ANALYSIS OF TWO-DIMENSIONAL CROSS-FLOW OF REACTIVE CONTAMINANT

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ABSTRACT

The advection-dispersion equation is commonly employed in studying solute migration in a flow. This study presents semi-analytical solution of two-dimensional contaminant flow models incorporating the cross-flow dispersion parameter and a decay term for evaluating groundwater contamination in a homogeneous finite medium. In deriving the model equations, it was assumed that there was a constant point-source concentration at the origin. Two models were considered: case 1 with Neumann boundary conditions and case 2 with associated Dirichlet boundary conditions. The cross-flow dispersion, horizontal dispersion, vertical dispersion, velocities and decay terms are time-dependent. The model equations were transformed and solved by combined parameter expanding method, Eigen-functions expansion method and direct integration method. The results which investigate the effect of change in the parameters on the concentration were discussed and represented graphically for suitable initial 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 $\alpha = 0.1$, The study revealed that as the decay parameter increases, the contaminant concentration decreases with time in the two cases considered, while in case 2, the contaminant concentration declines with both time and distances as the values of the parameters listed above increase.

TABLE OF CONTENTS

Contents **Pages**

CHAPTER TWO

CHAPTER THREE

CHAPTER FOUR

CHAPTER FIVE

LIST OF FIGURES

Figures **pages**

NOTATIONS

The following symbols are used in the project

K - permeability

V_p – pressure drop

D_x – horizontal dispersion

D_y – vertical dispersion

D_L – Longitudinal dispersion coefficient

D_T – vertical dispersion coefficient

s – concentration of contaminant attached to porous media

D_{LT} – cross-flow horizontal dispersion coefficient

D_{TL} – cross-cross-flow vertical dispersion coefficient

q – flow resistance parameter $\left[T^{-1}\right]$

c – solute concentration in the liquid phase $\left[ML^{-1}\right]$

v – seepage or average pure water velocity $\left[LT^{-1}\right]$

u – initial velocity $\left[LT^{-1}\right]$

c_0 – initial concentration $\left[ML^{-3}\right]$

R_i – initial concentration $\left[ML^{-3}\right]$

$R -$ retardation factor

$\tau -$non-dimensional time variable

$\alpha -$ decay parameter

$x -$the longitudinal direction of flow (L)

$D_n -$dispersion porosity of the different geologic formation

$t -$time variable

$k_d -$distribution coefficient

CHAPTER ONE

1.0 INTRODUCTION

1.1 Background to the Study

Groundwater is the water found beneath 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. Groundwater is usually 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 (Paladino *et al.*, 2018). Part of the reason for this is that surface water is more readily exposed to pollutants (from sources such as factories) than groundwater. Thus groundwater serves as an essential source of drinking water and other domestic use in most part of the world. However, its contamination is one of the most typical hydro-geological and environmental problems. Groundwater contamination occurs when pollutants are released to the ground and make their way down into groundwater. This type of water pollution can also occur naturally due to the presence of a minor and unwanted constituent, contaminant or impurity in the groundwater (Jaiswal *et al.,* 2011). The pollutant often creates a contaminant plume within an aquifer which spreads the pollutant over a wider area. Its advancing boundary, often called a plume edge, can intersect with groundwater wells or daylight into surface water such as seeps and springs making the water supplies unsafe for humans and wildlife. The movement of the plume may be analyzed through a hydrological transport model or groundwater model. Analysis of groundwater pollution may focus on soil characteristics and site geology, hydrogeology, hydrology and the nature of the contaminants. In many parts of the world, groundwater resources are under increasing threat from growing demands, wasteful use and contamination. The fare and transport of solute in soils and groundwater has long been a focus of experimental and theoretical research in subsurface hydrology. Solute transport in the soil and the groundwater is affected by a large number of physical, chemical and microbial processes, such as on-site sanitation systems, landfills, effluent from wastewater treatment plants, leaking sewers, petrol filling stations or from over application of fertilizers in agriculture and the properties of the media. Once the groundwater is contaminated, it is extremely difficult and costly to remove the contaminants from the groundwater (Gurganus, 1993). In many practical situations, one needs to predict the time behavior of a contaminated groundwater layer. Most of the groundwater contaminants are reactive in nature and they infiltrate through the Vadoze zone, reach the water-table, and continue to migrate in the direction of groundwater flow. Therefore, it is essential to understand the transport process of contaminants through the subsurface porous media.

1.2 Statement of the Research Problem

The importance of the utilization of groundwater resources continues to grow due to the increasing requirement for water for irrigation, drinking, commercial, agricultural and industrial proposes. From this, we can see that water become an even more important part of human life. Contaminated groundwater can enter the food chain and cause many life-threatening diseases and problems. The effect of drinking contaminated or dirty water causes waterborne disease. Contaminated water can cause many types of diarrheal diseases, including Cholera, and other serious illnesses, such as Guinea worm disease, Typhoid and Dysentery. The solution to this problem is to approximate when the water from the primary source of drinking will become a hazardous zone. Hence, sustainable management planning must be developed for groundwater systems. The main focus of this study is to consider the transport and fate of reactive contaminant and determine how to take care of problems associated with it. A number of mathematical models describing groundwater flow and solute transport in homogeneous and heterogeneous porous domain have been developed in the past (Lee & Kim, 2012). Several methods such as Laplace transform technique, Green's function method and generalized integral transform technique have been used to model and solve these problems in one - two and three dimensions. Despites all efforts, contaminants still remain a major problem that possess a threat, hence the need for this research.

1.3 Aim and Objectives of Study

The aim of this work is to carry out analysis of two-dimensional cross-flow of reactive contaminants.

The objectives are to;

i. extend the work of Lee and Kim (2012) on two-dimensional cross-flow by incorporating the decay and reactive contaminant term;

ii. solve the two-dimensional cross-flow model with Neumann boundary condition using Eigen-Function Expansion Technique;

iii. solve the two-dimensional cross-flow model with Dirichlet boundary condition using Eigen-Function Expansion Technique;

iv. obtain the graphical simulations of the solutions obtained;

v. find the effects of change of the parameters of the model on the concentration of the contaminant.

1.4 Justification of the Study

Groundwater contamination is a major problem related strongly to both; protection of environment and the need of water. Due to the increasing interest in groundwater protection, models for simulating contaminants fate and transport in the unsaturated zone are valuable and useful tools in many scientific and engineering applications. Several modeling approaches are available in the scientific literature, ranging from models that solve a single equation (solute transport) to more complex models that solve a set of governing equations (groundwater flow, solute transport, heat movement) due to the increasing concern of the healthy hydro–environment nature for the existence of life on earth. This problem has led to growing interest in the study of fate and transport of contaminants through a homogeneous finite aquifer.

1.5 Scope of the Study

This research work considers a two-dimensional contaminants flow model incorporating cross-flow dispersion and reaction term. This research however, does not put in to consideration, three-dimensional contaminant flow.

1.6. Definition of Terms

Advection – Dispersion Equation (ADE): The ADE relates one or more function and their derivatives either ordinary differential equation or partial differential equation.

Model: a simplified description of a system or process that can be used as an aide in analysis or design.

Porous Media: is a solid matrix that is partially filled by interconnected voids (pores) which can convey fluids under an applied gradient.

Surface water: bodies of water on or above the surface of the earth such as lakes, streams, ponds, wetlands

Aquifer: is a geological formation in an underground with structures or textures capable of storing and transmitting water such as springs and wells.

Ground Water: is the water stored underground which flow downward saturating soils or rocks and supplying springs and wells.

Ground Water Recharge: inflow of water to a ground water reservoir from the surface.

Discharge Rate: the rate at which water is removed from ground water reservoir.

Contamination: Is the introduction of any substance into the ground water as a result of man's activities causing significant degradation of water quality, deteriorating and restricting water usage.

Contaminants: physical, chemical, biological and radiological substances in water which are introduced by humans and are harmful.

Contaminate: to introduce a substance into waters that would cause the concentration of that substance to exceed the maximum contaminant level.

Contaminant Transport Model: is the application of a mathematical model to represent a regional ground water contamination problem.

Contamination Plume: is an area of degraded water in an aquifer resulting from migration of a contaminant.

Point Source: a source of pollution that can be traced to or is released at a definable single place.

Pollution: any aspect of water quality (physical, thermal, chemical, or biological) that interferes with an intended use.

Water Pollution: is an alteration of the physical, chemical or biological properties of a water resource making it harmful or less fit for any beneficial water purpose and usage.

Pollution Source: is the origin of ground water pollution.

Molecular Diffusion: is the mass spreading of contaminants under a chemical concentration gradient from an area of greater concentration towards an area of lower concentration.

Advection: is the mass transportation process of solutes in ground water system caused by the bulk movement of flowing ground water.

Leaching: a quantity of wood ashes, through which water passes and thus imbibes the alkali

Sub- surface: a surface which is sub manifold of another surface.

Adsorption: the adhesion of a liquid or gas on the surface of a solid material forming a thin film on the surface.

Porosity: a measure of how porous a material is, the ratio of the volume of pores to the total volume

Advection: the horizontal movement of a body of atmosphere (or other fluid) along with a contaminant transport of its temperature humidity. **Dispersion:** the state of being dispersed.

Diffusion: the movement of water vapor from regions of high concentration (high water vapor pressure) toward regions of lower concentration.

Hydrodynamic Dispersion: the dispersion or spreading of solutes, colloids, or heat in a groundwater system which is caused by variations in the velocity and direction of flow.

Retardation: the process by which a solute travel at a slower rate than the average linear velocity because of partitioning onto the solid phase of the porous medium.

Retardation factor: a dimensionless number expressing the relative velocity of a chemical in ground water to that of water. Retardation factor represents the delay in the contaminants migration due to linear and instantaneous adsorption to the solid phase.

Diffusion Coefficient: the coefficient relating solute flux due to diffusion to the concentration gradient.

Diffusivity: the ratio of conductivity to storage capacity

Distribution Coefficient: the measure of the tendency of a solute to sorb to the solid phase of a porous media.

Remediation: is the reduction in concentration of contaminants to some acceptable or usable level in ground water.

Percolation: is a process of downward movement of water and contaminants in the unsaturated zone influenced by gravity and hydraulic force to the ground water system.

Permeability: the ability of a material to allow the passage of a liquid such as water.

Homogenous: is a characteristic of the same or similar nature that is uniform in structure or composition throughout.

Homogeneity: the property of a parameter or system whose values are unchanged over space.

Heterogeneous: is a characteristic of dissimilar nature that is different in structure or composition.

Anthropogenic: created or caused, or induced by human actions

Concentration: the amount of dissolved or colloidal species in water

Infiltration: the movement of water from the surface of the land into the subsurface.

Permeability: the ease with which a porous media can transmit water or other fluids.

Plume: a three dimensional body of fluid emanating from a point source or point sources with a chemistry or physical composition differing from the ambient groundwater, atmosphere, or surface water body.

Source: any point by which fluid, colloids, or heat is added to a groundwater system.

Geology: the fields of study concerned with the structure, evolution and dynamics of the Earth and its natural mineral and energy resources.

Hydrogeology: is the area of geology that deals with the distribution and movement of groundwater in the soil and rocks of the Earth's crust.

Hydrology: is the science that encompasses the study of water on the Earth's surface and beneath the surface of the Earth, the occurrence and movement of water, the physical and chemical properties of water, and its relationship with the living and material components of the environment.

CHAPTER TWO

2.0 LITERATURE REVIEW

2.1 Groundwater Contaminant Transport Models

Immiscible solute or tracer particles of pollutants are major cause of degradation of the hydro-environment in the surface water bodies and aquifers, (Dilip *et al.,* 2011). In most cases, groundwater is safer and more reliable for use than surface water. One of the reason is that 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 in Nigeria as well as in other countries. However, the determination of the environmental indicators of many ecosystems has led to stringent environmental control and an increase in research into the fate of contaminant in water. The ability of practitioners and regulators to predict the extent and the rate of dispersion of pollution plumes can help them develop better pre-emptier or remedial strategies. The contaminant of soil and groundwater by chemicals has become an increasing concern in the recent past years. These chemicals enter the groundwater system by a wide variety of mechanisms including accidental spills, land disposal of domestics and industrial wastes and application of agricultural fertilizers. Once introduced into an aquifer, these contaminants are transported by flowing groundwater and degraded water qualities at nearby wells and streams. For improving the management and protection of groundwater resources, it is important to first understand the various processes that can control the transport of contaminant in groundwater. Prediction of the facts of groundwater contaminant can be to assess the effect of this chemical on local water resources and to evaluate the effectiveness of remedial actions. There is need for the study in the area of contaminant transport modeling for the prevention of unacceptable long-term environmental impact of the contaminant. There are two major methods applied in examining contaminant transport with regard to reactions in porous media. These methods are termed stochastic and deterministic (Flury *et al.,* 1998; Kia, 1991; Gao *et al.,* 2013). Stochastic methods deal with reaction coefficients and are considered to 'be stationary processes' (Loll & Moldrup, 2000; Sleep & McClure, 2001; Deceuster & Kaufmann, 2012), or they may be verified through a random hydraulic conductivity field (Miralles-Wilhem & Gelhar, 1996). As proper site-specific quantities are fundamental for simulation of contaminant transport, these models are expensive and unlikely to be used in practical cases (Gao *et al.,* 2013). The other approach is to analyze which of the deterministic methods could be simpler and more general compared to the stochastic methods (Gao *et al.,* 2013) by considering two dimensions for the soil medium and the possibility of it being developed without Laplace transformation. One approach to consider deterministically is to model the soil medium as a layered system in which each layer has its own constant coefficients of reaction (Wu *et al.,* 1997; Vanderborght & Vereecken, 2007; Lewis & Sjöstrom, 2010). In order to allow early detection of possible contamination of groundwater, Chegenizadeh *et al.,* (2014) developed a prediction model by introducing the concept of modeling of contamination transport through a soil matrix in a two-dimensional convection-dispersion equation for contaminant transport in a soil matrix. Their study includes the investigation of different reaction coefficients and time-dependent inlet boundary conditions, from which a numerical solution is derived.

Ghoraba *et al.,* (2013), investigated groundwater quality through hydro chemical analyses in order to assess the quality of water in samples taken from the canals, drains and groundwater. A 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. In their results, levels of water were determined and the values of solute concentration and distribution of water in the region at different times were evaluated. They also proposed a groundwater remediation scheme by using group of extraction wells at some region where the concentration values of ammonium contaminants are the up most according to hydro chemical analyses results. Also proposed scenario for cleaning to use a set of wells to pump contaminated groundwater extraction for treatment and reused in irrigation.

Ghose *et al.,* (2013), observed that in planning of water resource projects, the estimation of the availability of water plays an important role. The first step in the water availability estimation is the computation of runoff resulting from the precipitation on river catchments. The length of the run off measured in a stream may be of short period or long period depending upon the catchment characteristics. Therefore, keeping this in mind, their work focused on two different model generation – runoff rating curves, considering present day water level (H(t)) as input and present day runoff (Q(t)) as the model output; and runoff prediction models, considering 1 day lag water level (H(t - 1)), 2 day lag water level (H(t-2)) and 1 day lag runoff (Q(t - 1)) as inputs and 1 day ahead runoff (Q(t+1)) as the output of the model. Models developed which were used for prediction of runoff are Non-Linear Multiple Regression (NLMR) and Adaptive Neuro-Fuzzy Inference System (ANFIS). Both models were trained and tested to predict the performance of models. Genetic Algorithm (GA) is then coupled with NLMR model to obtain the condition of hydrological parameter for which the runoff is maximum.

Seyf-Laye *et al.,* (2012), developed 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 in the central Beijing area. They estimated current contaminant fluxes to the central area and site streams via groundwater by developing a program of groundwater model. The conceptual model developed for the site attempted to incorporate a complex stratigraphic profile in which groundwater flow and contaminant transport is strongly controlled by a shallow aquifer. Their model simulations indicated that a sharp drop in the hydraulic head occurs at the center of the model area, which generates a cone of depression and a continuous decline of head with respect to time as a result of heavy groundwater abstraction.

2.2 Groundwater Contaminant Models in One-Dimension

Mathematical modeling is a powerful tool in managing the groundwater resources and rehabilitation of polluted aquifers. The distribution and behavior of contaminant concentration along/against unsteady groundwater flow in aquifer is usually studied through mathematical modeling as it is an essential approach to formulate the geo-environmental problems and provides the best possible solution for reducing its impact on the environment. The pollutant's solute 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 (Singh, 2011), and is known as advection-diffusion equation (ADE). In one-dimension is contains two coefficients, one represents the diffusion parameter and the second represents the velocity of the advection of the medium. A one-dimensional solution can be suitable to model contaminant in laboratory columns, pollution in aquifers where the contamination source extends through the saturated zone in either transverse y and z directions or cases where dispersion in y and z directions can be neglected (Moranda *et al.,* 2018). Many one-dimensional exact analytical solutions in closed form have been proposed, and scientists' attention has been dedicated to solutions that have time-dependent sources (Chen *et al.,* 2017). A library of one-dimensional analytical models that encloses some solution with source decay was proposed by Van Genuchten *et al.,* (1982). Guerrero *et al.,* (2013) proposed a Duhamel theorem based approach in order to compute one-dimensional solution with time dependent boundary conditions and gave some solution in closed form for exponential source decay. The literature contains analytical solutions for solute transport in homogenous and heterogeneous porous media. Analytical solution in one-dimensional advection-dispersion transport equations in homogeneous medium have been collected in various compendiums. These analytical solutions are useful for providing contamination scenarios in risk analysis, to investigate the effects of chemical-physical parameters on contaminant transport, and also to validate the numerical models (Moranda *et al.,* 2018). Singh *et al.,* (2009), derived an analytical solution of solute concentration for space-time variation in unsteady flow in a homogeneous finite aquifer subjected to point source contamination under the conditions of the flow velocity in the aquifer of sinusoidal form and the flow velocity as an exponentially decreasing function. The sinusoidal form represents the seasonal variation in tropical regions. In their work, it is found that the time dependent velocity has a significant effect on the migration of pollutant in aquifers. Similarly, Singh *et al.* (2015), obtained analytical solutions for one-dimensional solute dispersion along uniform groundwater flow in a semi-infinite aquifer using the Laplace transform technique to describe the nature of the contaminant concentration with respect to space and time for Dirichlet and Cauchy-type boundary conditions. The results obtained for two expressions of temporally dependent dispersion, such as the sinusoidally and exponentially increasing forms, are more realistic as the time-dependent input concentration is considered at the source and more significant than the uniform source of the input concentration.

Moranda *et al.,* (2018), proposed an analytical solution in closed form of the advection-dispersion equation in one dimensional contaminated soils which is valid for non-conservative solutes with first order reaction, linear equilibrium sorption, and a time-dependent Robin boundary condition representing a combined production-decay release mechanism. Their governing equation is written as:

$$S\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2} - \upsilon\frac{\partial C(x,t)}{\partial x} - \lambda C(x,t) \tag{2.1}$$

subject to the following initial and boundary conditions

$$\left.\begin{aligned} &C(x,0) = 0, \quad C(0,t) = h(t) \\ &-D\frac{\partial C(x,t)}{\partial x} + \upsilon C(0,t) = \upsilon g(t) \end{aligned}\right\} \tag{2.2}$$

The above model is particularly useful to describe sources as the contaminant release due to the failure in underground tanks or pipelines, on Aqueous Phase Liquid pools, or radioactive decay series which shows that the use of the Robin boundary condition can underestimate concentration profiles.

Purkayastha and Kumar (2018), presented an analytical solution for the one-dimensional advection diffusion equation for studying the contaminant transport in groundwater. The solution obtained in their work is for spatially varying diffusivity and velocity terms along with time varying boundary conditions. The differential equation considered in their paper is in the form of Legendre Linear Differential Equation which is reduced to a linear differential equation having constant coefficients by a suitable transformation. The final solution for differential equation in the transformed domain is obtained by the method of Eigen-function expansions.

Yadav and Kumar (2017) described the analytical solution of spatially dependent solute transport in one-dimensional semi-infinite homogeneous porous domain assuming that the dispersion coefficient is considered spatially dependent, while seepage velocity is considered exponentially decreasing function of space. Dispersion parameter and velocity are directly proportional to each other; space dependent retardation factor was also taken. The nature of porous media and solute pollutant were considered chemically non-reactive. Initially porous domain was considered solute free and the input source condition was considered uniformly continuous. They presented the advection-dispersion equation in one-dimension with initial and boundary conditions as follows:

$$R(x,t)\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C}{\partial x}-u(x,t)C\right) \tag{2.4}$$

$$\left.\begin{aligned} &C(x,t)=0 &&;\ t=0, x\geq 0\\ &C(x,t)=C_0 &&;\ t>0, x=0\\ &\frac{\partial C(x,t)}{\partial x}=0 &&;\ t\geq 0, x\to\infty \end{aligned}\right\} \tag{2.5}$$

The following transformation was introduced to solve the advection dispersion equation by Laplace Transformation Techniques

$$\left.\begin{aligned} &u(x,t)=u_0 e^{-mx}\\ &D(x,t)\propto u\Rightarrow\ D(x,t)=D_0 e^{-mx}\\ &R(x,t)\propto u\Rightarrow\ R(x,t)=R_0 e^{-mx} \end{aligned}\right\} \tag{2.6}$$

It was gathered that the trends of solute concentration with distance travelled in presence of source contaminant and time are reducing in nature which may help to understand rehabilitation tendency of the contaminated aquifer in the domain which may help as the primary predictive tools in groundwater management system. From their obtained solution of dispersion equation and graphs, they also concluded that the contaminant concentration reduces with increasing retardation factor whereas increases with increasing time, dispersion parameter and flow resistance coefficients and vice-versa.

2.3 Groundwater Contaminant Model in Two-Dimensions

Limthanakul and Pochai (2020) proposed a two-dimensional mathematical model for long-term contaminated groundwater pollution measurement around a land fill. The model is governed by a combination of two models. The first model is a transient two-dimensional groundwater flow model that provides the hydraulic head of the groundwater.

$$S\frac{\partial H(x,z,t)}{\partial t}=\frac{\partial}{\partial x}\left(K_x\frac{\partial H(x,z,t)}{\partial x}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial H(x,z,t)}{\partial z}\right) \tag{2.7}$$

$$\left.\begin{aligned}
&H(x,z,0)=h(x,z)\\
&h(x,z,t)=h_L(z),\quad \forall z\in[0,I_z],\ x=0,\\
&\frac{\partial h(x,z,t)}{\partial z}=h_T(x),\quad \forall x\in[0,I_x],\ z=M_z,\\
&\frac{\partial h(x,z,t)}{\partial x}=h_R(z),\quad \forall z\in[0,I_z],\ x=M_x\\
&\frac{\partial h(x,z,t)}{\partial z}=h_B(x),\quad \forall x\in[0,I_x],\ z=0
\end{aligned}\right\} \tag{2.8}$$

The second model is a transient two-dimensional advection-diffusion equation that provides the groundwater pollutant concentration.

$$\frac{\partial c(x,z,t)}{\partial t}+u\frac{\partial c(x,z,t)}{\partial x}+w\frac{\partial c(x,z,t)}{\partial z}=D_x\frac{\partial^2 c(x,z,t)}{\partial x^2}+D_z\frac{\partial^2 c(x,z,t)}{\partial z^2}+Q \tag{2.9}$$

$$\left.\begin{aligned}
&H(x,z,0)=h(x,z)\\
&h(x,z,t)=h_L(z),\ \forall z\in[0,I_z],\ x=0,\\
&\frac{\partial h(x,z,t)}{\partial z}=h_T(x),\ \forall x\in[0,I_x],\ z=M_z,\\
&\frac{\partial h(x,z,t)}{\partial x}=h_R(z),\ \forall z\in[0,I_z],\ x=M_x\\
&\frac{\partial h(x,z,t)}{\partial z}=h_B(x),\ \forall x\in[0,I_x],\ z=0
\end{aligned}\right\} \tag{2.10}$$

The explicit finite difference technique was used to approximate the hydraulic head and the groundwater pollutant concentration. The simulations can be used to indicate when each simulated zone becomes a hazardous zone or a protection zone.

Cole *et al.,* (2017) considered (in two-dimensions) the steady state flow condition of the contaminant transport where inorganic contaminants in aqueous waste solutions are disposed off at the land surface where it would migrate through the vadoze zone to underground water through the model equation:

$$v\frac{\partial c}{\partial x} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) \tag{2.11}$$

with the boundary conditions:

$$\left.\begin{aligned} c(x,y) &= c_0; \quad x = 0,\ y = 0 \\ c(x,y) &\to 0; \quad x^2 + y^2 \to \infty \end{aligned}\right\} \tag{2.12}$$

The two-dimensional advection dispersion equation which is solute transport model without sorption or degradation was solved using change of variable method. The effect of Peclet number on the concentration of contaminant was investigated when the Peclet number is less that one and when the Peclet number is greater than one. The result obtained revealed that the contaminant concentration increases along x-direction and decreases along y direction for both values of the Peclet number - greater than one and less than one.

Chegenizadeh *et al.,* (2014) developed a prediction model that allows the early detection of possible contamination by introducing the concept of the modeling of contamination transport through a soil matrix and then presented a two-dimensional Convection-Dispersion Equation (CDE) for contaminant transport in a soil matrix. They investigated the effect of different reaction coefficients and time-dependent inlet boundary conditions, from which a numerical solution is derived. The governing equation is system of uncoupled 2-dimensionalConvection-Dispersion Equation (CDE). The equations were applied on the basis of constant water content, dispersion coefficient and velocity.

$$
\left.
\begin{aligned}
&\frac{\partial c_r}{\partial t} + \frac{\rho b}{\theta}\frac{\partial s}{\partial t} = D\frac{\partial^2 c_r}{\partial y^2} - \vartheta\frac{\partial c_r}{\partial y} - \mu(y)c_r \\
&\frac{\partial c_r}{\partial t} + \frac{\rho b}{\theta}\frac{\partial s}{\partial t} = D\frac{\partial^2 c_r}{\partial x^2} - \vartheta\frac{\partial c_r}{\partial x} - \mu(x)c_r \\
&K_d(x) = K_0 = Cosh^{-2}\left(\frac{x}{x_0}\right) \\
&K_d(y) = K_0 = Cosh^{-2}\left(\frac{y}{y_0}\right) \\
&R(x)\frac{\partial c_r}{\partial t} = D\frac{\partial^2 c_r}{\partial x^2} - \vartheta\frac{\partial c_r}{\partial x} - \mu c_r \\
&R(y)\frac{\partial c_r}{\partial t} = D\frac{\partial^2 c_r}{\partial y^2} - \vartheta\frac{\partial c_r}{\partial y} - \mu c_r \\
&R(x) = 1 + \frac{\rho b K_d(x)}{\theta} \\
&R(y) = 1 + \frac{\rho b K_d(y)}{\theta}
\end{aligned}
\right\} \qquad (2.13)
$$

Ujile (2013) and Singh *et al.* (2015) at different times studied the two dimensional contaminant flow with different boundary and initial conditions:

$$
\frac{\partial c}{\partial t} = D_x\frac{\partial^2 c}{\partial x^2} + D_y\frac{\partial^2 c}{\partial y^2} - u(t)\frac{\partial c}{\partial x} - v(t)\frac{\partial c}{\partial y} \qquad (2.14)
$$

In order to understand the movement and dispersion of solutes in the flow, Lee and Kim (2012) formulated the two-dimensional model:

$$
\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial s} = \frac{\partial}{\partial s}\left(D_{ss}\frac{\partial c}{\partial s} + D_{sn}\frac{\partial c}{\partial n}\right) + \frac{\partial}{\partial n}\left(D_{sn}\frac{\partial c}{\partial s} + D_{nn}\frac{\partial c}{\partial n}\right) \qquad (2.15)
$$

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 convective term are incorporated in order to see the behavior of the concentration.

2.4 Preferential Path and Transport Processes in Sub-Soil

Jarvis (2007) and Clothier *et al.,* (2008) defined Preferential flow as the fast, non-equilibrium flow of water infiltration in the soil that can reduce water and nutrient availability, threaten groundwater, and cause natural disasters such as avalanches, landslides, and mudslides. The residues in the soil are subjected to various processes, viz, adsorption, movement and degradation. Advection carries the contaminant at an average rate as a plug flow. However, in reality, the solute is seen to spread out from the flow path. This spreading or mixing phenomenon is called dispersion. At the microscopic level, the fluid flow within a porous medium is actually a movement along the tortuous three dimensional passages in voids. The local velocities in the passages are different from their macroscopic average values both in magnitude and in direction. Due to the complexity of the micro-geometry of the porous media, one has to describe the flow phenomena in porous media on a macroscopic basis. The spatial average method is a way to transfer properties of porous media from microscopic level to the macroscopic level. The dispersion consists of mechanical hydrodynamic dispersion and molecular diffusion. Mechanical dispersion refers to the spreading and mixing caused long variation in the velocity with which water moves and the fluid mixing due to the effect of unresolved heterogeneities in the permeability distribution.

The molecular diffusion is caused by the non-homogeneous distribution of contaminant in a fluid. The contaminant molecules in high concentration moves to the low concentration areas to form a uniform concentration distribution. Several mechanisms causing macroscopic mixing are generally accounted for in the dispersion coefficient, viz, mixing due to tortuosity, inaccessibility of pore water, recirculation due to flow restriction, macroscopic and hydrodynamic dispersion and turbulence in flow path. The formation of a dispersion coefficient tensor for an anisotropic medium requires five dispersivities by Bear (1972). The effect of preferential flow processes on hydrological processes has been widely discussed in the literature to predict soil solute transport and soil erosion (Nieber & Sidle, 2010; Zhang *et al.,* 2014 and Zhou *et al.,* 2013).

Various factors have influenced the formation, distribution, and differentiation of the preferential flow, leading to complex and diverse research on the preferential flow (Cheng *et al.,* 2011). Factors that affect preferential flow paths include soil types and structure, biological activities (channels of roots and earthworms), soil moisture content, and hydraulic conditions (Hardie *et al.,* 2011; Vannoppen, *et al.,* 2015; Yi, *et al.,* 2019). Soil types and structure have complex effects on preferential flow because of their spatial heterogeneities, which can directly change the hydraulic properties, quantities and distribution of soil macro-pores. Biological activities create complex channel systems that could serve as preferential flow paths, thereby further influencing the lateral and vertical movements of preferential flow (Bargues *et al.,* 2014). The role of antecedent soil water in preferential flow may differ under different soil and macro-pore conditions (Yao *et al.,* 2017). These factors primarily affect the density and distribution of preferential flow paths, altering the soil macro-porous structure and its connectivity through the soil, and consequently determining the scale and nature of the preferential flows. Hydraulic conditions such as rainfall intensity, duration and total rainfall affects the momentum balance of water flow driven primarily by gravity. Studies showed that increase in rainfall intensity can enhance preferential flow as a result of increased soil water pressure (Wu *et al.,* 2014). However, spatial changes of preferential flow under different amounts of precipitation have not been fully described and quantitatively tested, which are crucial to understanding the mechanism of preferential flow in different rainfall events. Jimoh *et al.,* (2017) used the Bubnov-Galerkin weighted residual method to solve a one-dimensional contaminant flow problem which is characterized by advection, dispersion and adsorption was discretized and solved to obtain the semi-analytical solution. The adsorption isotherm was assumed to be of Freudlich type. The results obtained were expressed in graphical form to show the effect of change in the parameters 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 dispersion and velocity coefficient decrease.

2.5 Saturated Porous Media

A porous medium or material is defined as a solid (often called a matrix) permeated by an interconnected network of pores (voids) filled with a fluid, (Yeh *et al.,* 2015). Experimental investigations have shown that variation of porosity and hydraulic gradient are responsible for the deviations from Darcy's law:

$$q = -\frac{k}{\mu}\nabla p \qquad (2.16)$$

(q= instantaneous flow rate, k = permeability, μ = dynamic viscosity of fluid ∇p = pressure drop), which is perfectly obeyed only when the fluid flow is laminar in porous media (Alabi *et al.,* 2009). Previous attempts to modify this equation considered only the effects of porosity of surface-active materials such as clay in causing deviations from Darcy's law. Alabi *et al., (*2009), considered both the effect of porosity of any porous medium and hydraulic gradient from recent experimental data to propose a general equation for both laminar and non-laminar or turbulent fluid flow in porous media at any hydraulic gradient, including the boundary conditions.

The analytical models are the available tools for investigating solute transport in porous media and for estimating potential for contaminant transport in groundwater. Analytical solutions are usually derived from the basis of physical principles and are free from numerical dispersion and other truncation errors that often occurred in numerical simulations. They also provided computationally-efficient tools for modeling the fate and transport of groundwater contaminants plumes (Clement, 2001). In general, the analytical models can be evaluated much more quickly than numerical solutions. In a given transport equation, analytical solution would differ according to the assumed domain geometry, the source geometry and boundary conditions. The ease of use, marks analytical transport models in obvious foremost step in any mass transport modeling. Analytical solutions of the advection-dispersion solute transport equation remain useful for a large number of applications in water science and engineering, hydrological science and engineering, environmental science and engineering (Das *et al.,* 2017). The dominant process of solute transport is advection moving aqueous chemical species along with fluid flow. Most of the solute transport modeling begins with advective transport. The advection-dispersion equation describes the spatial and temporal variation in solute concentration with specific initial and boundary conditions. The governing equation known as the constant-parameter advection-dispersion equation:

$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} \qquad (2.17)$$

may be derived for the case of steady and unsteady flows. The traditional advection-dispersion equation represents a standard model to predict the solute concentration in an aquifer which is based on conservation of mass and Fick's law of diffusion (Bear, 1972; Fried & Combarnous, 1971). The simulation of solute transport in rivers is frequently based on numerical models of the Advection-Dispersion Equation (Wallis, 2007).

Wexler (1989) presented analytical solutions to the advection- dispersion solute equation, for a variety of boundary conditions types and solute-sources configurations in one, two and three dimensional system having uniform groundwater flows. Solutions were presented in a simplified format, together with information on important assumption in derivation and limitations to their use.

Numerical modeling of pollutant migration in porous media has recently a great deal of attention due to an increased interest in the preservation of the quality of the environment and particularly of the protection of groundwater from various pollutants. The finite difference methods have traditionally been applied to solve flow and transport equations. One of the most important implementations of the finite difference approach is in the powerful code swift and its succeeding works.

2.6. Differential Equation (DE)

In mathematics, we call the changing entities as variables and the rate of change of one variable with respect to another as a derivative. Equations expressing a relationship among these variables and their derivatives are known as differential equations. In order words, a differential equation originate whenever a universal law is expressed by means of variables and their derivatives. Any equation containing differential coefficients is called a differential equation. The order of differential equation is the order of the highest differential coefficient contained in the differential equation while the degree of differential equation is the power to which the highest differential coefficient is raised when the equation is rationalized.

Ordinary Differential Equation (ODE): Ordinary differential equations are those equations that involve only one independent variable and only ordinary differential coefficients.

Partial Differential Equation (PDE): A partial differential equation is a mathematical equation that involves relations between two or more independent variables, an unknown function (dependent on those variables); and partial derivatives of the unknown function with respect to the independent variables. Partial differential equations are ubiquitous in mathematically-oriented scientific fields, such as physics and engineering. They are foundational in the modern scientific understanding of sound, heat, diffusion, electrostatics, electrodynamics, fluid dynamics, electricity, general relativity and quantum mechanics. They also arise from many purely mathematical considerations, such as differential geometry and the calculus of variation; among other notable applications, they are the fundamental tool in the proof of the Poincare conjecture from geometric topology. The order of a partial differential equation is the order of the highest derivative involved. Partial differential equations are used to mathematically formulate, and this aid the solution of physical and other problems involving functions of several variables, such as the propagation of heat or sound, fluid flow, elasticity, electrostatics and electrodynamics.

Example of partial differential equation:

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = 0 \qquad (2.18)$$

$$\frac{\partial \varphi}{\partial t} + \frac{\partial^2 \varphi}{\partial y^2} = 0 \qquad (2.19)$$

In partial differential equations, it is common to denote partial derivative using subscripts, that is

$$w_{xy} = \frac{\partial^2 w}{\partial x \partial y} \qquad (2.20)$$

There are several methods of solving a PDE which can be classified either as analytical or numerical methods. It is typically understood that any exact solution to a differential equation (DE) that can be expressed in terms of polynomial, logarithmic/exponential, and/or trigonometric functions (elementary functions) is an analytical solution. Most methods for analytically solving PDEs transform them into system of fairly comprehensive list of techniques which include – separation of variables, integral transform, integral equations, change of coordinates, dependent variable transforms, perturbation methods, impulse response techniques, calculus of variations, Eigen-function expansion.

2.7 Eigen-function Expansion Method

The method of Eigen-function expansion is one of the most elegant methods for various problems resulting from partial differential equations. It is the method in which a solution is represented in the form of a series in some functions closely related to an original problem. Physically, in the simplest cases this approach corresponds to superposition of stationary waves. Some applications of the method of Eigen-function date back to Euler, Ostrogradskii was first to develop its general formation. The method of Eigen-function is closely related to the Fourier method, or the method of separation of variables which is intended for finding a particular solution of a differential equation. However, many problems involve homogeneous reactions in the system or complicated coordinate systems making the governing PDE more complicated and maybe requiring a more sophisticated method to solve it. This is a typical diffusion – reaction problem in spherical coordinates with first order consumption. Solving this PDE with separation of variables can be somewhat confusing and cumbersome. One of the most often used methods of mathematical physics which is called Eigen-function expansion method has been a veritable tool for solving problems arising from aforementioned physical phenomenon by contemporary researchers (El-Raheem, 2011 and Olayiwola *et al.,* 2013).

CHAPTER THREE

3.0 MATERIALS AND METHODS

3.1. Model Formulation

We consider the transport of a contaminant through a homogeneous finite medium of length $x = L$ under transient state flow is assumed that at time $t = 0$, the flow is not clean (that is, the domain is solute free). 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 de 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. The dispersion D_L , D_T , D_{LT} and D_{TL} represent the horizontal dispersion coefficient, vertical dispersion coefficient and cross-flow dispersion coefficients respectively.

3.1.1 The cross-flow contaminant flow model

Following the work of Lee and Kim (2012), the cross-flow contaminant flow model can be formulated as follows:

$$\frac{\partial c}{\partial t} + \frac{\partial s}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = \frac{\partial}{\partial x}\left(D_L\frac{\partial c}{\partial x} + D_{LT}\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{TL}\frac{\partial c}{\partial x} + D_T\frac{\partial c}{\partial y}\right) - \alpha c \tag{3.1}$$

$$\frac{\partial c}{\partial t} + \frac{\partial s}{\partial t} = D_L\frac{\partial^2 c}{\partial x^2} + D_T\frac{\partial^2 c}{\partial y^2} + D_{LT}\frac{\partial^2 c}{\partial x\partial y} + D_{TL}\frac{\partial^2 c}{\partial y\,\partial x} - u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - \alpha c \tag{3.2}$$

$$\left(1 + kd\right)\frac{\partial c}{\partial t} = D_L\frac{\partial^2 c}{\partial x^2} + D_T\frac{\partial^2 c}{\partial y^2} + D_{LT}\frac{\partial^2 c}{\partial x\partial y} + D_{TL}\frac{\partial^2 c}{\partial y\,\partial x} - u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - \alpha c \tag{3.3}$$

where

D_L − Longitudinal dispersion coefficient

D_T – vertical dispersion coefficient

D_{LT} – cross-flow horizontal dispersion coefficient

D_{TL} – cross-cross-flow vertical dispersion coefficient

c – solute concentration in the liquid phase $\left[ML^{-1}\right]$

v – seepage or average pure water velocity $\left[LT^{-1}\right]$

u – initial velocity $\left[LT^{-1}\right]$

α – decay parameter

k_d – distribution coefficient

s – concentration of contaminant attached to porous media

$$\frac{\partial s}{\partial t} = k_d \frac{\partial c}{\partial t} \tag{3.4}$$

and $D_L, D_T, D_{LT}\ D_{TL}, u\ v$ are functions of t

Let $R = \left(1 + k_d\right)$ (3.5)

$$R\frac{\partial c}{\partial t} = D_{L_0} f(t)\frac{\partial^2 c}{\partial x^2} + D_{T_0} f(t)\frac{\partial^2 c}{\partial y^2} + 2D_{LT_0} f(t)\frac{\partial^2 c}{\partial x \partial y} - u_0 f(t)\frac{\partial c}{\partial x} - v_0 f(t)\frac{\partial c}{\partial y} - \alpha_0 f(t) c \tag{3.6}$$

Divide equation (3.6) through by $f(t)$

$$\frac{R}{f(t)}\frac{\partial c}{\partial t} = D_{L_0}\frac{\partial^2 c}{\partial x^2} + D_{T_0}\frac{\partial^2 c}{\partial y^2} + 2D_{LT_0}\frac{\partial^2 c}{\partial x \partial y} - u_0\frac{\partial c}{\partial x} - v_0\frac{\partial c}{\partial y} - \alpha_0 c \tag{3.7}$$

Introducing a new time variable,

$$\tau = \frac{1}{R}\int f(t)\,dt \tag{3.8}$$

where

$$f(t) = R\,e^{-qt} \tag{3.9}$$

$$\frac{\partial \tau}{\partial t} = \frac{f(t)}{R} \tag{3.10}$$

$$\frac{\partial t}{\partial \tau} = \frac{R}{f(t)} \tag{3.11}$$

Substituting equation (3.11) into equation (3.7), it becomes

$$\frac{\partial t}{\partial \tau}\frac{\partial c}{\partial t} = D_{L0}\frac{\partial^2 c}{\partial x^2} + D_{T0}\frac{\partial^2 c}{\partial y^2} + 2D_{LT0}\frac{\partial^2 c}{\partial x \partial y} - u_0\frac{\partial c}{\partial x} - v_0\frac{\partial c}{\partial y} - \alpha_0 c \tag{3.12}$$

$$\frac{\partial c}{\partial \tau} = D_{L0}\frac{\partial^2 c}{\partial x^2} + D_{T0}\frac{\partial^2 c}{\partial y^2} + 2D_{LT0}\frac{\partial^2 c}{\partial x \partial y} - u_0\frac{\partial c}{\partial x} - v_0\frac{\partial c}{\partial y} - \alpha_0 c \tag{3.13}$$

Introducing a space variable,

$$\eta = x + y\sqrt{\frac{D_{T0}}{D_{L0}}} \tag{3.14}$$

$$\frac{\partial c}{\partial x} = \frac{\partial c}{\partial \eta}\cdot\frac{\partial \eta}{\partial x} = \frac{\partial c}{\partial \eta} \tag{3.15}$$

$$\frac{\partial c}{\partial y} = \frac{\partial c}{\partial \eta}\cdot\frac{\partial \eta}{\partial y} = \sqrt{\frac{D_{T0}}{D_{L0}}}\frac{\partial c}{\partial \eta} \tag{3.16}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right) = \frac{\partial}{\partial \eta}\left(\frac{\partial c}{\partial \eta}\right) = \frac{\partial^2 c}{\partial \eta^2} \tag{3.17}$$

$$\frac{\partial c}{\partial y}=\frac{\partial}{\partial\eta}\cdot\frac{\partial\eta}{\partial y}=\frac{\partial}{\partial\eta}\left(\sqrt{\frac{D_{T0}}{D_{L0}}}\right) \tag{3.18}$$

$$\frac{\partial^2 c}{\partial y^2}=\frac{\partial^2}{\partial\eta^2}\cdot\left(\frac{\partial\eta}{\partial y}\right)^2=\frac{\partial^2}{\partial\eta^2}\left(\frac{D_{T0}}{D_{L0}}\right)=\frac{D_{T0}}{D_{L0}}\frac{\partial^2}{\partial\eta^2} \tag{3.19}$$

$$\frac{\partial^2}{\partial x\partial y}=\frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}\right)=\frac{\partial}{\partial\eta}\left(\sqrt{\frac{D_{T0}}{D_{L0}}}\right)\frac{\partial}{\partial\eta}=\sqrt{\frac{D_{T0}}{D_{L0}}}\frac{\partial^2}{\partial\eta^2} \tag{3.20}$$

Substituting into equation (3.13)

$$\frac{\partial c}{\partial\tau}=D_{L_0}\frac{\partial^2 c}{\partial\eta^2}+D_{T_0}\frac{D_{T_0}}{D_{L_0}}\frac{\partial^2 c}{\partial\eta^2}+2D_{LT_0}\frac{\partial^2 c}{\partial\eta^2}-u_0\frac{\partial c}{\partial\eta}-v_0\sqrt{\frac{D_{T_0}}{D_{L_0}}}\frac{\partial c}{\partial\eta}-\alpha_0 c \tag{3.21}$$

$$\frac{\partial c}{\partial\tau}=\left(D_{L_0}+\frac{D_{T_0}^2}{D_{L_0}}+2D_{LT_0}\sqrt{\frac{D_{T_0}}{D_{L_0}}}\right)\frac{\partial^2 c}{\partial\eta^2}-\left(u_0+v_0\sqrt{\frac{D_{T_0}}{D_{L_0}}}\right)\frac{\partial c}{\partial\eta}-\alpha_0 c \tag{3.22}$$

Let $D=D_{L_0}+\frac{D_{T_0}^2}{D_{L_0}}+2D_{LT_0}\sqrt{\frac{D_{T_0}}{D_{L_0}}}$, and $u=u_0+v_0\sqrt{\frac{D_{T_0}}{D_{L_0}}}$ (3.23)

Equation (3.22) can be written as

Case 1:

$$\frac{\partial c}{\partial\tau}=D\frac{\partial^2 c}{\partial\eta^2}-u\frac{\partial c}{\partial\eta}-\alpha c \tag{3.24}$$

The initial and boundary conditions are as chosen below

$$c(\eta,0)=c_i;\quad \tau=0 \tag{3.25}$$

$$c(0,\tau)=c_0\left(1+e^{-q\tau}\right);\qquad x=0 \tag{3.26}$$

$$\frac{\partial c}{\partial\eta}(l,\tau)=0,\quad \eta=l \tag{3.27}$$

By transforming the boundary and initial condition, the equation becomes

$$\left.\begin{aligned} \frac{\partial c}{\partial \tau} &= D\frac{\partial^2 c}{\partial \eta^2} - u\frac{\partial c}{\partial \eta} - \alpha c \\ c(\eta, 0) &= c_i \\ c(0, \tau) &= c_0(2 - q\tau) \\ \frac{\partial c}{\partial \eta}(l, \tau) &= 0 \end{aligned}\right\} \tag{3.28}$$

Non-dimensionalization

We non-dimensionalize equation (3.28) with the aid of the dimensionless variables

$$\left.\begin{aligned} c^* &= \frac{c}{c_0} \\ \eta^* &= \frac{\eta}{l} \\ \tau^* &= \frac{\tau u}{l} \end{aligned}\right\} \tag{3.29}$$

Equation (3.28) becomes

$$\frac{c_0}{\frac{l}{u}}\frac{\partial c^*}{\partial \tau^*} = D\frac{c_0\,\partial^2 c^*}{\partial (l\eta^*)^2} - u\frac{c_0\,\partial c^*}{\partial (l\eta^*)} - \alpha c_0 c^* \tag{3.30}$$

$$\frac{c_0 u}{l}\frac{\partial c^*}{\partial \tau^*} = \frac{Dc_0}{l^2}\frac{\partial^2 c^*}{\partial \eta^{*2}} - \frac{uc_0}{l}\frac{\partial c^*}{\partial \eta^*} - \alpha c_0 c^* \tag{3.31}$$

$$\frac{\partial c^*}{\partial \tau^*} = \frac{Dc_0}{l^2}\frac{l}{c_0 u}\frac{\partial^2 c^*}{\partial \eta^{*2}} - \frac{uc_0}{l}\frac{l}{c_0 u}\frac{\partial c^*}{\partial \eta^*} - \alpha c_0\frac{l c^*}{c_0 u} \tag{3.32}$$

$$\frac{\partial c^*}{\partial \tau^*} = \frac{D}{lu}\frac{\partial^2 c^*}{\partial \eta^{*2}} - \frac{\partial c^*}{\partial \eta^*} - \frac{\alpha l}{u}c^* \tag{3.33}$$

Where $D^* = \dfrac{D}{lu}$ (3.34)

The non-dimensionalized equation is

$$\frac{\partial c_*}{\partial \tau_*} = D_* \frac{\partial^2 c_*}{\partial \eta_*^2} - \frac{\partial c_*}{\partial \eta_*} - \alpha_* c_* \tag{3.35}$$

The non-dimensionalized equation with the initial and boundary conditions of equation (3.28) becomes

$$\left.\begin{aligned}
&\frac{\partial c_*}{\partial \tau_*} = D_* \frac{\partial^2 c_*}{\partial \eta_*^2} - \frac{\partial c_*}{\partial \eta_*} - \alpha_* c_* \\
&c_*(\eta, 0) = \frac{c_i}{c_0} \\
&c_*(0, \tau) = 2 - q\tau; \quad \tau \geq 0 \\
&\frac{\partial c_*}{\partial \eta}(1, \tau) = 0; \quad \eta = 1
\end{aligned}\right\} \tag{3.36}$$

The parameter expanding method is applied to the equation (3.36) as follows:

Let $c_*(\eta, \tau) = c_0(\eta, \tau) + \alpha c_1(\eta, \tau) + \ldots$

and $1 = b\alpha$ in the advection term of equation (3.36) as used in Olayiwola *et al*. (2013).

The following equation is obtained from equation (3.36)

$$\left.\begin{aligned}
\frac{\partial}{\partial \tau}\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + \ldots\right) = {} & D_* \frac{\partial^2}{\partial \eta^2}\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + \ldots\right) \\
& - b\alpha\left(\frac{\partial}{\partial \eta}\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + \ldots\right)\right) \\
& - \alpha\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + \ldots\right)
\end{aligned}\right\} \tag{3.37}$$

From equation (3.37) we generate the following equation

Order zero $\alpha^{(0)}$:

$$\left.\begin{aligned}
&\frac{\partial c_0}{\partial \tau} = D_* \frac{\partial^2}{\partial \eta^2} c_0(\eta,\tau) \\
&c_0(\eta, 0) = \frac{c_i}{c_0} \\
&c(0, \tau) = 2 - q\tau \\
&\frac{\partial c_0}{\partial \eta}(1,\tau) = 0
\end{aligned}\right\} \tag{3.38}$$

Order zero $\alpha^{(1)}$:

$$\left.\begin{aligned}
&\frac{\partial c_1}{\partial \tau} = D_* \frac{\partial^2}{\partial \eta^2} c_1(\eta,\tau) - b \frac{\partial}{\partial \eta} c_0(\eta, \tau) - c_0(\eta,\tau) \\
&c_0(\eta,0) = 0 \\
&c_1(0,\tau)=0 \\
&c_1(1,\tau)=0
\end{aligned}\right\} \tag{3.39}$$

The above equations (3.33) and (3.35) are transformed to satisfy the homogeneous boundary conditions. This is done by using the transformation:

$$g_0(\eta,\tau) = \alpha(\tau) + \eta\beta(\tau) \tag{3.40}$$

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

so that

$$c_0(\eta, \tau) = w_0(\eta, \tau) + g_0(\eta,\tau) \tag{3.41}$$

That is,

$$c_0(\eta, \tau) = w_0(\eta,\tau) + (2 - q\tau) + \eta(0) \tag{3.42}$$

Differentiating equation (3.42) we have

$$\frac{\partial c_0}{\partial \tau} = \frac{\partial c_0}{\partial w_0} \cdot \frac{\partial w_0}{\partial \tau} + \frac{\partial c_0}{\partial g_0} \cdot \frac{\partial g_0}{\partial \tau_0} \tag{3.43}$$

$$\frac{\partial c_0}{\partial \tau} = \frac{\partial w_0}{\partial \tau} - q \tag{3.44}$$

Also,

$$\frac{\partial c_0}{\partial \eta} = \frac{\partial c_0}{\partial w_0} \cdot \frac{\partial w_0}{\partial \eta} + \frac{\partial c_0}{\partial g} \cdot \frac{\partial g}{\partial \eta} \tag{3.45}$$

$$\frac{\partial c_0}{\partial \eta} = \frac{\partial w_0}{\partial \eta} + 0 \tag{3.46}$$

$$\frac{\partial^2 c_0}{\partial \eta^2} = \frac{\partial}{\partial \eta}\left(\frac{\partial w_0}{\partial \eta}\right) \tag{3.47}$$

$$\frac{\partial^2 c_0}{\partial \eta^2} = \frac{\partial^2 w_0}{\partial \eta^2} \tag{3.48}$$

Substituting back equations (3.44) and 3.48) into equation (3.38),

$$\frac{\partial w_0}{\partial \tau} - q = D_* \frac{\partial^2 w_0}{\partial \eta^2} \tag{3.49}$$

$$\frac{\partial w_0}{\partial \tau} = D^* \frac{\partial^2 w_0}{\partial \eta^2} + q \tag{3.50}$$

Also from the initial and boundary conditions,

$$c_0\left(0, \tau\right) = w_0\left(0, \tau\right) + 2 - q\tau = 2 - q\tau \tag{3.51}$$

$$w_0\left(0, \tau\right) = 0 \tag{3.52}$$

$$\Rightarrow \frac{\partial w_0}{\partial \eta}\left(1, \tau\right) = 0; \eta = 1 \tag{3.53}$$

For initial condition,

$$c_0(\eta, 0) = w_0(\eta, 0) + 2 = \frac{c_i}{c_0} \tag{3.54}$$

$$w_0(\eta, 0) = \frac{c_i}{c_0} - 2 \tag{3.55}$$

The transformed equation (3.38) becomes

$$\left.\begin{aligned} &\frac{\partial w_0}{\partial \tau} = D_* \frac{\partial^2 w_0}{\partial \eta^2} + q \\ &w_0(\eta, 0) = \frac{c_i}{c_0} - 2 \\ &w_0(0, \tau) = 0 \\ &\frac{\partial w_0}{\partial \eta}(1, \tau) = 0 \end{aligned}\right\} \tag{3.56}$$

Also from equation (3.39), we have

$$\frac{\partial c_1}{\partial \tau} = \frac{\partial w_1}{\partial \tau} \tag{3.57}$$

$$\frac{\partial c_1}{\partial \eta} = \frac{\partial w_1}{\partial \eta} \tag{3.58}$$

$$\frac{\partial^2 c_1}{\partial \eta^2} = \frac{\partial^2 w_1}{\partial \eta^2} \tag{3.59}$$

The transformed equation (3.39) becomes

$$\left.\begin{aligned} &\frac{\partial w_1}{\partial \tau} = D_* \frac{\partial^2 w_1}{\partial \eta^2} - b \frac{\partial w_0}{\partial \eta} - w_0 \\ &w_0(\eta, 0) = 0 \\ &w_0(0, \tau) = 0 \\ &\frac{\partial w_0}{\partial \eta}(1, \tau) = 0 \end{aligned}\right\} \tag{3.60}$$

Equation (3.56) is solved by the method of Eigen-function expansion as follows:

The solution by Eigen-function expansion is of the form as used by Olayiwola *et al.* (2013)

$$w(\eta,\tau) = \sum_{n=1}^{\infty} w_n(\tau)\sin\frac{(2n-1)}{2l}\pi\eta \tag{3.61}$$

where

$$w_n(\tau) = \int_0^{\tau} e^{-D^*\left(\frac{(2n-1)\pi}{2l}\right)^2(\tau-t)} \cdot F_n(t)\,dt + b_n e^{-D^*\left(\frac{(2n-1)\pi}{2l}\right)^2\tau} \tag{3.62}$$

$$F_n(\tau) = \frac{2}{l}\int_0^{l} F(\eta,\tau)\sin\frac{(2n-1)}{2l}\pi\eta\,d\eta \tag{3.63}$$

$$b_n = \frac{2}{l}\int_0^{l} f(\eta)\sin\frac{(2n-1)}{2l}\pi\eta\,d\eta \tag{3.64}$$

In this case, $l = 1$

From equation (3.56), $f(\eta) = \frac{c_i}{c_0} - 2$:

$$b_n = \frac{2}{l}\int_0^{l}\left(\frac{c_i}{c_0} - 2\right)\sin\frac{(2n-1)}{2}\pi\eta\,d\eta \tag{3.65}$$

$$b_n = 2\left(\frac{c_i}{c_0} - 2\right)\int_0^{l}\sin\frac{(2n-1)}{2}\pi\eta\,d\eta \tag{3.66}$$

$$b = 2\left(\frac{c_i}{c_0} - 2\right)\left(-\frac{2}{(2n-1)\pi}\cos\frac{(2n-1)}{2}\pi\eta\right)_0^1 \tag{3.67}$$

$$b_n = -\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0} - 2\right)(0-1) \tag{3.68}$$

$$\therefore b_n = \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right) \tag{3.69}$$

From equation (3.56), $F(x,\tau)=q$

$$F_n(\tau)=\frac{2}{1}\int_0^1 q\sin\frac{(2n-1)}{2}\pi\eta\, d\eta \tag{3.70}$$

$$F_n(\tau)=2q\int_0^1 \sin\frac{(2n-1)}{2}\pi\eta\, d\eta \tag{3.71}$$

$$F_n(\tau)=-2q\frac{2}{(2n-1)\pi}\left[\cos\frac{(2n-1)}{2}\pi\eta\right]_0^1 \tag{3.72}$$

$$\therefore F_n(\tau)=\frac{4q}{(2n-1)\pi} \tag{3.73}$$

Substitute $b_n(\tau)$ and $F_n(\tau)$ into equation (3.62)

$$w_n(\tau)=\int_0^\tau e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau-t)}\cdot\frac{4q}{(2n-1)\pi}\,dt+\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau} \tag{3.74}$$

$$w_n(\tau)=\frac{4q}{(2n-1)\pi}\int_0^\tau e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau-t)}\,dt+\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau} \tag{3.75}$$

$$w_n(\tau)=\frac{4q}{(2n-1)\pi}\left[\frac{4}{D^*(2n-1)^2\pi^2}e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau-t)}\right]_0^\tau+\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau} \tag{3.76}$$

$$w_n(\tau)=\frac{4q}{(2n-1)\pi}\frac{4}{D^*(2n-1)^2\pi^2}\left[1-e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right]+\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau} \tag{3.77}$$

$$w_n(\tau)=\frac{16q}{D^*(2n-1)^3\pi^3}\left[1-e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right]+\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c}\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau} \quad (3.78)$$

$$w_n(\tau)=\frac{16q}{D^*(2n-1)^3\pi^3}-\frac{16q}{D^*(2n-1)^3\pi^3}e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau}+\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c}-2\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau} \quad (3.79)$$

$$w_n(\tau)=\frac{16q}{D^*(2n-1)^3\pi^3}-\left(\frac{16q}{D^*(2n-1)^3\pi^3}-\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)} \quad (3.80)$$

Therefore $c_0(\eta,\tau)=w_0(\eta,\tau)+g_0(\eta,\tau)$ (3.81)

$$c_0(\eta,\tau)=\sum_{n=1}^{\infty}w_n(\tau)\sin\frac{(2n-1)}{2}\pi\eta+g_0(\tau) \quad (3.82)$$

$$c_0(\eta,\tau)=2-q\tau+\sum_{n=1}^{\infty}w_n(\tau)\sin\frac{(2n-1)}{2}\pi\eta \quad (3.83)$$

$$c_0(\eta,\tau)=2-q\tau+\sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3}-\left(\frac{16q}{D^*(2n-1)^3\pi^3}-\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times\sin\frac{(2n-1)}{2}\pi\eta \quad (3.84)$$

Recall

$$w_0=\sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3}-\left(\frac{16q}{D^*(2n-1)^3\pi^3}-\frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times\sin\frac{(2n-1)}{2}\pi\eta \quad (3.85)$$

$$\frac{\partial w_0}{\partial\eta}=\sum_{n=1}^{\infty}\left(\frac{8q}{D^*(2n-1)^2\pi^2}-\left(\frac{8q}{D^*(2n-1)^2\pi^2}-2\left(\frac{c_i}{c_0}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times\cos\frac{(2n-1)}{2}\pi\eta \quad (3.86)$$

Equation (3.60) is solved by the method of Eigen-function expansion as follows:

The solution by Eigen-function expansion is of the form

$$w(\eta,\tau)=\sum_{n=1}^{\infty} w_n(\tau)\sin\frac{(2n-1)}{2l}\pi\eta \tag{3.87}$$

where

$$w_n(\tau)=\int_0^{\tau} e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau-t)}\cdot F_n(t)\,dt+b_n e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2\tau} \tag{3.88}$$

$$F_n(\tau)=\frac{2}{l}\int_0^{l} F(\eta,\tau)\sin\frac{(2n-1)}{2}\pi\eta\, d\eta \tag{3.89}$$

$$b_n(\tau)=\frac{2}{l}\int_0^{l} F(\eta)\sin\frac{(2n-1)}{2}\pi\eta\, d\eta \tag{3.90}$$

In this case, $l=1$

From equation (3.60)

$$b_n(\tau)=\frac{2}{1}\int_0^{1} 0\cdot\sin\frac{(2n-1)}{2}\pi\eta\, d\eta \tag{3.91}$$

$$b_n(\tau)=0 \tag{3.92}$$

From equation (3.60),

$$F(\eta,\tau)=-b\frac{\partial w_0}{\partial\eta}-w_0 \tag{3.93}$$

$$F_n(\tau)=\frac{2}{1}\int_0^{1}\left(-b\frac{\partial w_0}{\partial\eta}-w_0\right)\cdot\sin\frac{(2n-1)}{2}\pi\eta\, d\eta \tag{3.94}$$

$$F_n(\tau) = -2b\int_0^1 \sum_{n=1}^{\infty}\left(\frac{8q}{D^*(2n-1)^2\pi^2} - \left(\frac{8q}{D^*(2n-1)^2\pi^2} - \left(\frac{c_i}{c_0} - 2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2l}\right)^2(\tau)}\right)\times \cos\frac{(2n-1)}{2}\pi\eta \sin\frac{(2n-1)}{2}\pi\eta \, d\eta$$

$$-2\int_0^1 \sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0} - 2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2l}\right)^2(\tau)}\right)\times \sin\frac{(2n-1)}{2}\pi\eta \sin\frac{(2n-1)}{2}\pi\eta \, d\eta \tag{3.95}$$

$$F_n(\tau) = -2b\sum_{n=1}^{\infty}\left(\frac{8q}{D^*(2n-1)^2\pi^2} - \left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0} - 2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times \frac{1}{2}\int_0^1 \sin(2n-1)\pi\eta \, d\eta$$

$$-2\sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{2}{(2n-1)\pi}\left(\frac{c_i}{c_0} - 2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times \int_0^1 \sin^2\frac{(2n-1)}{2}\pi\eta \, d\eta \tag{3.96}$$

$$F_n(\tau) = -2b\sum_{n=1}^{\infty}\left(\frac{8q}{D^*(2n-1)^2\pi^2} - \left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0} - 2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2l}\right)^2(\tau)}\right)\times \frac{1}{2}\int_0^1 \sin(2n-1)\pi\eta \, d\eta$$

$$-2\sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{2}{(2n-1)\pi}\left(\frac{c_i}{c_0} - 2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times \frac{1}{2}\int_0^1 \left(1 - \cos(2n-1)\pi\eta\right) d\eta \tag{3.97}$$

$$\sum_{n=1}^{\infty} F_n(\tau) = -2b\sum \left(\frac{8q}{D^*(2n-1)^2\pi^2} - \left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2l}\right)^2(\tau)}\right)\times \frac{1}{2(2n-1)\pi}\left[-\cos(2n-1)\pi\eta\right]_0^1$$

$$-2\sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times \frac{1}{2}\left(\eta - \frac{\sin(2n-1)\pi\eta}{(2n-1)\pi}\right)_0^1 \qquad (3.98)$$

$$\sum_{n=1}^{\infty} F_n(\tau) = -2b\sum^{\infty}\left(\frac{8q}{D^*(2n-1)^2\pi^2} - \left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)\times \frac{1}{(2n-1)\pi} \qquad (3.99)$$

$$-\sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{\text{[redacted]}\,2n\,\text{[redacted]}\,1\,\text{[redacted]}}\left(\frac{c_i}{c}-2\right)\right)e^{-D^*\left(\frac{(2n-1)\pi}{2}\right)^2(\tau)}\right)$$

We Substitute $b_n(\tau)$ and $F_n(\tau)$ into equation (3.62).

Recall that

$$b_n(\tau) = 0 \qquad (3.100)$$

$$w_n(\tau) = \int_0^{\tau} e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi(\tau-t)}\left(\frac{-2b}{(2n-1)\pi}\sum_{n=1}^{\infty}\left(\frac{8q}{D^*(2n-1)^2\pi^2} - \left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0}-2\right)\right)e^{-D\left(\frac{2n-1}{2}\right)^2\pi t}\right)\right)dt$$

$$-\int_0^{\tau} e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi(\tau-t)}\sum_{n=1}^{\infty}\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right)e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi t}\right)dt \qquad (3.101)$$

$$= \int_0^\tau \left(-\sum_{n=1}^{\infty} \frac{-2b}{(2n-1)^2\pi} \left(\frac{8q}{D^*(2n-1)^2\pi^2} e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2(\tau-t)} - \left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right) \right) dt$$

$$-\int_0^\tau \sum_{n=1}^{\infty} \left(\frac{16q}{D^*(2n-1)^3\pi^3} e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2(\tau-t)} - \left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right) dt \qquad (3.102)$$

$$= -\sum_{n=1}^{\infty} \frac{2b}{(2n-1)\pi} \left(\left[\frac{8q}{D^*(2n-1)^2\pi^2} \frac{4}{D^*(2n-1)^2\pi^2} e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2(\tau-t)} \right]_0^\tau - \left[t\left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2 t} \right]_0^\tau \right)$$

$$-\sum_{n=1}^{\infty} \left(\left[\frac{16q}{D^*(2n-1)^3\pi^3} \frac{4}{D^*(2n-1)^2\pi^2} e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2(\tau-t)} \right]_0^\tau - \left[t\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right]_0^\tau \right) \qquad (3.103)$$

$$= -\sum_{n=1}^{\infty} \frac{2b}{(2n-1)\pi} \left(\frac{8q}{D^*(2n-1)^2\pi^2} \frac{4}{D^*(2n-1)^2\pi^2} \left(1 - e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau}\right) - \tau\left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right)$$

$$-\sum_{n=1}^{\infty} \left(\frac{16q}{D^*(2n-1)^3\pi^3} \frac{4}{D^*(2n-1)^2\pi^2} \left(1 - e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau}\right) - \tau\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right) \qquad (3.104)$$

$$= -\sum_{n=1}^{\infty} \frac{2b}{(2n-1)\pi} \left(\frac{32q}{(D^*)^2(2n-1)^4\pi^4} \left(1 - e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau}\right) - \tau\left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right)$$

$$-\sum_{n=1}^{\infty} \left(64q$$ [redacted] $$\left(1 - e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau}\right) - \tau\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right) \qquad (3.105)$$

The solution of order one is therefore

$$c_1(\eta,\tau) = -\sum_{n=1}^{\infty}\sum_{n=1}^{\infty} \frac{2b}{(2n-1)\pi} \left(\frac{32q}{(D^*)^2(2n-1)^4\pi^4} \left(1 - e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau}\right) - \tau\left(\frac{8q}{D^*(2n-1)^2\pi^2} - 2\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right) \sin\left(\frac{2n-1}{2}\right)\pi\eta$$

$$-\sum_{n=1}^{\infty}\sum_{n=1}^{\infty} \left(\frac{64q}{(D^*)^2(2n-1)^5\pi^5} \left(1 - e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau}\right) - \tau\left(\frac{16q}{D^*(2n-1)^3\pi^3} - \frac{4}{(2n-1)\pi}\left(\frac{c_i}{c_0}-2\right)\right) e^{-D^*\left(\frac{2n-1}{2}\right)^2\pi^2\tau} \right) \times \sin\left(\frac{2n-1}{2}\right)\pi\eta \qquad (3.106)$$

Therefore, the solution of the cross-flow dispersion problem in (3.24) is

$$c(\eta,\tau) = c_0(\eta,\tau) + \alpha c_1(\eta,\tau) \tag{3.107}$$

where $c_0(\eta,\tau)$ and $c_1(\eta,\tau)$ are given in equations (3.84) and (3.106) respectively

Case 2:

In this case, the boundary conditions are of the Dirichlet type and the flow was initially not solute free as given below:

$$\left.\begin{aligned}
&\frac{\partial c}{\partial \tau} = D\frac{\partial^2 c}{\partial \eta^2} - u\frac{\partial c}{\partial \eta} - \alpha c\\
&c(\eta,0) = c_i; \quad \tau = 0\\
&c(0,\tau) = c_0\left(1+e^{-q\tau}\right)\\
&c(1,\tau) = 0; \quad \eta = 1
\end{aligned}\right\} \tag{3.108}$$

By transforming the boundary and initial condition, just like as in case 1, the initial boundary value problem (3.108) becomes

$$\left.\begin{aligned}
&\frac{\partial c}{\partial \tau} = D\frac{\partial^2 c}{\partial \eta^2} - u\frac{\partial c}{\partial \eta} - \alpha c\\
&c(\eta,0) = c_i\\
&c(0,\tau) = c_0(2-q\tau)\\
&c(1,\tau) = 0; \quad \eta = 1
\end{aligned}\right\} \tag{3.109}$$

Non-dimensionalization

We non-dimensionalize equation (3.109) using the following dimensionless variables.

$$\left.\begin{aligned} c^{*} &= \frac{c}{c_0} \\ \eta^{*} &= \frac{\eta}{l} \\ \tau^{*} &= \frac{\tau u}{l} \end{aligned}\right\} \tag{3.110}$$

Equation (3.109) becomes

$$\frac{c_0}{\frac{l}{u}}\frac{\partial c^{*}}{\partial \tau^{*}} = D\frac{c_0\,\partial^2 c^{*}}{\partial \left(l\eta^{*}\right)^2} - u\frac{c_0\,\partial c^{*}}{\partial \left(l\eta^{*}\right)} - \alpha c_0 c^{*} \tag{3.111}$$

$$\frac{c_0 u}{l}\frac{\partial c^{*}}{\partial \tau^{*}} = \frac{Dc_0}{l^2}\frac{\partial^2 c^{*}}{\partial \eta^{*2}} - \frac{uc_0}{l}\frac{\partial c^{*}}{\partial \eta^{*}} - \alpha c_0 c^{*} \tag{3.112}$$

$$\frac{\partial c^{*}}{\partial \tau^{*}} = \frac{Dc_0}{l^2}\frac{l}{c_0 u}\frac{\partial^2 c^{*}}{\partial \eta^{*2}} - \frac{uc_0}{l}\frac{l}{c_0 u}\frac{\partial c^{*}}{\partial \eta^{*}} - \alpha c_0 c^{*}\frac{l}{c_0 u} \tag{3.113}$$

$$\frac{\partial c^{*}}{\partial \tau^{*}} = \frac{D}{lu}\frac{\partial^2 c^{*}}{\partial \eta^{*2}} - \frac{\partial c^{*}}{\partial \eta^{*}} - \frac{\alpha l}{u} c^{*} \tag{3.114}$$

Where $\frac{D}{lu}$ is taken as D^{*}

The non-dimensionalized equation is

$$\frac{\partial c^{*}}{\partial \tau^{*}} = D^{*}\frac{\partial^2 c^{*}}{\partial \eta^{*2}} - \frac{\partial c^{*}}{\partial \eta^{*}} - \alpha^{*} c^{*} \tag{3.115}$$

The non-dimensionalized equation with the initial and boundary conditions of equation (3.109) becomes

$$\left.\begin{aligned}
&\frac{\partial c_*}{\partial \tau} = D_* \frac{\partial^2 c_*}{\partial \eta^2} - \frac{\partial c_*}{\partial \eta} - \alpha c_* \\
&c_*(\eta, 0) = \frac{c_i}{c_0} \\
&c_*(0,\tau) = (2 - q\tau) \qquad \tau \geq 0 \\
&c_*(l, \tau) = 0; \quad \eta = l
\end{aligned}\right\} \tag{3.116}$$

The parameter expanding method is applied to the equation (3.116) as follows

Let

$$c^*(\eta, \tau) = c_0(\eta, \tau) + \alpha c_1(\eta, \tau) + ... \tag{3.117}$$

and $1 = b\alpha$ in the advection term of equation (3.116) as used in Olayiwola *et al.* (2013).

The following equation is obtained from equation (3.116).

$$\left.\begin{aligned}
&\frac{\partial}{\partial \tau}\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + ...\right) = \\
&D_* \frac{\partial^2}{\partial \eta^2}\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + ...\right) \\
&- b\alpha \frac{\partial}{\partial \eta}\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + ...\right) \\
&- \alpha\left(c_0(\eta,\tau) + \alpha c_1(\eta,\tau) + \alpha^2 c_2(\eta,\tau) + ...\right)
\end{aligned}\right\} \tag{3.118}$$

From equation (3.118), we generate the following equation

Order zero $\alpha^{(0)}$:

$$\left.\begin{aligned}
&\frac{\partial c_0}{\partial \tau} = D_* \frac{\partial^2}{\partial \eta^2} c_0(\eta,\tau) \\
&c_0(\eta, 0) = \frac{c_i}{c_0} \\
&c_0(0, \tau) = (2 - q\tau) \\
&c_0(l, \tau) = 0
\end{aligned}\right\} \tag{3.119}$$

Order one $\alpha^{(1)}$:

$$\left.\begin{aligned}
&\frac{\partial c_1}{\partial \tau} = D_* \frac{\partial^2}{\partial \eta^2} c_0(\eta,\tau) - b\frac{\partial}{\partial \eta} c_0(\eta,\tau) - c_0(\eta,\tau)\\
&c_1(\eta,0) = 0\\
&c_1(0,\tau) = 0\\
&c_1(1,\tau) = 0
\end{aligned}\right\} \tag{3.120}$$

The above equation (3.119) and (3.120) are transformed to satisfy the homogeneous boundary conditions. This is done by using the transformation:

$$g_0(\eta,\tau) = \alpha(\tau) + \frac{\eta}{l}\left(\beta(\tau) - \alpha(\tau)\right) \tag{3.121}$$

$$g_0(\eta,\tau) = (2-q\tau) + \eta\left(0-(2-q\tau)\right) \tag{3.122}$$

$$c_0(\eta,\tau) = w_0(\eta,\tau) + g_0(\eta,\tau) \tag{3.123}$$

$$c_0(\eta,\tau) = w_0(\eta,\tau) + 2 - q\tau + \eta(0) - \eta(2-q\tau) \tag{3.124}$$

$$c_0(0,\tau) = w_0(0,\tau) + (2-q\tau) = 2 - q\tau \tag{3.125}$$

$$\Rightarrow w_0(0,\tau) = 0 \tag{3.126}$$

$$c_0(1,\tau) = w_0(1,\tau) + (2-q\tau) - (2-q\tau) = 0 \tag{3.127}$$

$$\Rightarrow w_0(1,\tau) = 0 \tag{3.128}$$

$$c_0(\eta,0) = w_0(\eta,\tau) + 2 - 2\eta = \frac{c_i}{c_0} \tag{3.129}$$

$$\Rightarrow w_0(\eta,0) = \frac{c_i}{c_0} + 2(\eta - 1)$$

Differentiating equation (3.124), with respect to τ we have

$$\frac{\partial c_0}{\partial \tau} = \frac{\partial w_0}{\partial \tau} + (\eta - 1)q \tag{3.130}$$

Also,

$$\frac{\partial c_0}{\partial \eta} = \frac{\partial c_0}{\partial w_0}\frac{\partial w_0}{\partial \eta} + \frac{\partial c_0}{\partial g_0}\frac{\partial g_0}{\partial \eta} \tag{3.131}$$

$$\frac{\partial c_0}{\partial \eta} = \frac{\partial w_0}{\partial \eta} - (2 - q\tau) \tag{3.132}$$

$$\frac{\partial^2 c_0}{\partial \eta^2} = \frac{\partial}{\partial \eta}\left(\frac{\partial w_0}{\partial \eta}\right)\frac{\partial \eta}{\partial \eta} \tag{3.133}$$

$$\frac{\partial^2 c_0}{\partial \eta^2} = \frac{\partial^2 w_0}{\partial \eta^2} \tag{3.134}$$

By substituting equation (3.130) and (3.134) in equation (3.119), the following equations are obtained

$$\frac{\partial w_0}{\partial \tau} + (\eta - 1)q = D_* \frac{\partial^2 w_0}{\partial \eta^2} \tag{3.135}$$

$$\frac{\partial w_0}{\partial \tau} = D_* \frac{\partial^2 w_0}{\partial \eta^2} - (\eta - 1)q \tag{3.136}$$

The transformed equation (3.119) becomes

$$\left.\begin{aligned}
&\frac{\partial w_0}{\partial \tau} = D_* \frac{\partial^2 w_0}{\partial \eta^2} - q(\eta - 1)\\
&w_0(\eta, 0) = \frac{c_i}{c_0} + 2(\eta - 1)\\
&w_0(0, \tau) = 0\\
&w_0(1, \tau) = 0
\end{aligned}\right\} \tag{3.137}$$

Also, from equation (3.120),

$$\frac{\partial c_1}{\partial \tau} = \frac{\partial w_1}{\partial \tau} \tag{3.138}$$

$$\frac{\partial c_1}{\partial \eta} = \frac{\partial w_1}{\partial \eta} \tag{3.139}$$

$$\frac{\partial^2 c_1}{\partial \eta^2} = \frac{\partial^2 w_1}{\partial \eta^2} \tag{3.140}$$

The transformed equation (3.120) becomes

$$\left.\begin{aligned}
&\frac{\partial w_1}{\partial \tau} = D^* \frac{\partial^2 w_1}{\partial \eta^2} - b\frac{\partial w_0}{\partial \eta} - w_0 \\
&w_0(\eta, 0) = 0 \\
&w_0(0,\tau) = 0 \\
&w_0(1,\tau) = 0
\end{aligned}\right\} \tag{3.141}$$

Equation (3.119) is solved by the method of Eigen-function expansion as follows.

The solution by Eigen-function expansion is of the form:

$$w(\eta,\tau) = \sum_{n=1}^{\infty} w_n(\tau)\sin\frac{n\pi\eta}{l} \tag{3.142}$$

where

$$w_n(\tau) = \int_0^{\tau} e^{-D^*\left(\frac{n\pi}{l}\right)^2 (t-\tau)} \cdot F_n(t)\,dt + b_n e^{-D^*\left(\frac{n\pi}{l}\right)^2 t} \tag{3.143}$$

$$F_n(\tau) = \frac{2}{l}\int_0^l F(\eta,\tau)\sin\frac{n\pi}{l}\eta\, d\eta \tag{3.144}$$

$$b_n = \frac{2}{l}\int_0^l F(\eta)\sin\frac{n\pi}{l}\eta\, d\eta \tag{3.145}$$

In this case, $l = 1$

From equation (3.137)

$$b_n = \frac{2}{1}\int_0^1 \left(\frac{c_i}{c_0} + 2(\eta - 1) \right) \cdot \sin n\pi\eta \, d\eta \tag{3.146}$$

$$b_n = 2\frac{c_i}{c_0}\int_0^1 \sin n\pi\eta \, d\eta + 4\int_0^1 (\eta - 1)\sin n\pi\eta \, d\eta \tag{3.147}$$

$$b_n = -\frac{2c_i}{c_0}\frac{1}{n\pi}\cos n\pi\eta \Big|_0^1 + 4\left[-\frac{1}{n\pi}(\eta - 1)\cos n\pi\eta \right]_0^1 - \frac{1}{n\pi}\int_0^1 \cos n\pi\eta \, d\eta \tag{3.148}$$

$$b_n = -\frac{2c_i}{n\pi c_0}(\cos n\pi - 1) + 4\left[-\frac{1}{n\pi} \right](0 + 1) - \frac{4}{n\pi}\frac{1}{n\pi}\sin n\pi\eta \Big|_0^1 \tag{3.149}$$

$$b_n = -\frac{2c_i}{n\pi c_0}(\cos n\pi - 1) - \frac{4}{n\pi} \tag{3.150}$$

$$b_n = -\frac{2}{n\pi}\left[\frac{c_i}{c_0}(\cos n\pi - 1) + 2 \right] \tag{3.151}$$

From equation (3.144), $F(\eta, \tau) = q(\eta - 1)$

$$F_n(\tau) = 2\int_0^1 q(\eta - 1)\sin n\pi\eta \, d\eta \tag{3.152}$$

$$F_n(\tau) = -2q\left[-\frac{1}{n\pi}(\eta - 1)\cos n\pi\eta \right]_0^1 - \frac{1}{n\pi}\int_0^1 \cos n\pi\eta \, d\eta \tag{3.153}$$

$$F_n(\tau) = -2q\left[-\frac{1}{n\pi}(0 + 1) - \frac{1}{n\pi}\frac{1}{n\pi}\sin n\pi\eta \Big|_0^1 \right] \tag{3.154}$$

$$F_n(\tau) = \frac{2q}{n\pi} \tag{3.155}$$

$b_n(\tau)$ and $F_n(\tau)$ are substituted into $w_n(\tau)$ (3.62) to obtain:

$$w_n(\tau) = \int_0^{\tau} e^{-D^*(n\pi)^2(t-\tau)} \cdot \frac{2q}{n\pi}\,dt + \left(-\frac{2c_i}{n\pi c_0}(\cos n\pi - 1) - \frac{4}{n\pi}\right) e^{-D^*\left(\frac{n\pi}{l}\right)^2 t} \tag{3.156}$$

$$w_n(\tau) = -\frac{2q}{n\pi}\frac{1}{D^*(n\pi)^2} e^{-D^*(n\pi)^2(t-\tau)}\Bigg|_0^1 - \left(\frac{2c_i}{n\pi c_0}(\cos n\pi - 1) - \frac{4}{n\pi}\right) e^{-D^*(n\pi)^2\tau} \tag{3.157}$$

$$w_n(\tau) = -\frac{2q}{D^*(n\pi)^3}\left[1 - e^{-D^*(n\pi)^2\tau}\right] - \frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi - 1) + 2\right) e^{-D^*(n\pi)^2\tau} \tag{3.158}$$

$$c_0(\eta,\tau) = w_0(\eta,\tau) + g_0(\eta,\tau) \tag{3.159}$$

$$w_0(\eta,\tau) = \sum_{n=1}^{\infty} w_n(\tau)\sin n\pi\eta \tag{3.160}$$

$$c_0(\eta,\tau) = (2 - q\tau)(1-\eta) + \sum_{n=1}^{\infty}\left(\frac{2q}{D^*(n\pi)^3}\left[1 - e^{-D^*(n\pi)^2\tau}\right] - \frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi - 1) + 2\right) e^{-D^*(n\pi)^2\tau}\right)\sin n\pi\eta \tag{3.161}$$

Recall that

$$w_0(\eta,\tau) = \sum_{n=1}^{\infty}\left(\frac{2q}{D^*(n\pi)^3}\left[1 - e^{-D^*(n\pi)^2\tau}\right] - \frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi - 1) + 2\right) e^{-D^*(n\pi)^2\tau}\right)\sin n\pi\eta \tag{3.162}$$

$$\frac{\partial w_0}{\partial \eta} = \sum_{n=1}^{\infty}\left(-\frac{4q}{D^*(n\pi)^2}\left[1 - e^{-D^*(n\pi)^2\tau}\right] - 2\left(\frac{c_i}{c_0}(\cos n\pi - 1) + 2\right) e^{-D^*(n\pi)^2\tau}\right)\cos n\pi\eta \tag{3.163}$$

By substituting equations (3.123) and (3.125) in the equation (3.60), gives

$$\begin{aligned}\frac{\partial w_1}{\partial \tau} = D^*\frac{\partial^2 w_1}{\partial \eta^2} &- b\sum_{n=1}^{\infty}\left(\frac{2q}{D^*(n\pi)^2}\left[1 - e^{-D^*(n\pi)^2\tau}\right] - 2\left(\frac{c_i}{c_0}(\cos n\pi - 1) + 2\right) e^{-D^*(n\pi)^2\tau}\right)\cos n\pi\eta \\ &- \sum_{n=1}^{\infty}\left(\frac{2q}{D^*(n\pi)^3}\left[1 - e^{-D^*(n\pi)^2\tau}\right] - \frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi - 1) + 2\right) e^{-D^*(n\pi)^2\tau}\right)\sin n\pi\eta\end{aligned} \tag{3.164}$$

From equation (3.164) above

$$F(\eta,\tau)=-b\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{2}}\left[1-e^{-D^{*}(n\pi)^{2}\tau}\right]-2\left(\frac{c_i}{c_0}(\cos n\pi-1)+2\right)e^{-D^{*}(n\pi)^{2}\tau}\right)\cos n\pi\eta$$
$$-\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{3}}\left[1-e^{-D^{*}(n\pi)^{2}\tau}\right]-\frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi-1)+2\right)e^{-D^{*}(n\pi)^{2}\tau}\right)\sin n\pi\eta \tag{3.165}$$

$$F_n(\tau)=-2\int_0^1\left(-b\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{2}}\left[1-e^{-D^{*}(n\pi)^{2}\tau}\right]-2\left(\frac{c_i}{c_0}(\cos n\pi-1)+2\right)e^{-D^{*}(n\pi)^{2}\tau}\right)\cos n\pi\eta\right)\sin n\pi\eta\,d\eta \tag{3.166}$$
$$-2\int_0^1\left[\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{3}}\left[1-e^{-D^{*}(n\pi)^{2}\tau}\right]-\frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi-1)+2\right)e^{-D^{*}(n\pi)^{2}\tau}\right)\sin n\pi\eta\right]\sin n\pi\eta\,d\eta$$

$$=-2\int_0^1\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{3}}\left[1-e^{-D^{*}(n\pi)^{2}\tau}\right]-\frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi-1)+2\right)e^{-D^{*}(n\pi)^{2}\tau}\right)\sin^{2}n\pi\eta\,d\eta \tag{3.167}$$

$$F_n(\tau)=-\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{3}}\left[1-e^{-D^{*}(n\pi)^{2}\tau}\right]-\frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi-1)+2\right)e^{-D^{*}(n\pi)^{2}\tau}\right) \tag{3.168}$$

From equation (3.143)

$$\tau_w^n(\tau)=\int_0^{\tau}e^{-D^{*}(n\pi)^{2}(\tau-t)}\left[-\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{3}}\left[1-e^{-D^{*}(n\pi)^{2}t}\right]-\frac{2}{n\pi}\left(\frac{c_i}{c_0}(\cos n\pi-1)+2\right)e^{-D^{*}(n\pi)^{2}t}\right)\right]dt$$

$$=\int_0^{\tau}e^{-D^{*}(n\pi)^{2}(\tau-t)}\left(-\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{3}}\left[1-e^{-D^{*}(n\pi)^{2}t}\right]-\frac{2}{n\pi}\left[\frac{c_i}{c_0}(\cos n\pi-1)+2\right]e^{-D^{*}(n\pi)^{2}t}\right)\right)dt$$

$$=\int_0^{\tau}-\sum_{n=1}^{\infty}\left(\frac{2q}{D^{*}(n\pi)^{3}}\left[e^{-D^{*}(n\pi)^{2}(\tau-t)}-e^{-D^{*}(n\pi)^{2}\tau}\right]dt+\frac{2}{n\pi}\left[\frac{c_i}{c_0}(\cos n\pi-1)+2\right]\int_0^{\tau}e^{-D^{*}(n\pi)^{2}\tau}dt\right)$$

$$=-\sum_{n=1}^{\infty}\frac{2q}{D^{*}(n\pi)^{3}}\left[\frac{1}{D^{*}(n\pi)^{2}}e^{-D^{*}(n\pi)^{2}(\tau-t)}-te^{-D^{*}(n\pi)^{2}\tau}\right]_0^{\tau}+\frac{2}{n\pi}\left[\frac{c_i}{c_0}(\cos n\pi-1)+2\right]te^{-D^{*}(n\pi)^{2}\tau}$$

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

(3.169)

(3.170)

(3.171)

(3.172)

(3.173)

$$c_1(\eta,\tau) = w_1(\eta,\tau) \tag{3.174}$$

$$c_1(\eta,\tau) = -\sum\left(\sum \frac{2q}{D^*(n\pi)^3}\left[\frac{1}{D^*(n\pi)^2}\left(1-e^{-D^*(n\pi)^2\tau}\right) - \tau e^{-D^*(n\pi)^2\tau}\right]\right)\sin n\pi\eta + \sum\left(\sum \frac{2}{n\pi}\left[\frac{c_i}{c_0}\left(\cos n\pi - 1\right) + 2\right]\tau e^{-D^*(n\pi)^2\tau}\right)\sin n\pi\eta \tag{3.175}$$

The general solution of the equation (3.108) is therefore

$$c(\eta,\tau) = c_0(\eta,\tau) + \alpha c_1(\eta,\tau) \tag{3.176}$$

where $c_0(\eta,\tau)$ and $c_1(\eta,\tau)$ are given in equation (3.161) and (3.175) respectively.

CHAPTER FOUR

4.0 RESULTS AND DISCUSSIONS

4.1 Results

In this section, the solutions obtained for the two cases considered are expressed in graphical forms with the aid of the Mathematical software called MAPLE 16. Under each of the graphs, brief interpretation and discussions were made. 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 $\alpha = 0.1$.

4.1.1 Graphical representation of the solution for case 1 with Neumann Boundary Condition

The solution obtained in equation (3.84) and (3.106) for case 1are presented in graphs in this section.

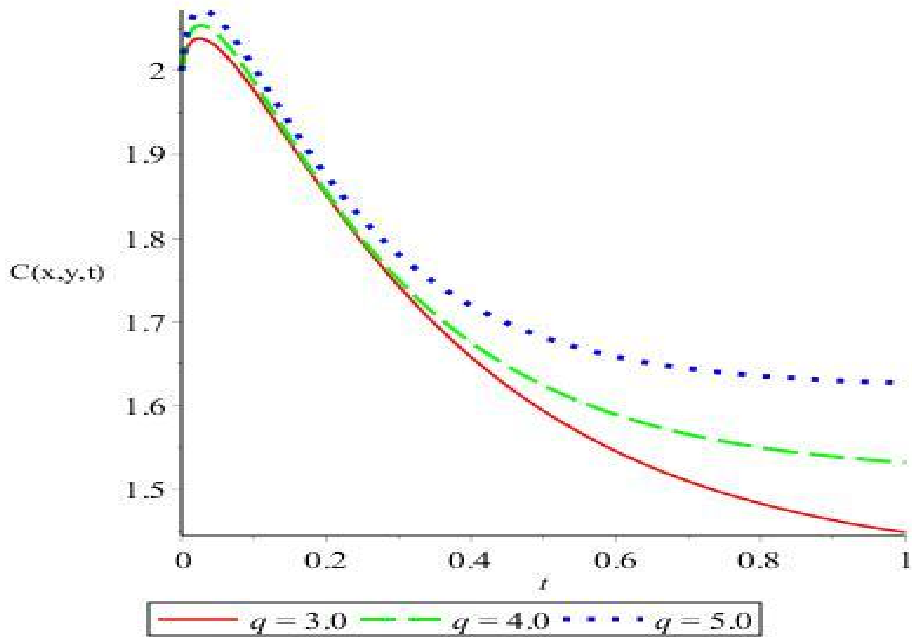

Figure 4.1: Contaminant Concentration Profile with Time for Varying Flow Resistance Coefficient.

The graph in Figure 4.1 shows that the contaminant concentration decreases with time but decreases faster as the flow resistance coefficient decreases.

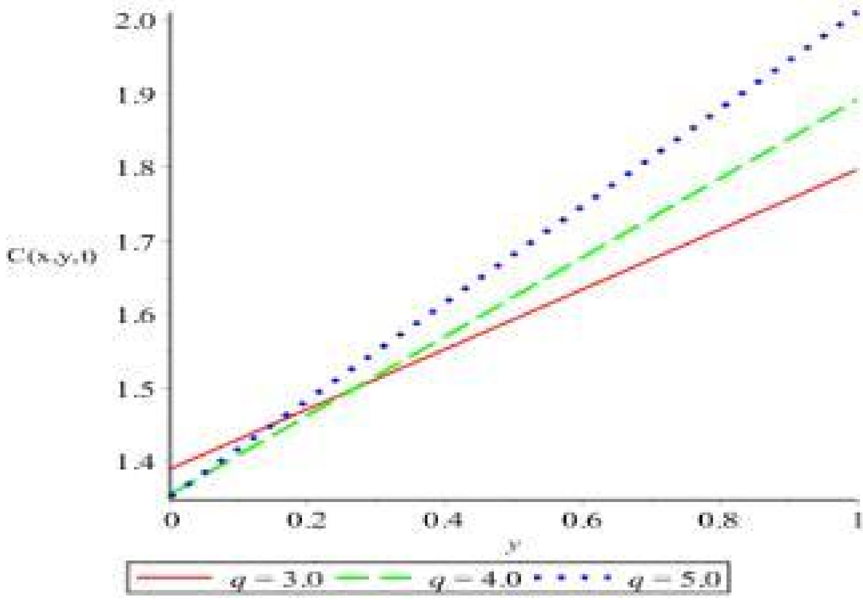

Figure 4.2: Contaminant Concentration Profile with Vertical Distance y for Varying Flow Resistance Coefficient.

The graph in Figure 4.2 reveals that the contaminant concentration increases with increase in vertical distance as the flow resistance coefficient increases.

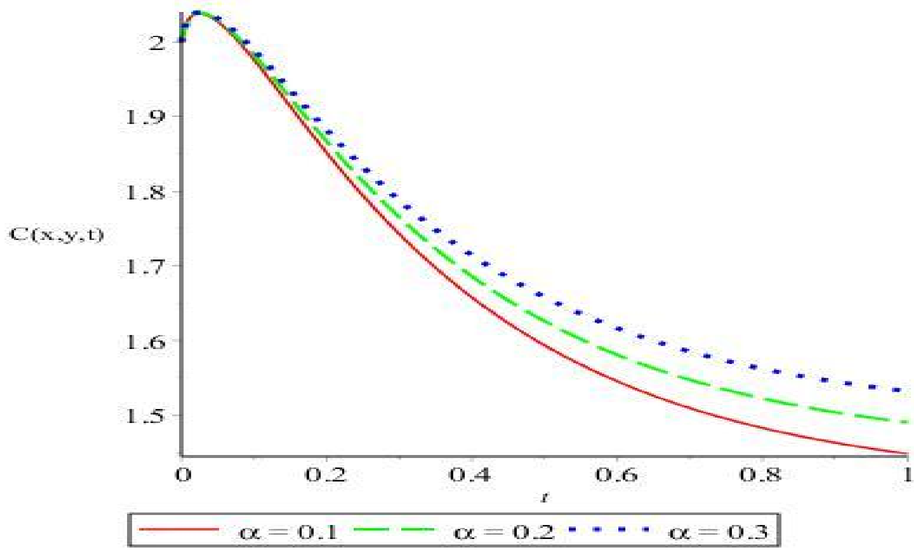

Figure 4.3: Contaminant Concentration Profile with Time for Varying Decay Parameter.

In Figure 4.3 above, the contaminant concentration decline with increase in time but tends to decrease faster as the decay coefficient decreases.

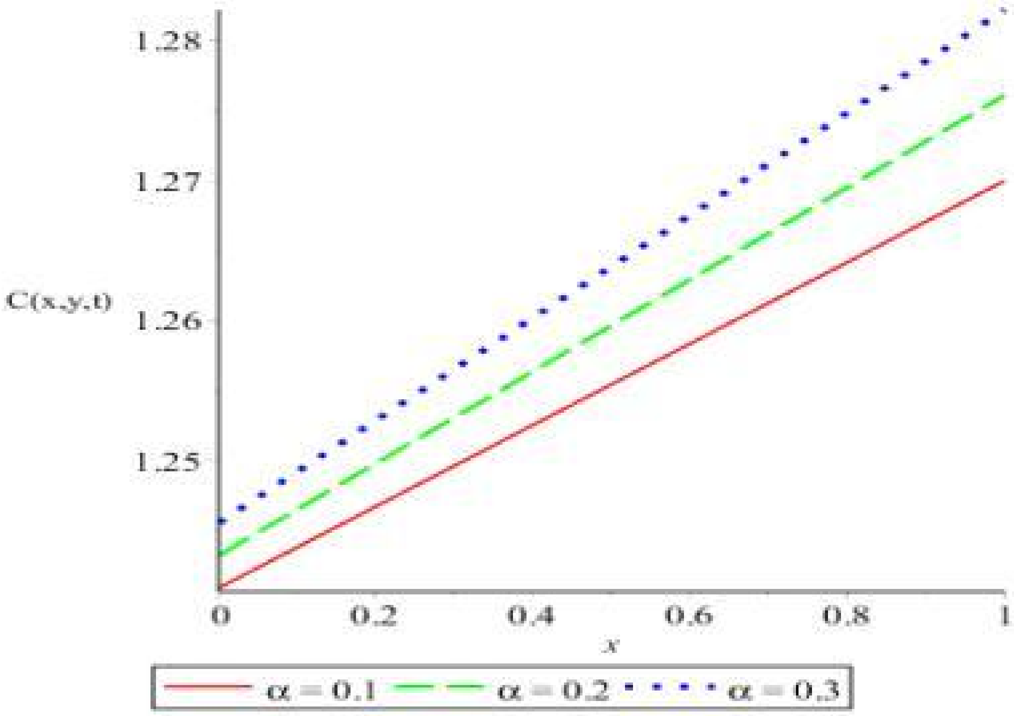

Figure 4.4: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Decay Coefficient.

The graph in Figure 4.4 shows that the contaminant concentration increases with increase in horizontal distance as decay coefficient increases. The contaminant concentration increases faster for higher values of decay parameter.

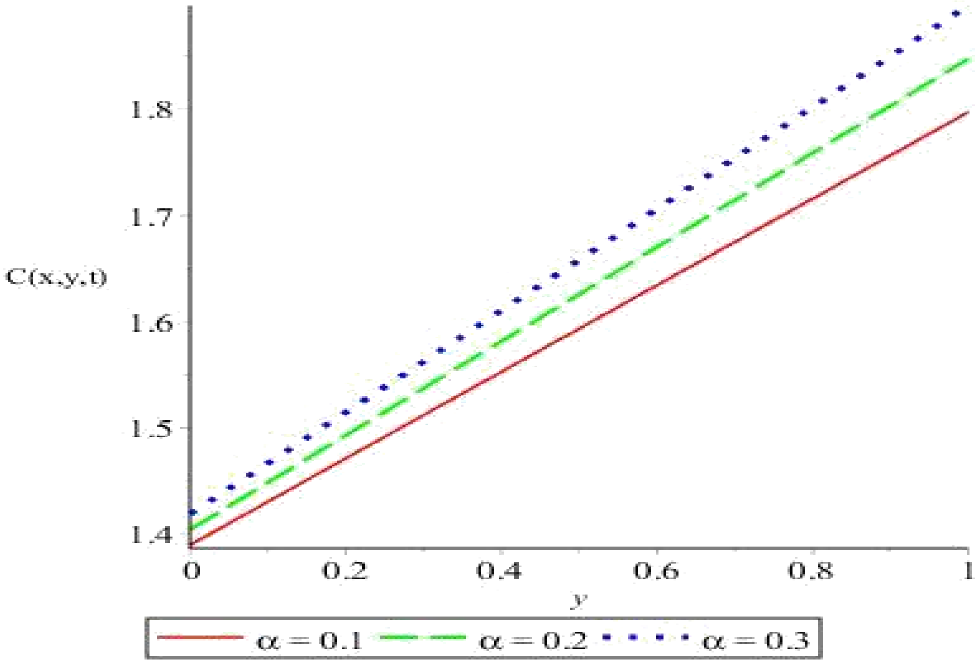

Figure 4.5: Contaminant Concentration Profile with Vertical Distance *y* for Varying Initial Decay Coefficient.

Figure 4.5 show that as the value of decay coefficient increases, the contaminant concentration increases faster with increase in vertical distance.

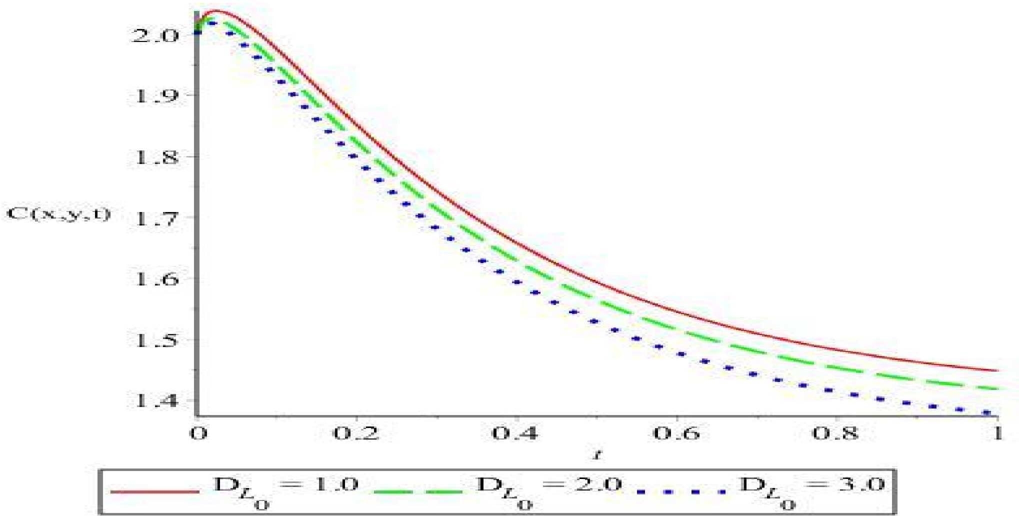

Figure 4.6: Contaminant Concentration Profile with Time for Varying Longitudinal Dispersion Coefficient.

The effect of increasing the horizontal dispersion coefficient is shown in the Figure 4.6 above. The graph reveals that the contaminant concentration decreases with increase in time as the horizontal dispersion coefficient increases.

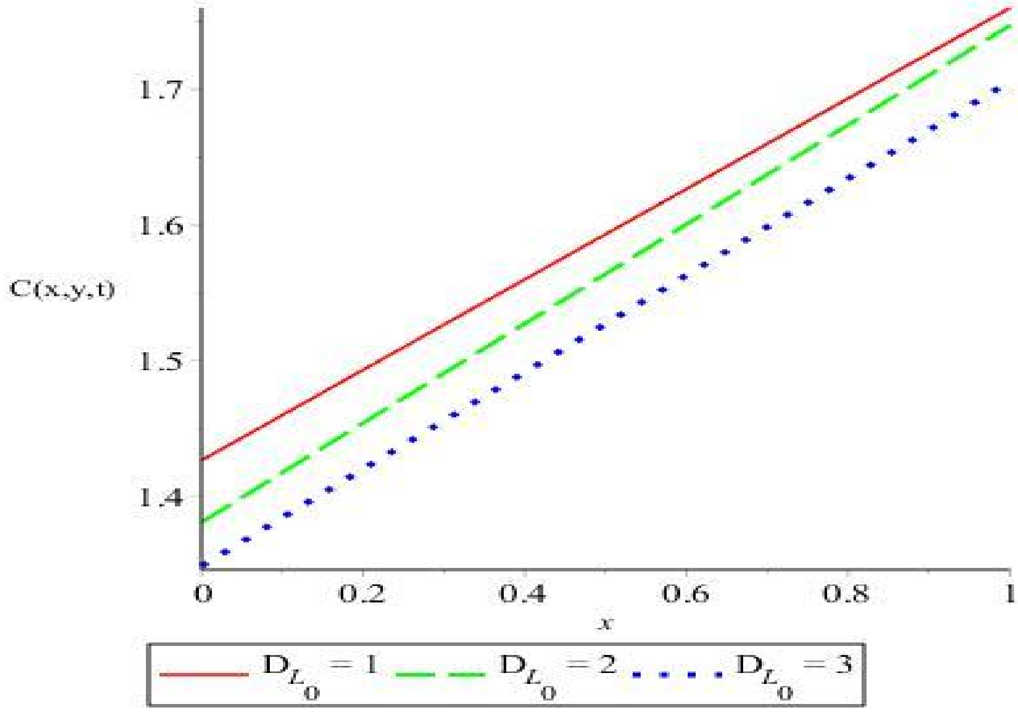

Figure 4.7: Contaminant Concentration Profile with Distance *x* for Varying Horizontal Dispersion Coefficient.

In Figure 4.7, the effect of increasing the horizontal dispersion coefficient is shown. The graph shows that the contaminant concentration increases with increase in the horizontal distance.

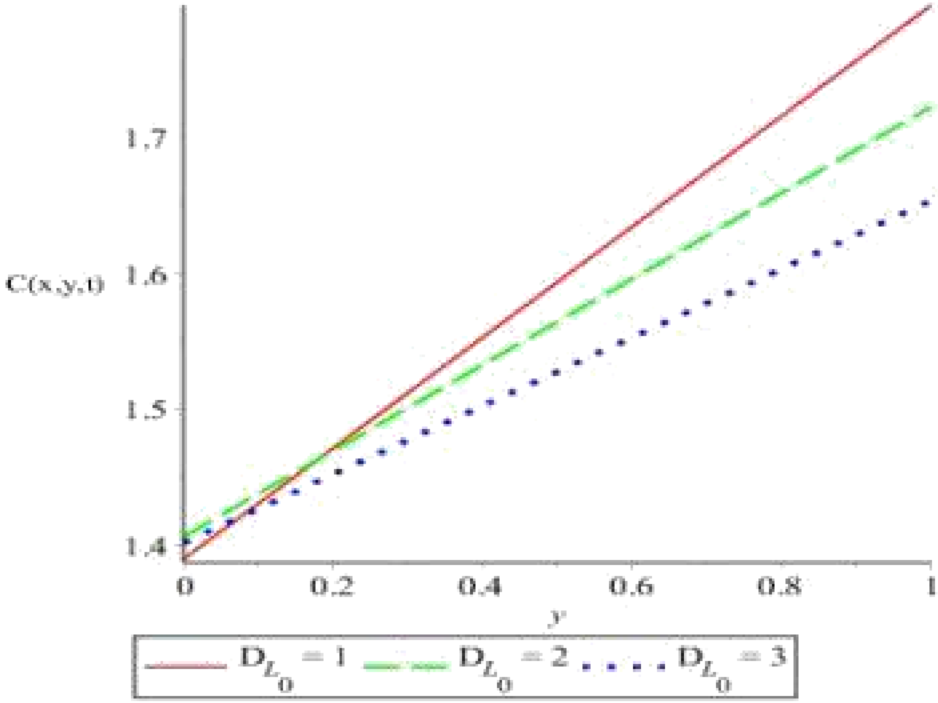

Figure 4.8: Contaminant Concentration Profile with Vertical Distance y for Varying Initial Horizontal Dispersion Coefficient.

The above graph in Figure 4.8 shows that as the horizontal dispersion coefficient increases, the contaminant concentration increases in the horizontal direction.

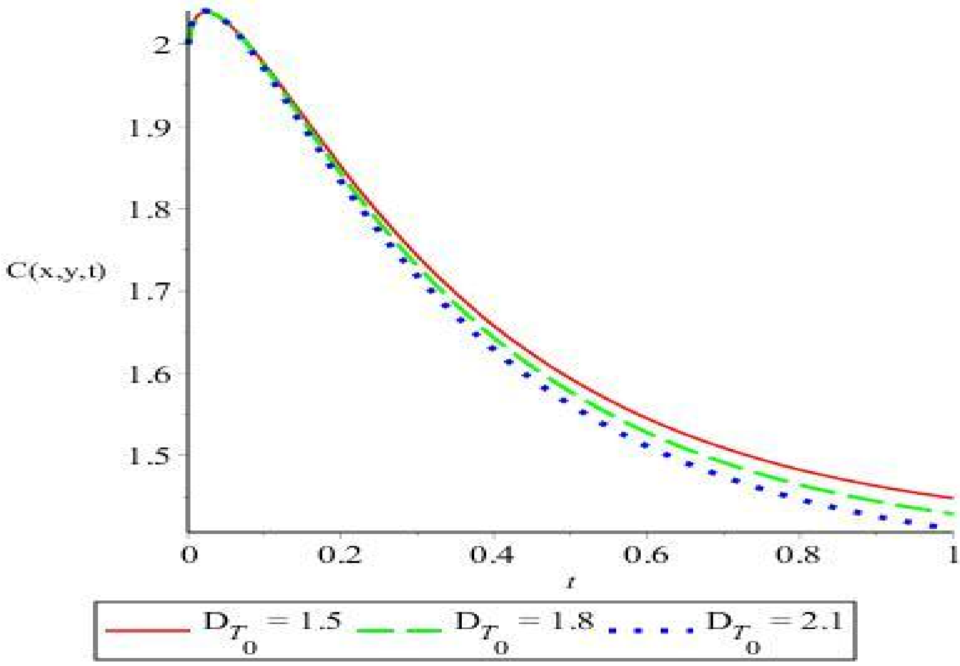

Figure 4.9: Contaminant Concentration Profile with Time for Varying Vertical Dispersion Coefficient.

The graph in figure 4.9 reveals that the contaminant concentration decline with time as the vertical dispersion coefficient increases but decreases faster for higher values of the vertical dispersion coefficient.

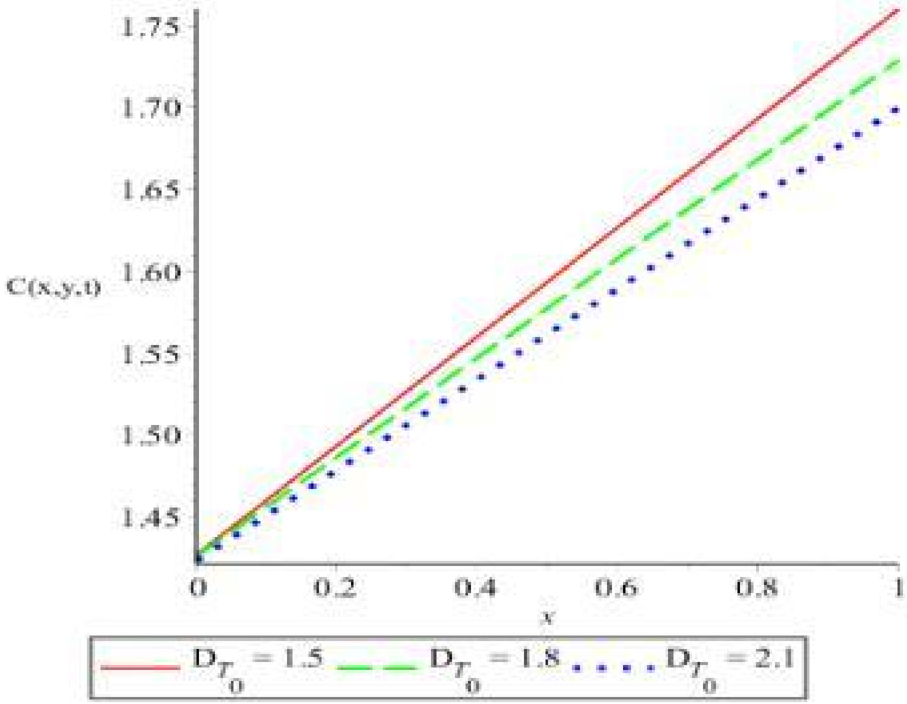

Figure 4.10: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Vertical Dispersion Coefficient.

Figure 4.10 reveals that the contaminant concentration increases with increase in the vertical dispersion coefficient but faster as the value of vertical dispersion coefficient decreases.

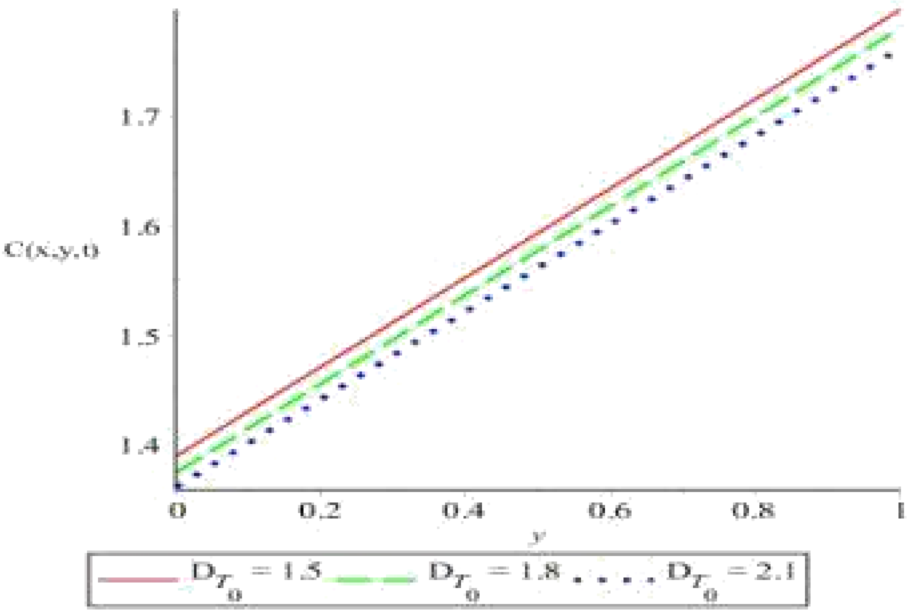

Figure 4.11: Contaminant Concentration Profile with Vertical Distance y for Varying Initial Horizontal Dispersion Coefficient.

The impact of increasing the value of the vertical dispersion is shown in Figure 4.11 above. The graph shows that the contaminant concentration increases with increase in vertical distance.

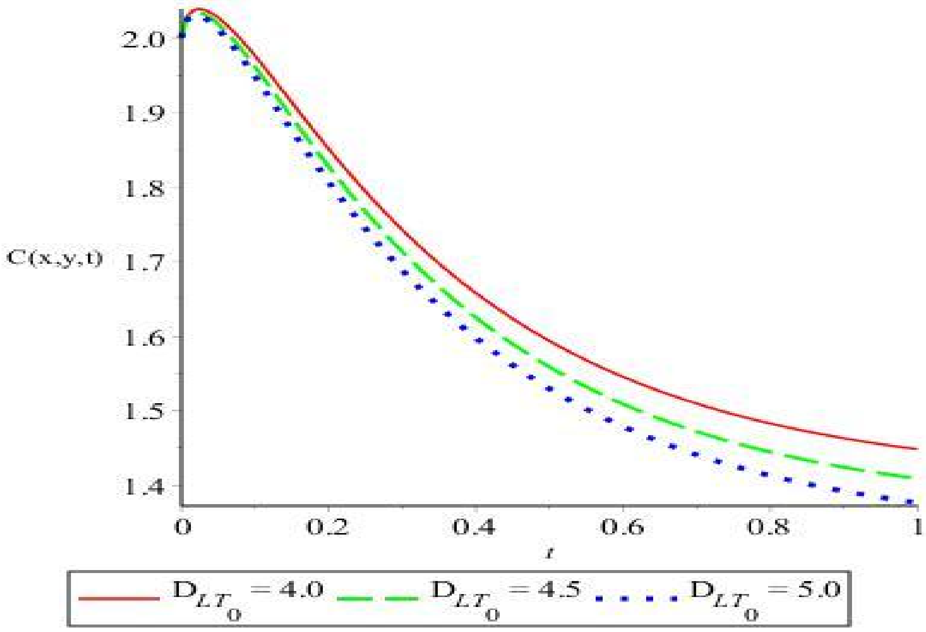

Figure 4.12: Contaminant Concentration Profile with Time for Varying Cross-flow Dispersion Coefficient.

In the figure 4.12 above, the contaminant concentration decreases with time as the cross-flow dispersion coefficient increases and decreases faster for higher values of the cross-flow dispersion coefficient.

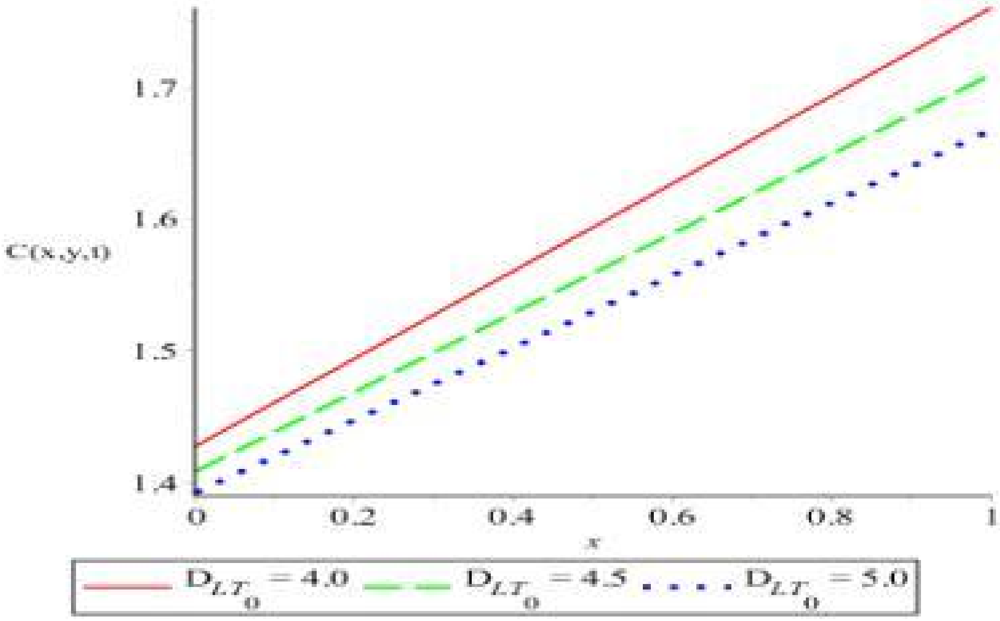

Figure 4.13: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Cross-flow Dispersion Coefficient.

The graph in the Figure 4.03 shows that the concentration of the contaminant increases as the horizontal distance increases. It increases faster as the cross-flow dispersion coefficient decreases.

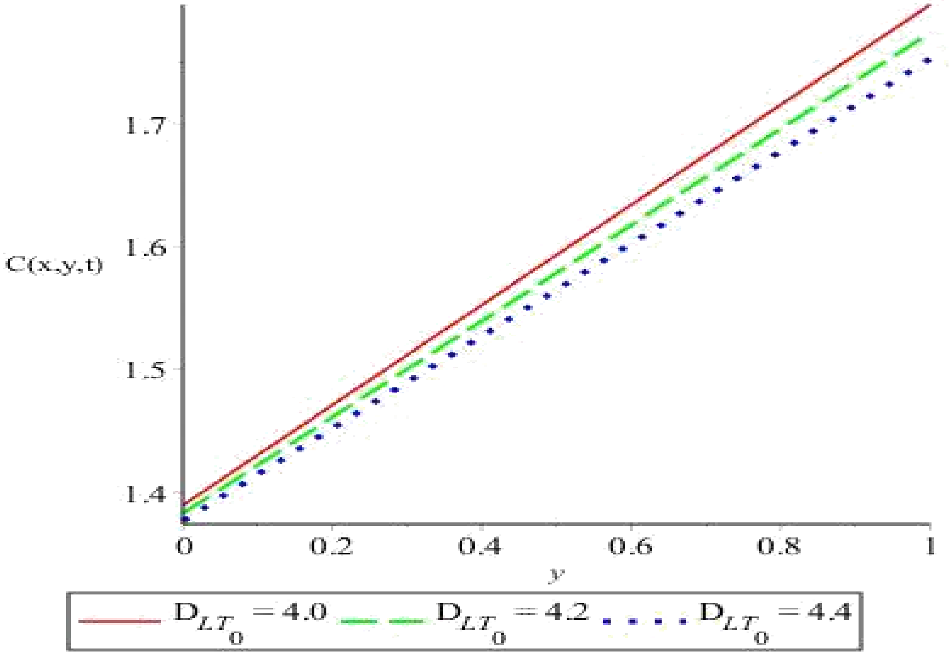

Figure 4.14: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Cross-flow Dispersion Coefficient.

The graph in Figure 4.14 shows that the contaminant concentration increases along the vertical direction as the cross-flow dispersion coefficient increases.

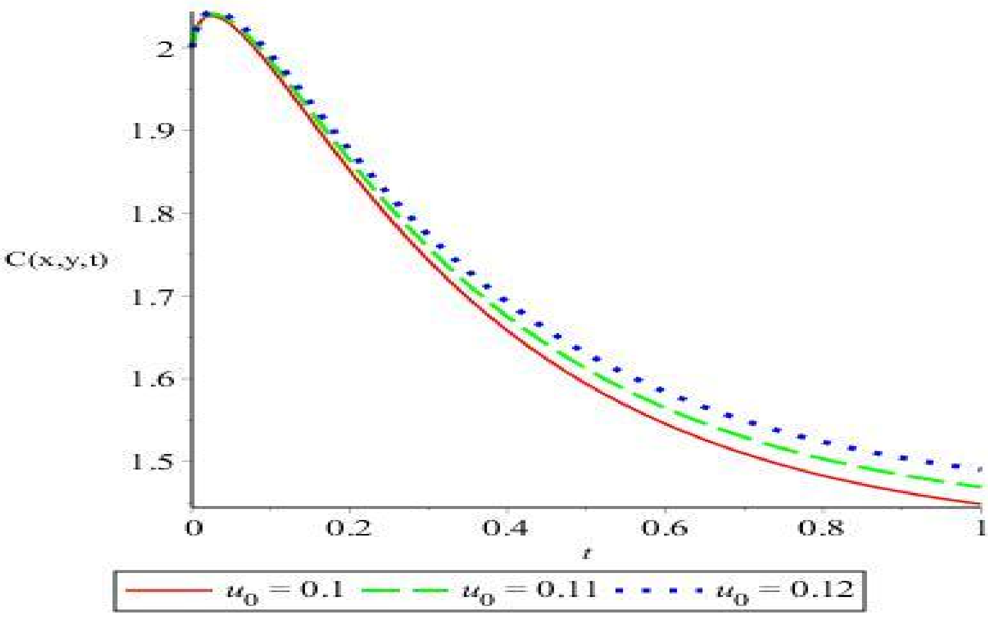

Figure 4.15: Contaminant Concentration Profile with Time for Varying Initial Horizontal Velocity Coefficient.

In Figure 4.15, the contaminant concentration decline with time as the initial horizontal velocity increases.

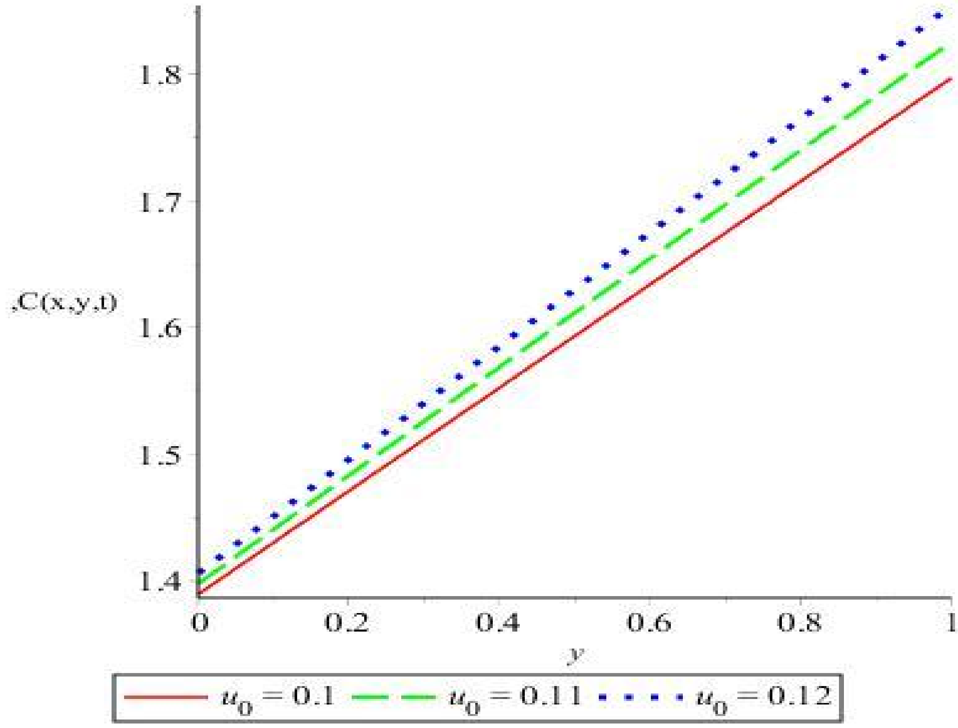

Figure 4.16: Contaminant Concentration Profile with Horizontal Distance *y* for Varying Initial Horizontal Velocity Coefficient.

Figure 4.16 shows that the contaminant concentration increases in the vertical direction as the initial horizontal velocity increases.

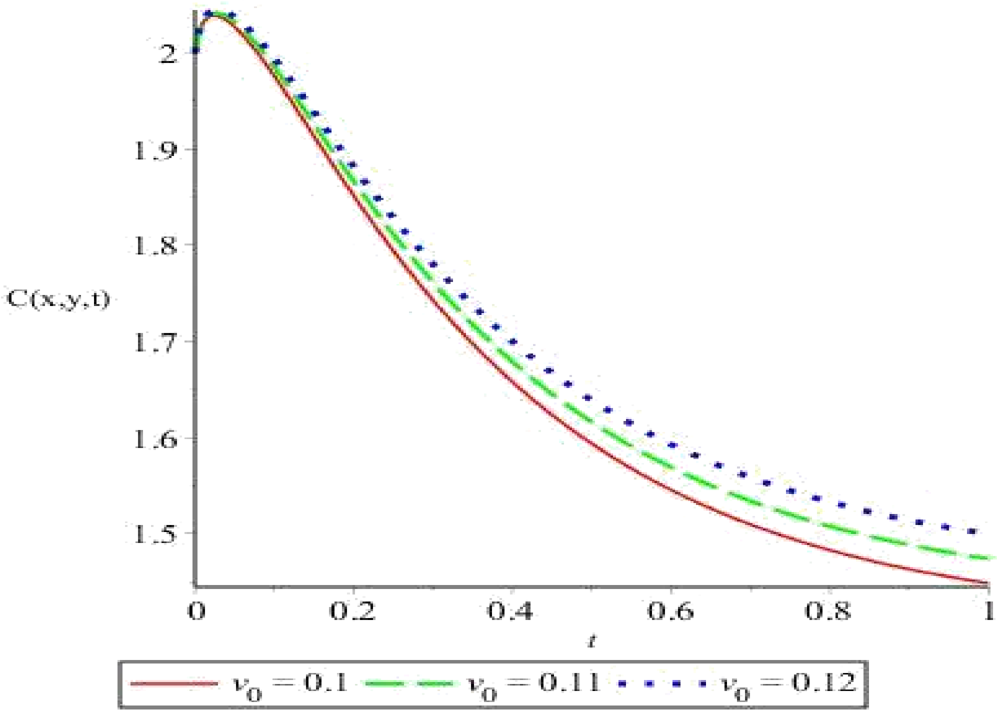

Figure 4.17: Contaminant Concentration Profile with Time for Varying Initial Horizontal Velocity Coefficient.

In the Figure 4.17 above, on increasing the value of the initial vertical velocity, the contaminant concentration decline with time.

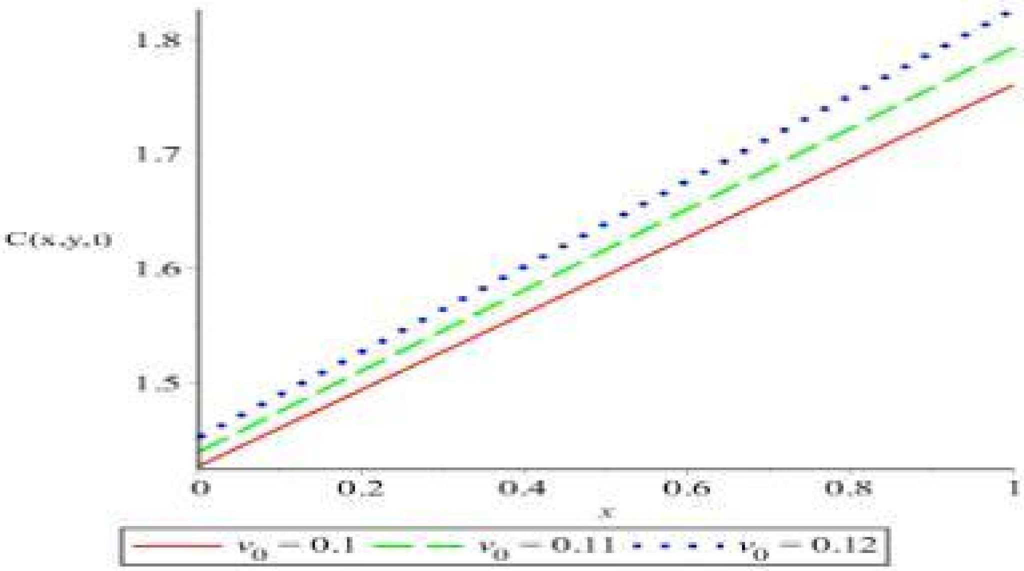

Figure 4.18: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Horizontal Velocity Coefficient.

The graph in the figure 4.18 above shows that the contaminant concentration increases as the horizontal distance increases for increasing value of the vertical velocity coefficient.

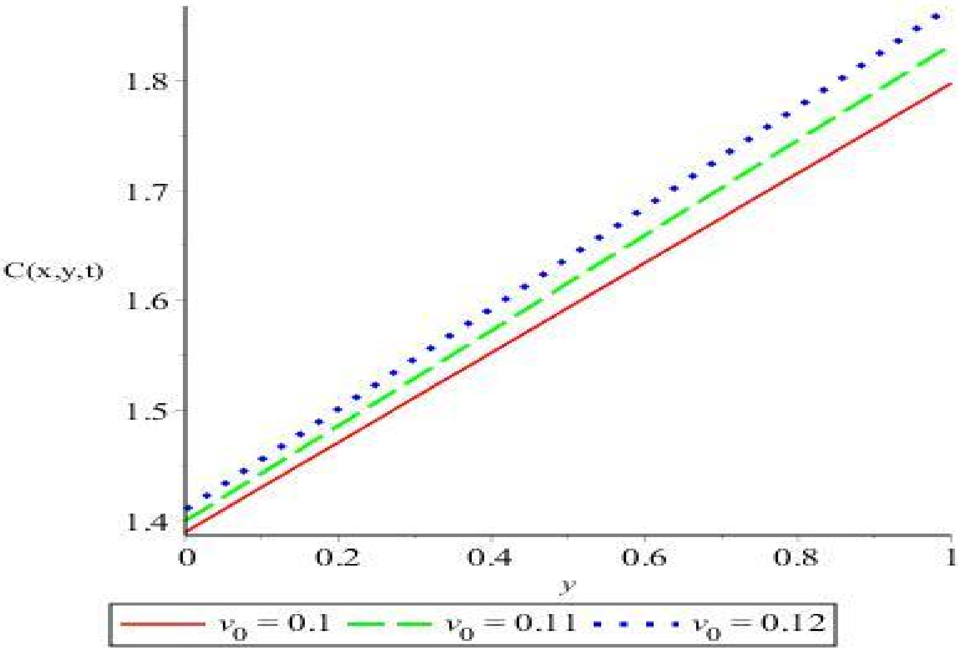

Figure 4.19: Contaminant Concentration Profile with Vertical Distance *y* for Varying Initial Horizontal Velocity Coefficient.

The graph in Figure 4.19 shows the effect of increasing vertical initial velocity on the concentration. It reveals that the contaminant concentration increases as the vertical initial velocity coefficient increases.

4.1.2 Graphical Representation of the Solution for Case Two with the Dirichlet Boundary Conditions.

In this section, the solution obtained in equation (3.161) and (3.175) for case two are presented in graphs below:

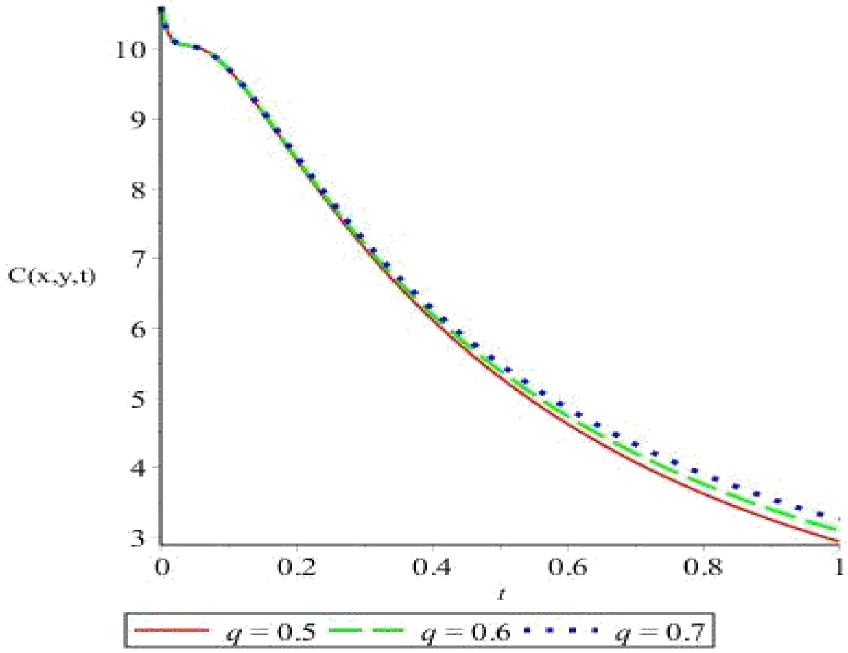

Figure 4.20: Contaminant Concentration Profile with Time for Varying Flow Resistance Coefficient.

The effect of the flow resistance parameter on the concentration of the contaminant is shown in Figure 4.20. It reveals the concentration decline with time as the floe resistance parameter increases.

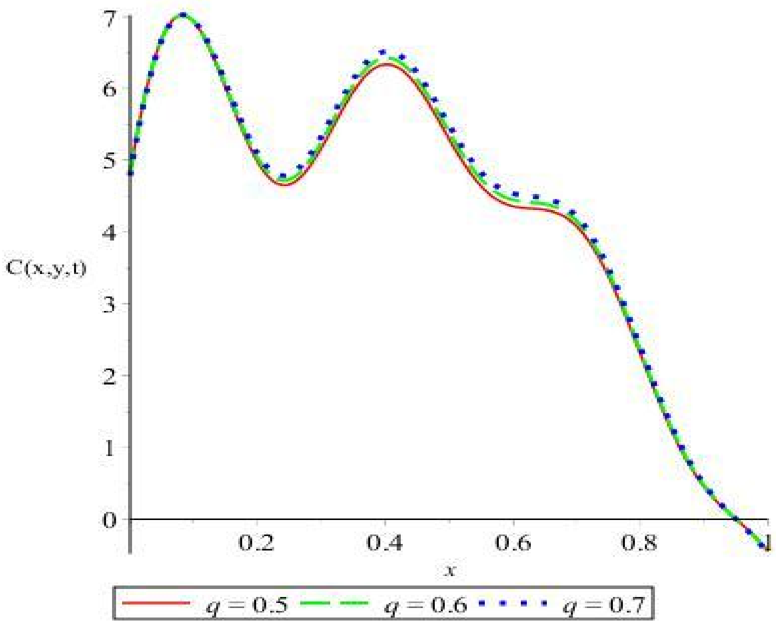

Figure 4.21: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Flow Resistance Coefficient.

In the Figure 4.21, the graph shows that the concentration moves sinusoidally in the horizontal direction and later decline sharply for growing values of flow resistance parameter.

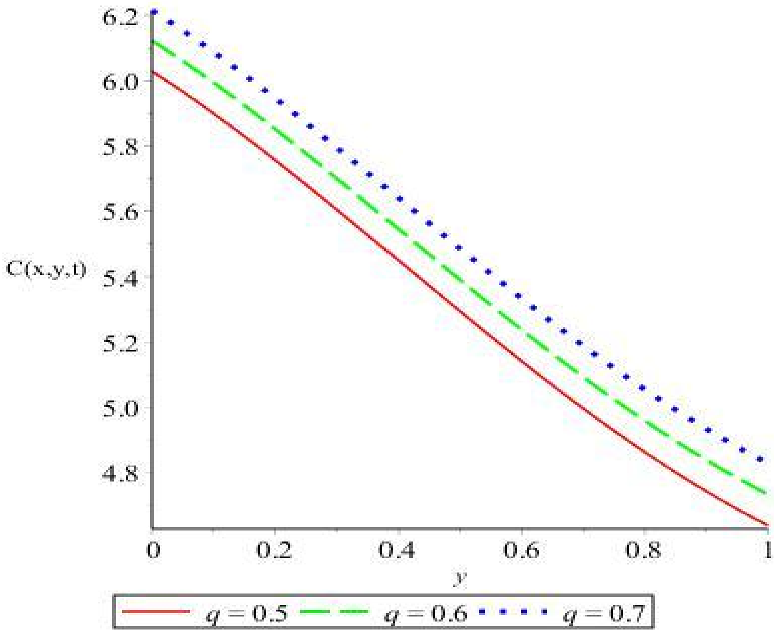

Figure 4.22: Contaminant Concentration Profile with Vertical Distance y for Varying Flow Resistance Coefficient.

The graph in Figure 4.22 above shows that the contaminant concentration decline with increasing vertical distance as the flow resistance parameter increases.

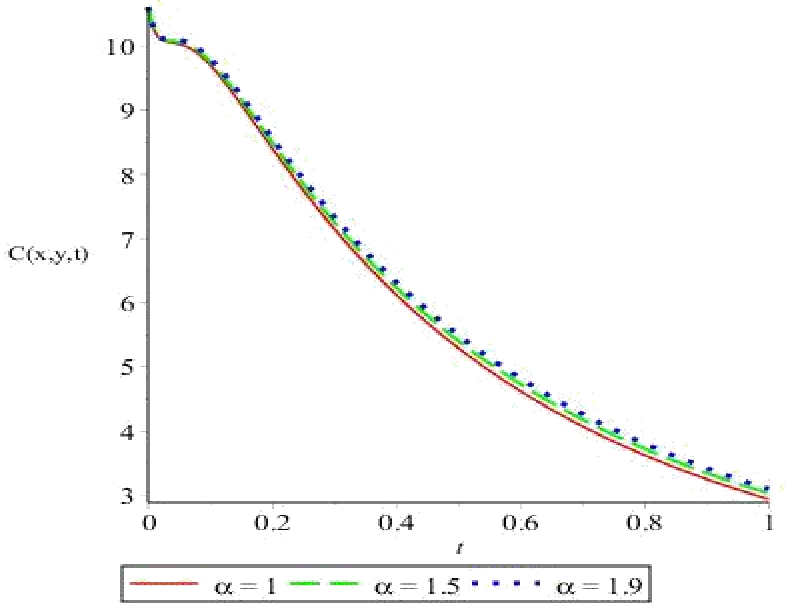

Figure 2.23: Contaminant Concentration Profile with Time for Varying Decay Parameter.

Figure 4.23 shows the impact of increasing the decay coefficient on the contaminant concentration. The graph shows that the concentration decline with time as the decay coefficient increases.

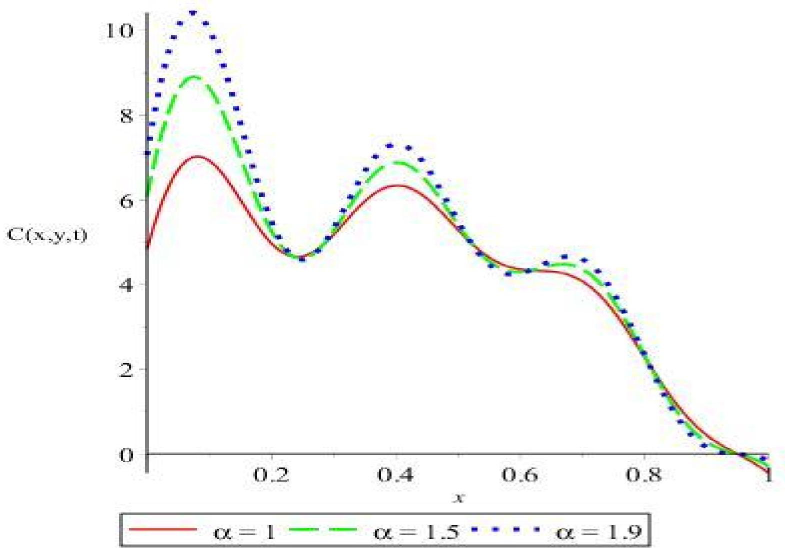

Figure 4.24: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Decay Coefficient.

In Figure 4.24, the effect of increasing the value of decay coefficient on the concentration is shown. The graph shows that the concentration moves sinusoidally and decline sharply as the decay coefficient increases.

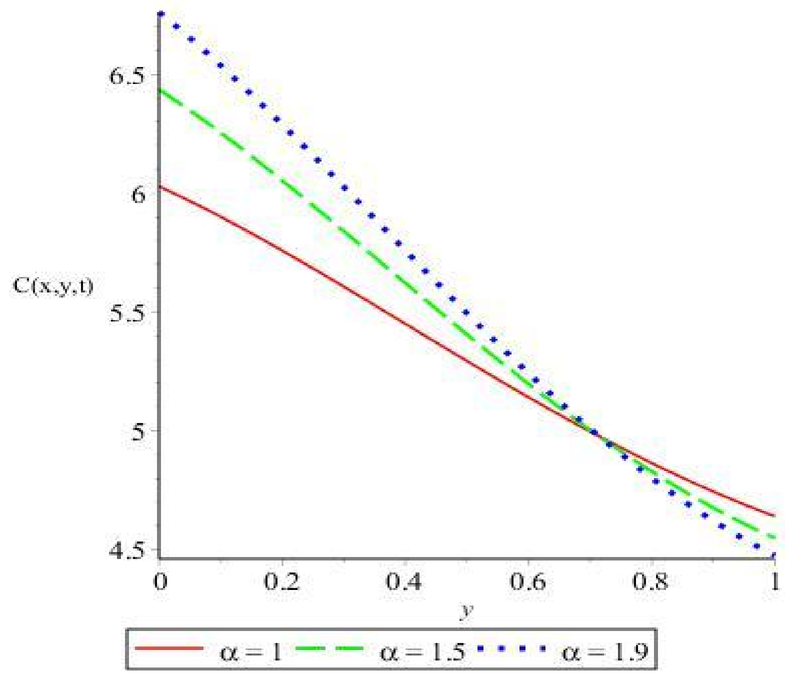

Figure 4.25: Contaminant Concentration Profile with Horizontal Distance *y* for Varying Initial Decay Coefficient.

The effect of increasing the decay coefficient is also shown in figure 4.25 above. The graph shows that the contaminant concentration decline along the vertical spatial direction as the decay coefficient increases.

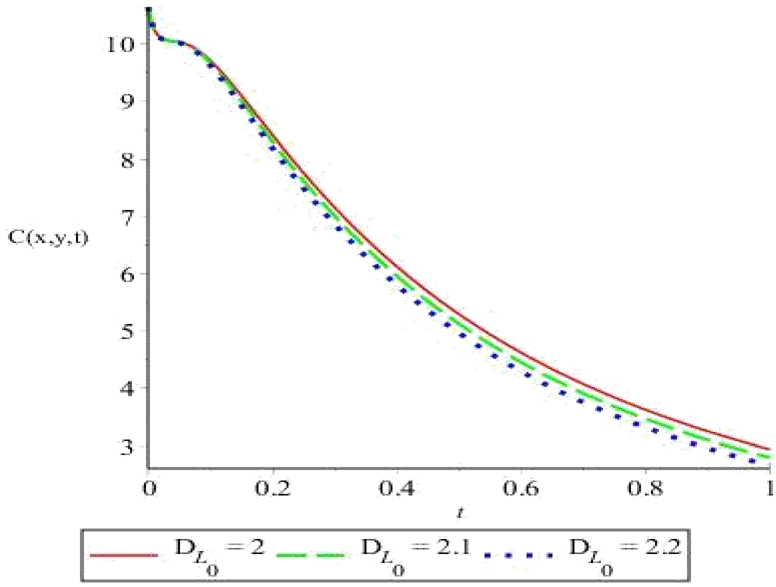

Figure 4.26: Contaminant Concentration Profile with Time for Varying Longitudinal Dispersion Coefficient.

Figure 4.26 shows the impact of increasing the horizontal dispersion on the concentration. The graph shows that the contaminant concentration decline with time as the horizontal dispersion increases.

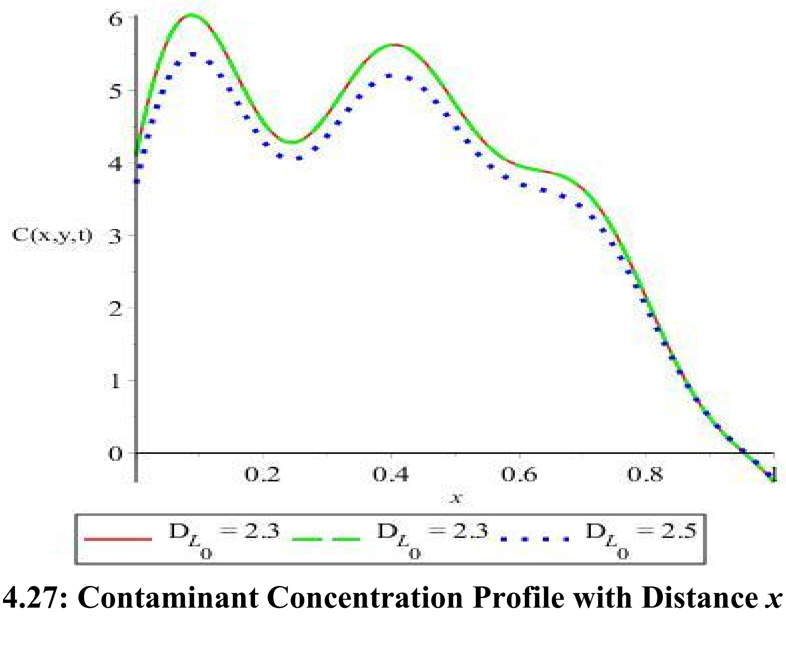

Figure 4.27: Contaminant Concentration Profile with Distance *x* for Varying Horizontal Dispersion Coefficient.

In the Figure 4.27, the contaminant concentration moves sinusoidally and then decline sharply which the effect of increasing the Horizontal Dispersion Coefficient on the concentration.

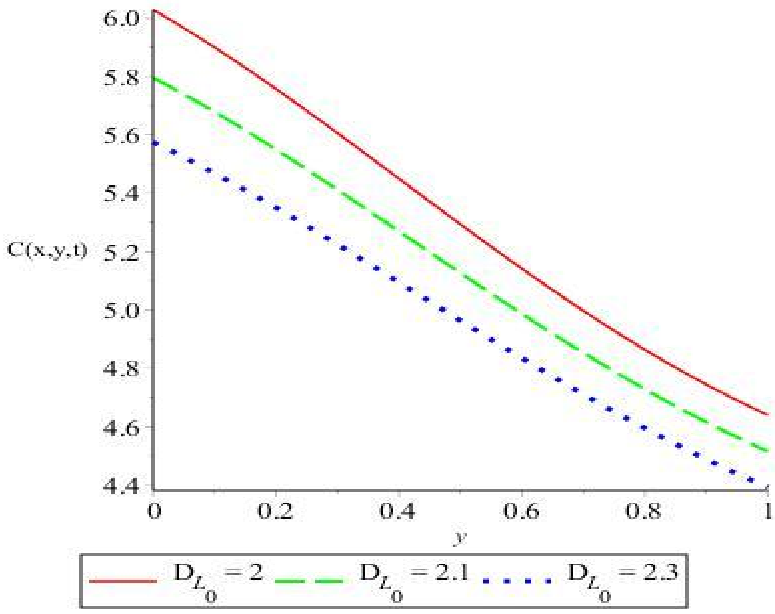

Figure 4.28: Contaminant Concentration Profile with Vertical Distance y for Varying Initial Horizontal Dispersion Coefficient.

The graph in Figure 4.28 shows the impact of varying the Horizontal Dispersion Coefficient on the concentration. The contaminant concentration decline along the vertical spacial direction as the Horizontal Dispersion Coefficient increases.

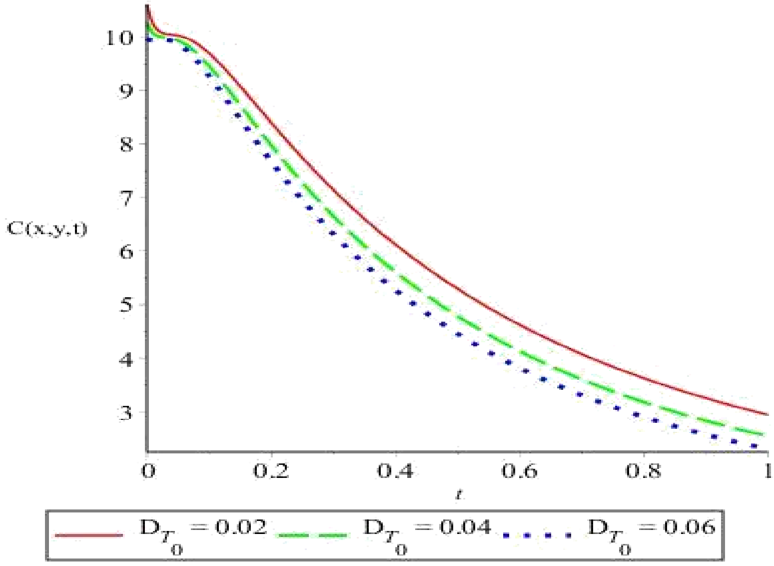

Figure 4.29: Contaminant Concentration Profile with Time for Varying Vertical Dispersion Coefficient.

In the Figure 4.29 above, the effect of increasing the initial vertical dispersion is shown. The graph shows that the concentration of contaminant decline with time as the initial vertical dispersion increases.

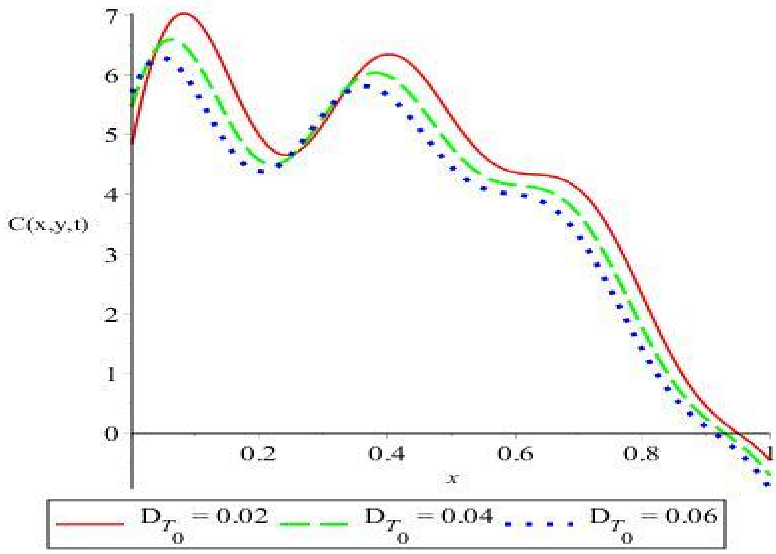

Figure 4.30: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Vertical Dispersion Coefficient.

The graph in Figure 4.30 shows the behavior of the contaminant along the horizontal direction as the initial vertical dispersion increases. From the graph, the contaminant concentration behaves sinusoidally and then decline sharply.

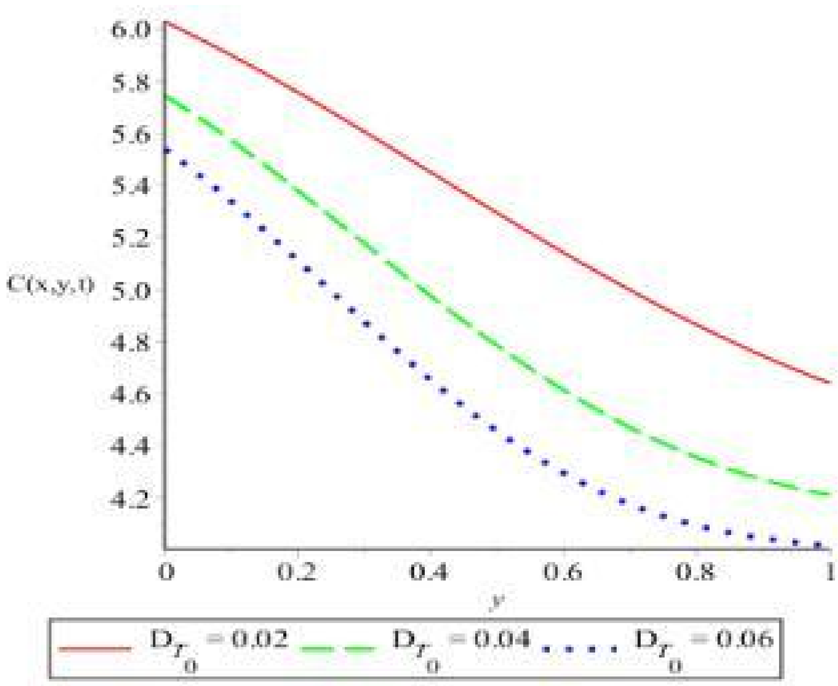

Figure 4.31: Contaminant Concentration Profile with Vertical Distance y for Varying Initial Horizontal Dispersion Coefficient.

Figure 4.31 shows the behavior of the contaminant concentration on the vertical direction as the initial vertical dispersion increases. The graph shows that the concentration decline with increasing initial vertical dispersion.

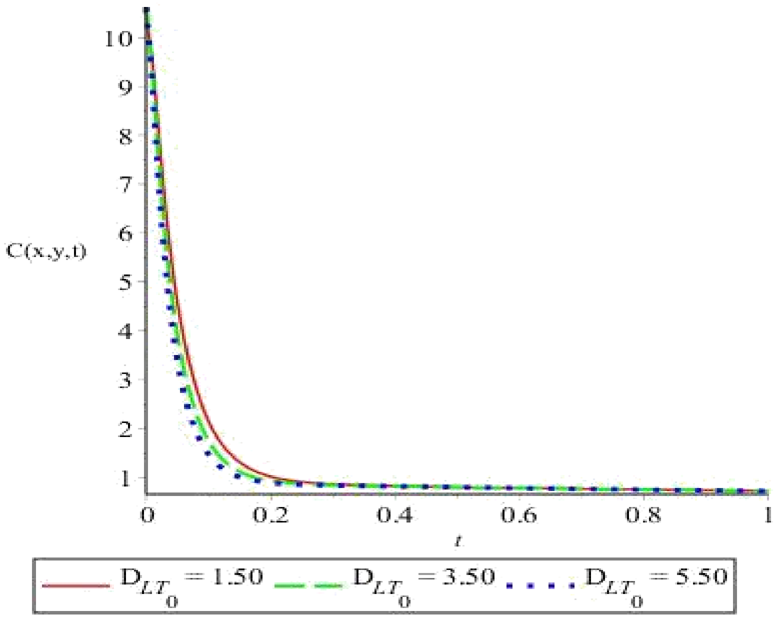

Figure 4.32: Contaminant Concentration Profile with Time for Varying Cross-flow Dispersion Coefficient.

Figure 4.32 shows the effect of varying the cross-flow dispersion on the concentration with time. The graph reveals that the concentration decline with time.

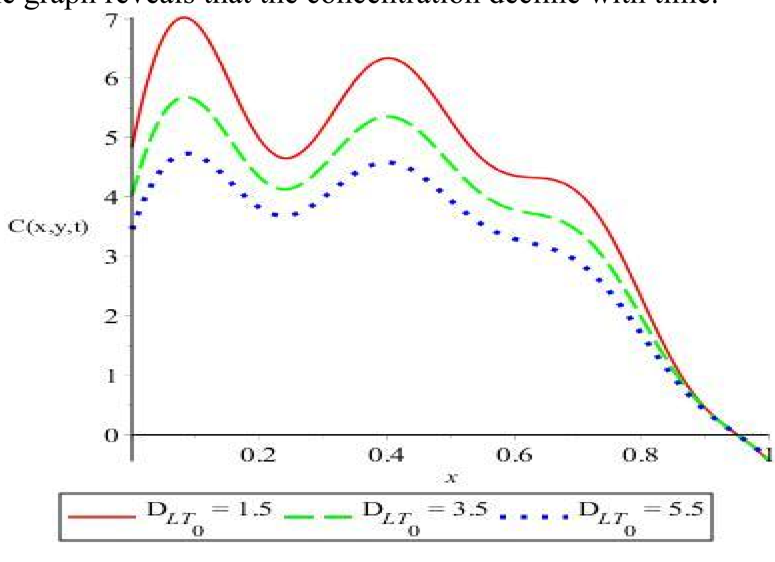

Figure 4.33: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Cross-flow Dispersion Coefficient.

The graph in Figure 4.33 shows that the contaminant concentration behaves sinusoidally along the horizontal direction and decline sharply as the Initial Cross-flow Dispersion Coefficient increases.

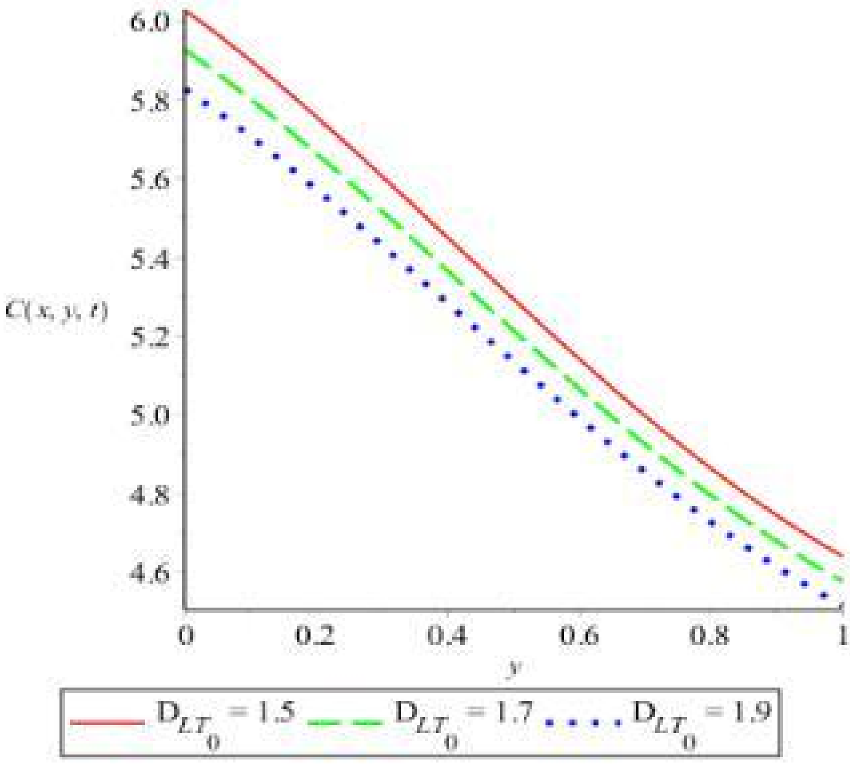

Figure 4.34: Contaminant Concentration Profile with Vertical Distance y for Varying Initial Cross-flow Dispersion Coefficient.

In the Figure 4.34, the contaminant concentration decreases along the vertical direction as the Initial Cross-flow Dispersion Coefficient increases.

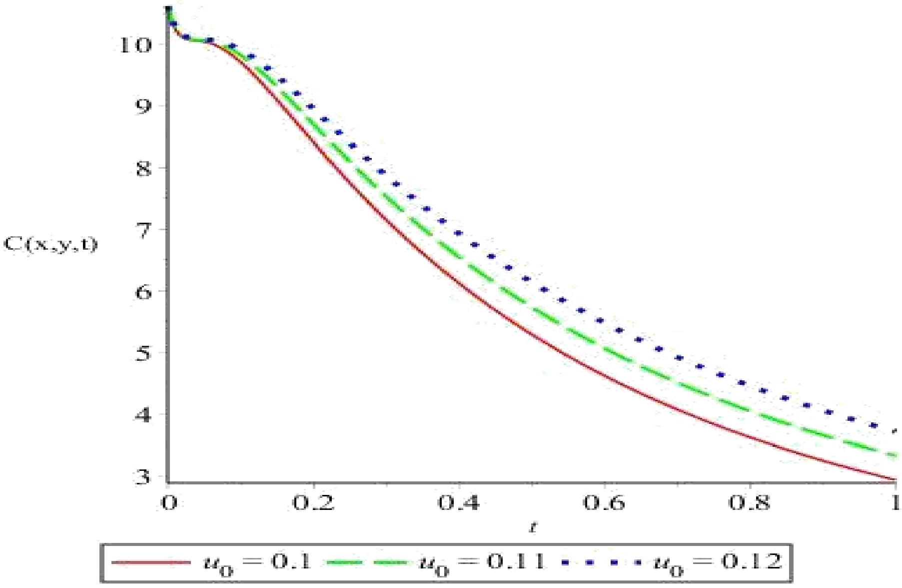

Figure 4.35: Contaminant Concentration Profile with Time for Varying Initial Horizontal Velocity Coefficient.

The behavior of the contaminant concentration as the initial horizontal velocity increases is shown in Figure 4.35 above. The graph revealed that the concentration decline with time.

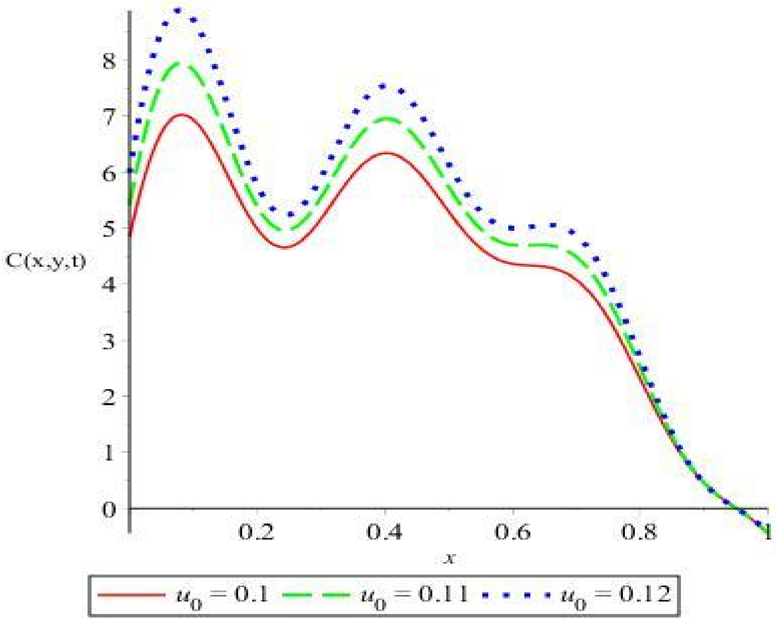

Figure 4.36: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Initial Horizontal Velocity Coefficient.

The effect of changing velocity in the horizontal direction is shown in Figure 4.36. The graph shows that the contaminant concentration decline sinusoidally along the horizontal direction as the horizontal velocity increases.

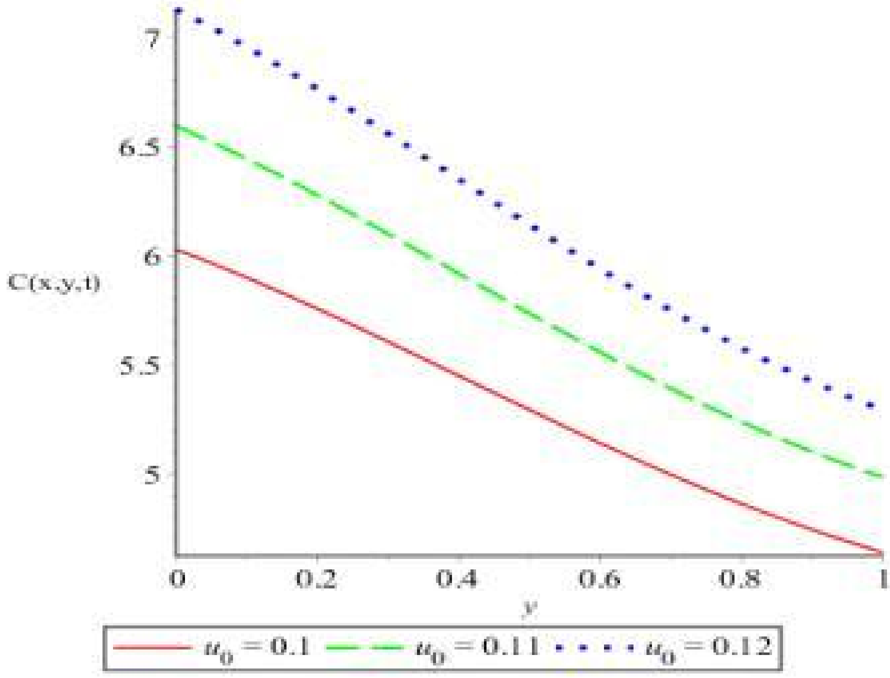

Figure 4.37: Contaminant Concentration Profile with Vertical Distance y for Varying Horizontal Velocity Dispersion Coefficient.

The graph in Figure 4.37 shows the behavior of the contaminant along the vertical direction as the initial velocity increases. From the graph, the contaminant concentration decreases as the initial horizontal velocity increases.

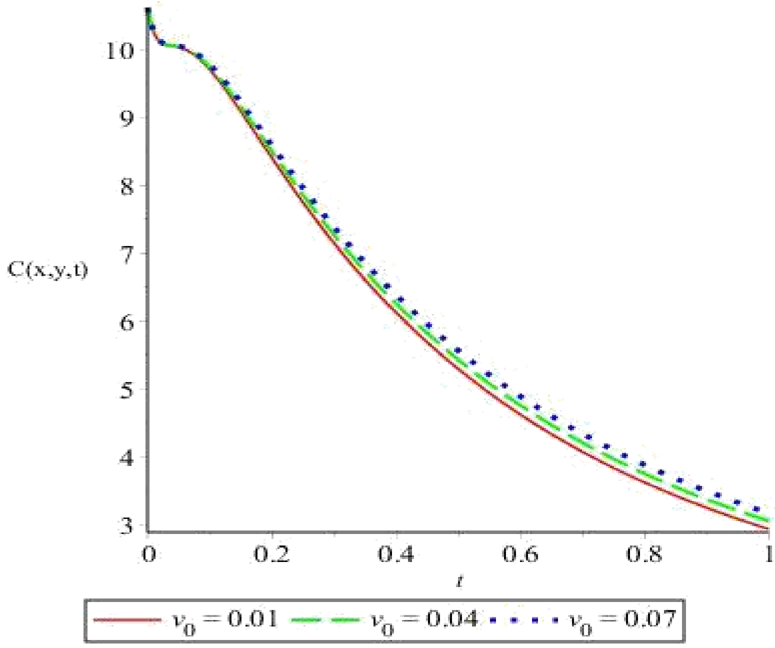

Figure 4.38: Contaminant Concentration Profile with Time for Varying Initial Horizontal Velocity Coefficient.

Figure 4.38 shows the impact of increasing the initial vertical velocity on the concentration. The graph revealed that the contaminant concentration decline with time.

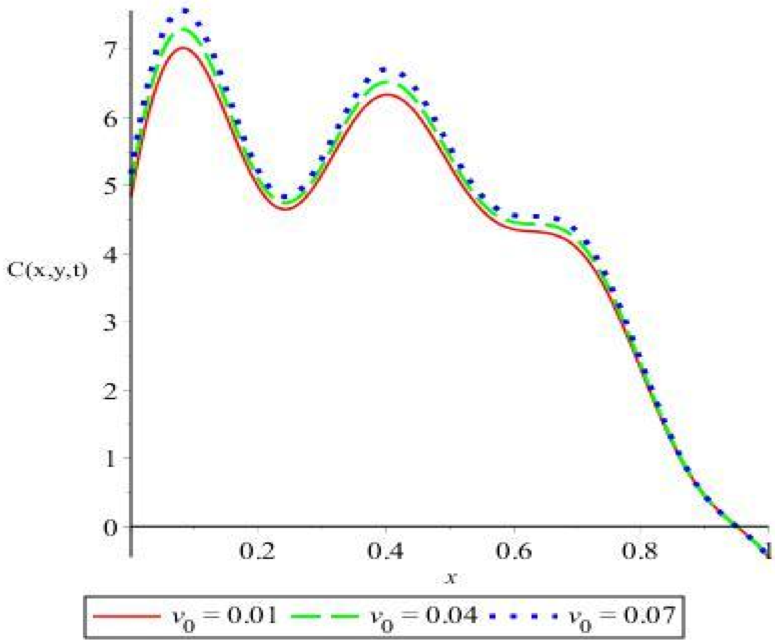

Figure 4.39: Contaminant Concentration Profile with Horizontal Distance *x* for Varying Horizontal Velocity Coefficient.

In Figure 4.39, the contaminant concentration moves sinusoidally and decline sharply along the horizontal direction as the initial vertical velocity increases.

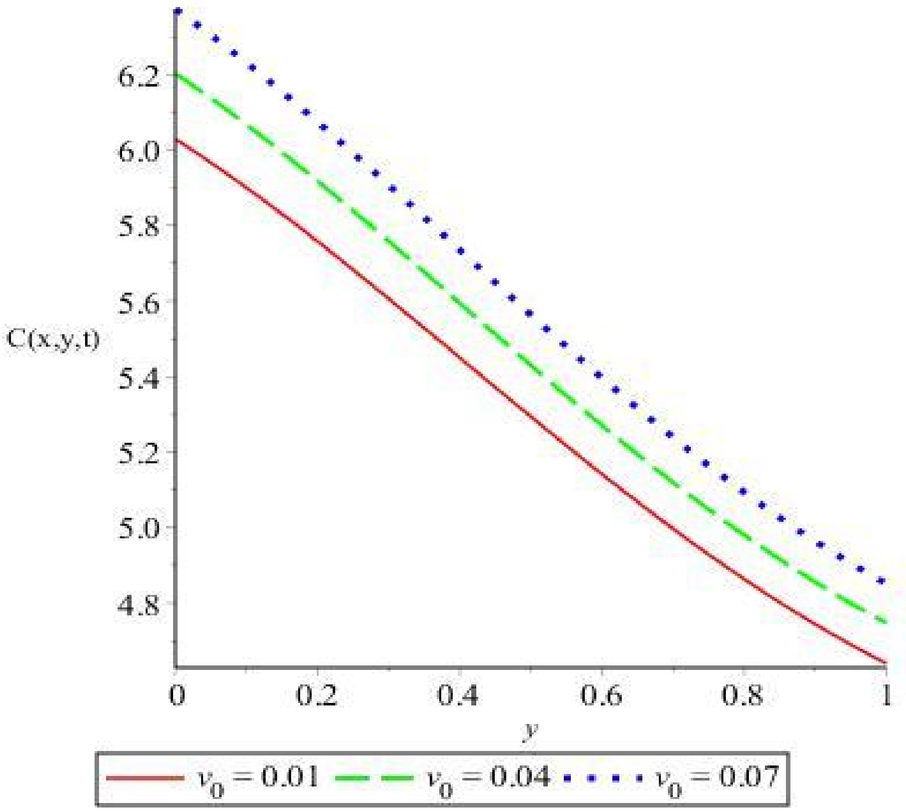

Figure 4.40: Contaminant Concentration Profile with Vertical Distance *y* for Varying Horizontal Velocity Coefficient.

The effect of increasing the horizontal velocity coefficient on the concentration is shown in Figure 4.40. The graph shows that the contaminant concentration decline with increase in initial vertical velocity in the vertical direction.

4.2 Discussion

In this section, the graphs presented in section 4.1.1 and 4.1.2 are analyzed and discussed. In Figures 4.1, 4.3, 4.15 and 4.17, the behaviors of the contaminant concentration are shown. The graphs show that the contaminant concentration decreases with time as the flow resistance parameter, decay parameter, horizontal velocity and vertical velocity increases respectively. It is also very clear from Figures 4.6, 4.9 and 4.12 that the contaminant concentration decline sharply with time as the horizontal, vertical and cross-flow dispersion coefficients decrease.

The graphs in Figures 4.4, 4.7, 4.10, 4.13, 4.16 and 4.18 are the concentration profile of the contaminant concentration with the horizontal distance. The graphs reveal that the contaminant concentration increases along the horizontal spatial direction as the values of decay coefficient, horizontal dispersion coefficient, vertical dispersion coefficient, cross-flow dispersion coefficient, horizontal and vertical velocity coefficients increase.

Similarly, Figures 4.2, 4.5, 4.8, 4.11, 4.14 and 4.19 are concentration profile of contaminant with the vertical distance. the analyses show that the contaminant concentration increases along the vertical direction as the values of flow resistance parameter, decay coefficient, horizontal dispersion coefficient, vertical dispersion coefficient, cross-flow dispersion coefficient, and the vertical velocity increase respectively.

In section 4.1.2, the graphs presented are analyzed as follows: Figures 4.20, 4.23, 4.35 and 4.38 are contaminant concentration profile with time The graphs revealed that the contaminant concentration decline with time as the flow resistance parameter, decay coefficient, horizontal and vertical velocity coefficients increases respectively. In Figures 4.26, 4.29 and 4.32, it was observed that the concentration decline sharply with time as the horizontal dispersion, vertical dispersion and cross-flow dispersion coefficient increase respectively. Similarly, in Figures 4.21, 4.24, 4.27, 4.30,4.33,4.36 and 4.39, the contaminant concentration decreases sinusoidally along the horizontal space as the flow resistance parameter, decay coefficient, horizontal dispersion, vertical dispersion, cross-flow dispersion, horizontal and vertical velocities increase.

Lastly, the contaminant concentration profile presented in Figures 4.22, 4.25, 4.28,4.31, 4.34, 4.37 and 4.40 revealed that the contaminant concentration decreases along the vertical direction as the values of flow resistance parameter, decay coefficient, horizontal dispersion, vertical dispersion, cross-flow dispersion, horizontal and vertical velocity coefficients increase.

CHAPTER FIVE

5.0 CONCLUSION AND RECOMMENDATIONS.

5.1 Conclusion

Two cases of contaminant flow models that incorporate the cross-flow dispersion and decay parameter were formulated. Case 1 was associated with the Neuman boundary conditions and Case 2 with the Dirichlet boundary conditions. The two problems have been solved by using combination of parameter expanding method, Eigen-Functions expanding technique and direct integration method.

The results obtained 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.

The following conclusions were made:

(i) In Case 1, 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 $\alpha = 0.1$, while the concentration of the contaminant increases along the co- ordinate axis (x and y) as parameters values increases.

(ii) In Case 2, the contaminant concentration decline with time as the values of the parameters increases, while, in contrast to results in Case 1, the concentration of the contaminant decline along the co-ordinate axis.

5.2 Contribution to Knowledge

Lee and Kim (2012) did not actually solve but formulated the two-dimensional model, in this study, the decay (α) and reaction term were incorporated and solved using Eigen-function expansion technique for: (i) Neumann boundary condition and (ii) Dirichlet boundary condition. Findings reveal that as the decay parameter increases from $\alpha = 0.1$ to $\alpha = 0.3$, the contaminant concentration declines faster to zero.

5.3 Recommendations

(i) In this research, an exponential form of velocity was assumed and used. Further research can adopt a sinusoidal form.

(ii) In Case 2, the value of the initial horizontal velocity was chosen to be greater than the vertical velocity. Future researcher may try the converse.

(iii) This research results may be recommended to the geologist as it may guide them to know exactly when and where the contaminant concentration is zero in order to locate their well in suitable location.

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