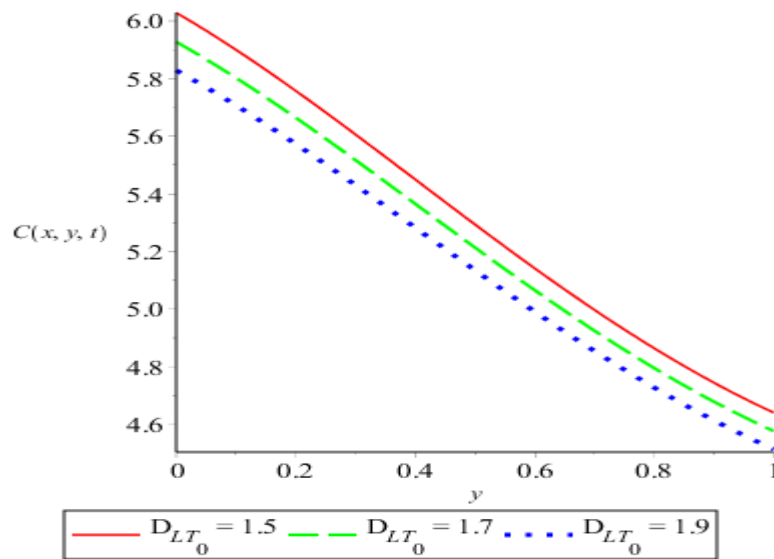


Figure 12: Concentration Profile of Contaminant Concentration with Vertical Distance y for varying Initial Cross-flow Dispersion Coefficient.

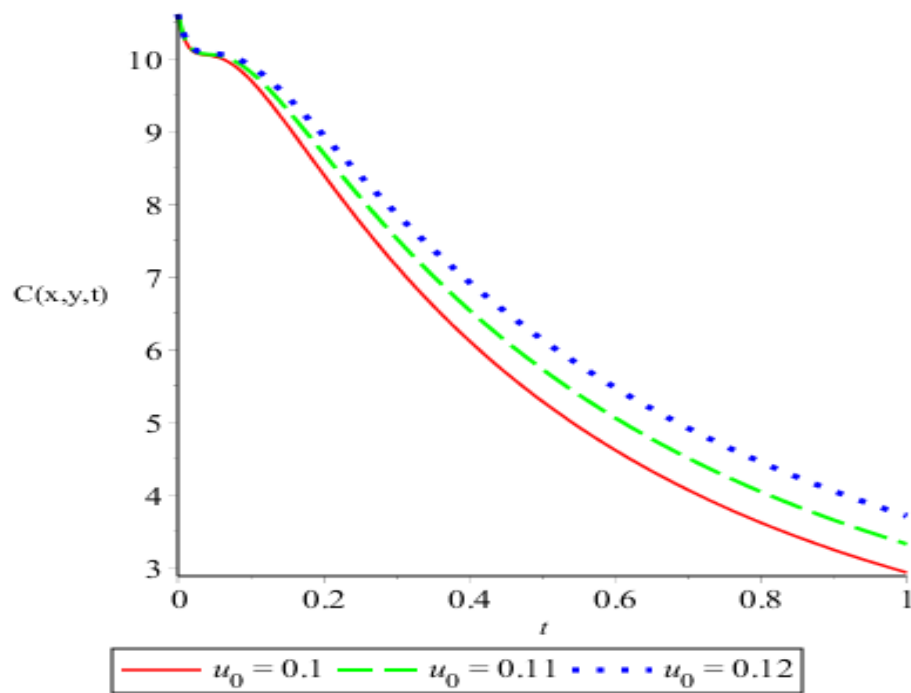


Figure 13: Concentration Profile of Contaminant Concentration with Time for Varying Initial Horizontal Velocity Coefficient.

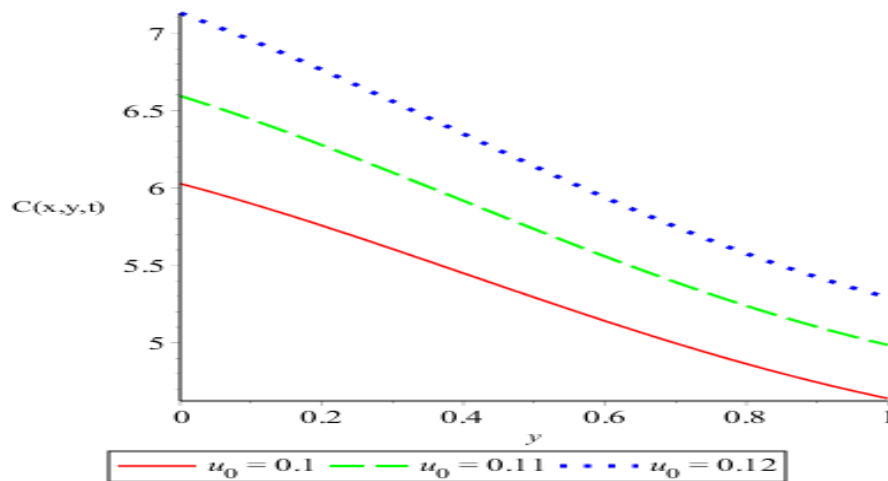


Figure 14: Concentration Profile of Contaminant Concentration with Vertical Distance y for Varying Horizontal Velocity Dispersion Coefficient.

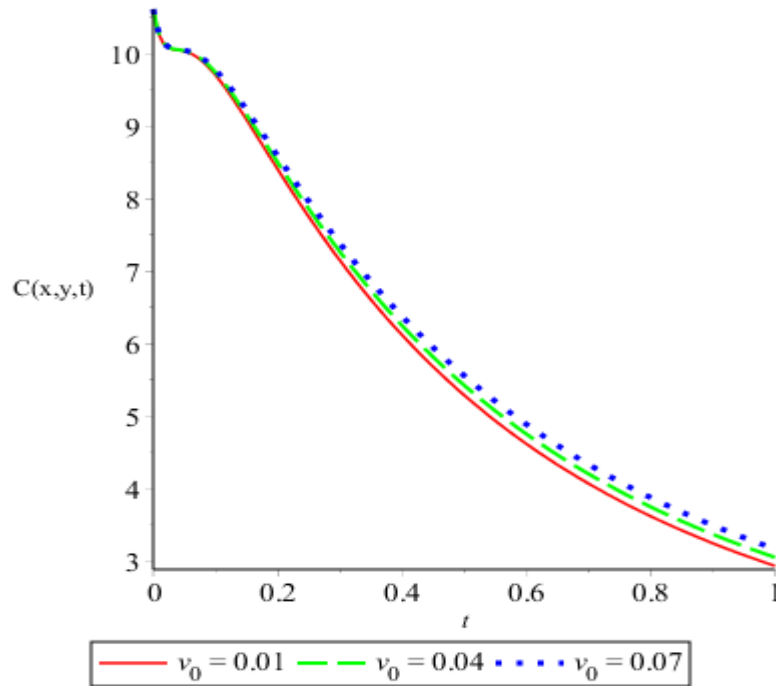


Figure 15: Concentration Profile of Contaminant Concentration with Time for Varying Initial Horizontal Velocity Coefficient.

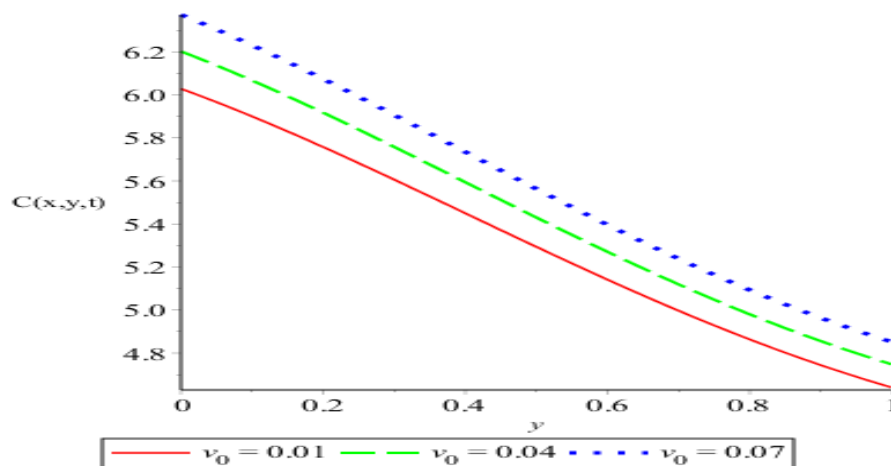


Figure 16: Concentration Profile of Contaminant Concentration with Vertical Distance y for Varying Horizontal Velocity Coefficient.

CONCLUSION

The contaminant flow model that incorporates the cross-flow dispersion and decay parameter was formulated with associated Dirichlet boundary conditions. The problems was solved by using combination of parameter expanding method, Eigen-Functions expanding technique and direct integration method.

The behaviors of the flow were expressed in graphical form in order to study and interpret the behavior of the concentration of the contaminant as the values of the parameters are varied. Findings show that

the concentration of the contaminant decreases with time for increasing values of the parameters, $D_{L0} = 1.0$, $D_{T0} = 1.5$, $D_{LT0} = 4.0$, $q = 3.0$, $u_0 = 0.1$, $v_0 = 0.1$ and $\alpha = 0.1$.

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