MATHEMATICAL MODELLING OF UNDERGROUND WATER CONTAMINATION

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DECLARATION

I declare that this project is my original work and has not been submitted to any other university or institution for award of any degree. No portion will be reproduced without my permission or permission of the university.

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DEDICATION

This research work is dedicated to my lecturers, family members and my colleagues who encouraged me to carry out this task.

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NOMENCLATURE

Nomenclature	
Parameter	**Definition**
c	nitrogen concentration in the soil column
θ	water content
ρ	soil bulk density
Z	is the space coordinate measured positive downward
K_N	the adsorption coefficient for nitrogen
q	water flux
ϕ	reactions terms either sinks or sources
$D(\theta)$	apparent diffusion coefficient
R	retardation factor
v	water velocity
C_s	concentration of all sources or sinks
Pe	Peclet number

ABSTRACT

Groundwater pollution is a major cause of many health hazards in our society. The pollution comes as a result of human indifference to waste disposal, industrial effluents, chemical spills etc. One major contaminant of underground water is nitrogen; which stems from excessive application of nitrogen-containing fertilisers, chemical spillage, etc. Its transport as it percolates through the porous media of ground surface layer to the underground water can be modelled mathematically by the advection-diffusion equation; advection (transport of contaminants by a bulk of the fluid parcel) and diffusion (random movement of the solutes i.e. contaminants, during transport). A linear model that incorporates both source and sinks is formulated and then non-dimensionalised by introducing suitable dimensionless variables and parameters. A finite difference scheme is developed for the problem using the Crank-Nilcoson scheme. The resulting algebraic equations are solved simultaneously at each time step to unravel the effect of the parameters on the concentration of nitrogen at each soil layer. The findings show that raising diffusion increases in concentration of nitrogen but increase in Peclet number leads to decreases in the concentration.

Chapter 1

INTRODUCTION

1.1 Background Information

Groundwater contamination occurs when unwanted constituent is released and makes its way into groundwater. The contaminant covers a wide area due to dispersion and water movement within the aquifer. The amount of contaminants reaching the aquifer is determined mostly by soil characteristics and the nature of contaminant. Due to these factors determining the amount of contaminants leaching, it is possible to predict transport of these contaminants into an aquifer. Because of slow movement of groundwater, concentration of pollutants changes along the same path as groundwater (Atangana, 2018). Many of these pollutants leach into underground water via micropores. Also, the potential for contamination increases in places surrounding pumping wells because water from the zone of contribution is drawn into the well and the surrounding aquifer. Some boreholes draw water from surface water. Due to these, pollutants present in surface water reach groundwater. However, if the distance between the underground water source and source of pollutant is greater, effects of contaminations will dwindle due to natural process such as oxidation, biological degradation and adsoprtion (Talabi and Kayode, 2019).

Underground water contamination occurs due to naturally occurring pollutants and also because of human activities; Arsenic and fluoride are examples of naturally occurring contaminants. The presence of high percentage of fluoride in potable water results in dental and skeletal fluorosis cases. Groundwater contamination is primarily as a results of human activities. Over the past several years, human society has come up with large number of chemical substances that have ended into the environment. Examples of human activities that have contributed to groundwater contamination include; on-site sanitation systems in which if the distance between pit latrines and underground water supply is least, then pathogens leach from pit latrines, pass unsaturated zones and contaminate groundwater. Sewage also contribute to groundwater contamination. Untreated sewage when they infiltrate, they pose health hazards such as diarrhoea and skin lesions to the users of boreholes. Also in treated sewage, urine and faeces contain micropollutants which are partly removed and the rest released into surface water where they reach underground water. Another example of human activities is the excessive application of fertilizers and pesticides. The use of nitrogen-containing fertilizers in high percentages leads to contamination of underground water by nitrates. This is because much of nitrogen not used up by plants transforms into nitrates which leaches easily. Run-off pesticides when it leaches into groundwater cause human health problems. Mining of iron and metal processing plants are the primary contributors of the presence of metals in groundwater. Oil spills from pipelines and underground storage tanks contain benzene and other soluble petroleum hydrocarbons that rapidly percolate into the groundwater (Emmanuel *et al.*, 2009).

Contamination of groundwater poses serious consequences to living organisms. Drinking contaminated groundwater can result in various diseases such as cholera, hepatitis, blue baby syndrome, among others. Hence, the best strategy to address the health problems associated with using contaminated underground water is preventing contaminants leaching to groundwater. This project is motivated to study the transport of the contaminants from the upper ground layer to the depth where it goes back into circulation. The flow is equipped with linear source and linear sink terms and it is considered to be one-dimensional because the contaminants are assumed to be evenly distributed at each layer of the soil and the Darcy's law is applicable(Singh *et al.*, 2016).

1.2 Statement of the Problem

Due to the rampant challenges of contamination of underground water, which in turn leads to poisoning of portable waters, it becomes very vital to investigate the motion of contaminants from the source on the ground surface to the underground water. Studies on groundwater have always focused on either source or sink but not both. The few studies that have considered the presence of both sink and source have only considered a constant source term. In this project, a mathematical model is formulated to model the movements of contaminants in permeable media in the presence of both linear source and sink terms. The dynamics of the flow is studied to reveal the effects of diffusivity, Peclet number, and velocity of flow on the movements of the contaminants from the ground level to the underground water.

1.3 Objectives

These are the goals our study is trying to achieve.

1.3.1 General objective

This study analyses the dynamics of underground water contamination in the presence of both sink and source.

1.3.2 Specific objectives

The specific objectives of this project are

i. to formulate a mathematical model for predicting the movements of contaminants through porous media.

ii. to nondimensionalise the flow equations and introduce flow parameters that render the equation dimensionless.

iii. to study the effects of the flow parameters that emerge from nondimensionalisation on the flow dynamics.

iv. to select remedial action to control or remove and treat contaminated groundwater.

1.4 Significance of the Study

Contamination of underground water is mostly associated to the excessive use of chemicals, such as fertilizers, or spillage of oil and other petroleum products. The contaminated underground water percolates through the soil and joins the portable water which is used for quenching thirst and added to food to be consumed. This contaminated underground water leads to outbreak of diseases such as diarrhoea (which is largely derived from poor water sanitation). Therefore, the control of the microbial quality of groundwater for drinking and other consumption uses should be the first priority in all places, given the immediate and potential consequences of waterborne diseases. However, use of chemicals such as fertilizers which can accumulate over time may render a source unusable hence requires priority for prevention and remedial strategies. This study provides information on control strategies that can be adopted by the environmental health scientist.

Chapter 2

LITERATURE REVIEW

Many studies have addressed contaminant transport in the unsaturated zone. This is because, unsaturated zone is the first sub-surface to be connected with the surface applied with agricultural chemicals (fertilizers). Hence, the surface and sub-surface agricultural chemical concentrations and subsequent environmental impacts are closely linked to the physical, biological and chemical dynamics. The basic law governing the movement of contaminants in a fluid through a permeable medium is Darcy's law (Brown, 2002). This law is valid where the porous media is saturated with fluid. The equation for estimating the contaminant transport in the vadose zone is mass-balance equation that provides a loading.

The analytical result is contrasted to a numerical solution. To discuss the correctness of the answer, the root mean square error technique is employed. Truncation error is explored in terms of numerical dispersion and velocity terms. The Peclet number's influence is explored. The graphical representation of unsteady velocity expressions is investigated. The study might be used as a preliminary forecasting tool for groundwater resource management. Among studies that examine the problem of contaminants fate and transport, physically-based deterministic model for the vadose zone are generally solutions of the Richard's equation merged with a one dimensional solution of the Adjective-Dispersive Equation (ADE) for representing a vertical flow and movement (in the z-direction) and assuming horizontal flow vectors are not significant.

Some applications of mathematical modelling in protection of groundwater environment are outlined by Slesicki (2009). The applications outlined include the usefulness of mathematical models of pollutant transport, implementation of numerical model and incorporation of mathematical models in geographical information systems. Li and Merchant (2013) diversified the groundwater pollution by considering effect of climatic change and land-use change. The research introduced a modelling approach to predict a plausible way to enhance quality groundwater in the future, putting into consideration several groundwater vulnerabilities. Akbar *et al.* (2016) explored mass transfer of nanofluid in a porous medium in which particles are injected into or suctioned out of the flow. The results indicated that heat transfer rate increases for the spherical particles in the case of the injection while an inverse conduct is watched for suction. Singh *et al.* (2016) presented a one-dimensional solute transport model using advection-dispersion equation in a finite aquifer with first-order decay and zero-order production. The model is rendered dimensionless by introducing some dimensionless variables and parameters. The dimensionless equation is investigated for several types of velocities. The results indicate that concentration rises in time. Also, the contaminant concentration is lowest at the source as a result of rising zero-order production parameter. Das *et al.* (2017) furthered the work of Singh *et al.* (2016) by focusing on the varying velocity fields to study the flow of the contaminated groundwater. Laplace integral Transform Technique is used to seek the analytical solution of the derived mathematical model by considering several forms of the velocity expressions.

Abd-Elaty *et al.* (2019) used some existing numerical models for contaminant transport to integrate surface water and groundwater and understand the contamination process of the groundwater from polluted drains. One important note from the research is that polluted drains should be located in a low permeability layer to minimize the water degradation. McLean *et al.* (2019) diverted attention towards the use of statistical tools for estimating groundwater contamination. The research is centred in using fewer data to achieve the same accuracy that large data can achieve for groundwater contamination. Nelson and Williams (2019) did a mathematical treatment of water flow in saturated heterogeneous porous media and showed that Darcy's law should be cautiously applied in modelling contaminant transport. It was inferred that there are cases where Darcy's law does not hold. Luo *et al.* (2022) used the genetic algorithm, alongside the inversion method, to measure contamination extent in groundwater and the outcome indicated that the TSASM-TRGA is more reliable, accurate and stable than the GCSI. Agrawal *et al.* (2022) proposed polynomial approximation as a method to measure to groundwater contamination as against the classical inverse source method.

Clearly, most studies have been carried out with the assumptions that either only sink or only source is present in the flow process. The few studies that considered the presence of both terms always assume that one is constant while the other is linear. In the present study, the simultaneous presence of both source and sink are considered. The sink and the source are assumed to be linearly proportional to the concentration. The flow is restricted to the the case where Darcy's law is typically applicable. The transport phenomenon of contaminated water down the ground is approximated by a one-dimensional flow since the direction of flow is generally downward. The soil is assumed to be isotropic so that the physical properties remain the same in different directions. The effects of diffusivity, Peclet number, and constant velocity on the concentration of the contaminants below the ground surface are studied and depicted as graphs.

Chapter 3

METHODOLOGY

3.1 Governing equations

The process of transportation of contaminants in ground water can be modelled by the solute transport modelling of the Advection Diffusion Equation (ADE). The transport of the contaminant is as a result of the random motion of the contaminants in each fluid parcel carrying the contaminant. The assumption of the model is that concentration of the solute are homogeneous across each soil layer and downward also; with concentrations varying solely in the downstream direction. Dispersion effects remain unchanged spatially but time-dependent, and solutes are conservative in an unsteady field (Singh *et al.*, 2016). According to Singh *et al.* (2016), the partial differential equation governing the one-dimensional transport of nitrogen in soil column into groundwater considering advection, dispersion and sinks and sources is described in the following equation

$$(\theta + \rho K_N)\frac{\partial c}{\partial \tau} = \frac{\partial}{\partial Z}\left(\theta D(\theta)\frac{\partial c}{\partial Z} - qc\right) - \phi \qquad (3.1.1)$$

where c is the concentration of nitrogen in the soil column, θ is water content, ρ is soil bulk density, Z is the space coordinate measured positive downward, the adsorption K_N coefficient for nitrogen is defined as

$$K_N = \frac{1-n}{n}, \ (n \text{ is geological formations' permeability}) \qquad (3.1.2)$$

q is water flux, ϕ is reactions terms either sinks or sources, and $D(\theta)$ is apparent diffusion coefficient. Rearranging equation (3.1.1) gives

$$(\theta+\rho K_N)\frac{\partial c}{\partial \tau}=\left(\theta\frac{\partial (D(\theta))}{\partial Z}+D(\theta)\frac{\partial \theta}{\partial Z}\right)\frac{\partial c}{\partial Z}+\theta D(\theta)\frac{\partial^2 c}{\partial Z^2}-q\frac{\partial c}{\partial Z}-\phi \quad (3.1.3)$$

For the case where θ is independent of z, the first term becomes zero and the equation becomes

$$(\theta+\rho K_N)\frac{\partial c}{\partial \tau}=\theta D(\theta)\frac{\partial^2 c}{\partial Z^2}-q\frac{\partial c}{\partial Z}-\phi \quad (3.1.4)$$

and dividing through by θ, we get

$$\left(1+\frac{\rho K_N}{\theta}\right)\frac{\partial c}{\partial \tau}=D(\theta)\frac{\partial^2 c}{\partial Z^2}-\frac{q}{\theta}\frac{\partial c}{\partial Z}-\frac{\phi}{\theta}. \quad (3.1.5)$$

Setting the retardation factor R, water velocity v and concentration C_s of all sources or sinks as

$$R=\left(1+\frac{\rho K_N}{\theta}\right),\ v=\frac{q}{\theta},\ C_s=\frac{\phi}{\theta}, \quad (3.1.6)$$

the equation becomes

$$R\frac{\partial c}{\partial \tau}=D\frac{\partial^2 c}{\partial Z^2}-v\frac{\partial c}{\partial Z}-C_s. \quad (3.1.7)$$

For the situation where source (or sink) is proportional to concentration, we have the governing equation as

$$R\frac{\partial c}{\partial \tau}=D\frac{\partial^2 c}{\partial Z^2}-v\frac{\partial c}{\partial Z}-\mu c. \quad (3.1.8)$$

In the presence of both sources and sinks, the equation becomes

$$R\frac{\partial c}{\partial \tau}=D\frac{\partial^2 c}{\partial Z^2}-v\frac{\partial c}{\partial Z}-\mu c+\gamma c. \quad (3.1.9)$$

Dimensionless equations are obtained by introducing the dimensionless variables

$$\tau=\frac{Lt}{v},\ Z=Lz \quad (3.1.10)$$

so that

$$\frac{vR}{L}\frac{\partial c}{\partial t} = \frac{D}{L^2}\frac{\partial^2 c}{\partial z^2} - \frac{v}{L}\frac{\partial c}{\partial z} - \mu c + \gamma c \Rightarrow R\frac{\partial c}{\partial t} = \frac{D}{Lv}\frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} - \frac{(\mu-\gamma)L}{v}c, \quad (3.1.11)$$

and finally, we have the dimensionless equation

$$R\frac{\partial c}{\partial t} = \frac{1}{Pe}\frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} - (\mu^* - \gamma^*)\, c \quad (3.1.12)$$

where Pe is the Peclet number defined as

$$Pe = \frac{Lv}{D},\ \mu^* = \frac{\mu L}{v},\ \gamma^* = \frac{\gamma L}{v}. \quad (3.1.13)$$

The associated initial conditions are given as

$$c(0,t) = c_0,\ t > 0 \quad (3.1.14)$$

$$c(z,0) = c^*,\ 0 \le z \le L \quad (3.1.15)$$

$$\frac{\partial c}{\partial z} = 0, \text{ as } z \to \infty \quad (3.1.16)$$

3.2 Finite difference method

A finite difference approximations to the derivatives of a function $u(x)$ on an interval (a,b) is described below. Divide the interval (a,b) into n equal subintervals so that we have the sequence $a = x_0, x_1, \cdots x_{n-1}, x_n = b$ and with the step size defined as $h = {(b-a)}/{n}$. Hence,

$$x_i = x_{i-1} + h = x_0 + ih. \quad (3.2.1)$$

For brevity, we write

$$u(x_i) = u_i,\ u'(x_i) = u'_i,\ \cdots. \quad (3.2.2)$$

By Taylor expansion

$$
\begin{aligned}
u_{i+1} &= u(x_{i+1}) = u(x_i + h) \\
&= u(x_i) + hu'(x_i) + \frac{h^2}{2!}u''(x_i) + \frac{h^3}{3!}u'''(x_i) + O\left(h^4\right), \\
&= u_i + hu'_i + \frac{h^2}{2!}u''_i + \frac{h^3}{3!}u'''_i + O\left(h^4\right),
\end{aligned} \tag{3.2.3}
$$

where $O\left(h^4\right)$ denotes fourth and higher powers of h. Truncating the series after the h^3 term and rearranging gives the first order forward difference approximation

$$\frac{u_{i+1} - u_i}{h} = u'_i + O(h). \tag{3.2.4}$$

In similar manner, starting with u_{i-1}, we derive the first order backward difference approximation to u'_i as

$$\frac{u_i - u_{i-1}}{h} = u'_i + O(h). \tag{3.2.5}$$

The second order central difference approximation to u''_i is obtained by adding the Taylor expansions of u'_{i+1} and u'_{i-1} and truncating at $O\left(h^4\right)$ and it is given as

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = u''_i + O\left(h^2\right). \tag{3.2.6}$$

Meanwhile, by subtracting the Taylor expansions of u'_{i-1} from u'_{i+1}, the second order central difference approximation to u'_i is obtained as

$$\frac{u_{i+1} - u_{i-1}}{2h} = u'_i + O\left(h^2\right). \tag{3.2.7}$$

So far, the function $u(x)$ has been considered as a function in one variable but the problem at hand is a function of two variables. Now, consider a function $u = u(x,t)$ and we let h and k be the mesh sizes on the x- and t- axes respectively. We have

$$x_{i\pm m} = x_i \pm mh \text{ and } t_{j\pm n} = t_j \pm nk \tag{3.2.8}$$

and denote $u\left(x_i,t_j\right)=u_i^j$. The first forward difference for $\frac{\partial u}{\partial t}$ is written as

$$\left.\frac{\partial u}{\partial t}\right|_{\left(x_i,t_j\right)}=\frac{u_i^{j+1}-u_i^j}{k}. \tag{3.2.9}$$

and the central difference for $\frac{\partial^2 u}{\partial x^2}$,

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{\left(x_i,t_j\right)}=\frac{u_i^{j+1}-2u_i^j+u_{i-1}^j}{h^2}. \tag{3.2.10}$$

3.3 Derivation of the finite difference scheme

The dimensionless governing equation to solve is

$$R\frac{\partial c}{\partial t}=\frac{1}{Pe}\frac{\partial^2 c}{\partial z^2}-\frac{\partial c}{\partial z}-\left(\mu^*-\gamma^*\right)c \tag{3.3.1}$$

with the initial conditions

$$c\left(0,t\right)=c_0,\ t>0 \tag{3.3.2}$$

$$c\left(z,0\right)=c^*,\ 0\leq z\leq L \tag{3.3.3}$$

$$\frac{\partial c}{\partial z}=0,\ \text{ as } z\to\infty. \tag{3.3.4}$$

The time derivative at the point $\left(x_i,t_j\right)$ is approximated by the forward difference approximation

$$\frac{\partial c}{\partial t}=\frac{c_i^{j+1}-c_i^j}{k}. \tag{3.3.5}$$

The spatial first derivative at the points (x_i, t_j) and (x_i, t_{j+1}) are approximated by the central difference approximations

$$\frac{\partial c}{\partial z} = \frac{c_{i+1}^{j} - c_{i-1}^{j}}{2h}, \text{ and} \tag{3.3.6}$$

$$\frac{\partial c}{\partial z} = \frac{c_{i+1}^{j+1} - c_{i-1}^{j+1}}{2h}. \tag{3.3.7}$$

and taking the average, we have

$$\frac{\partial c}{\partial z} = \frac{c_{i+1}^{j+1} - c_{i-1}^{j+1} + c_{i+1}^{j} - c_{i-1}^{j}}{4h}. \tag{3.3.8}$$

The spatial second derivative at the points (x_i, t_j) and (x_i, t_{j+1}) are approximated by the central difference approximation

$$\frac{\partial^2 c}{\partial z^2} = \frac{c_{i+1}^{j} - 2c_{i}^{j} + c_{i-1}^{j}}{h^2} \text{ and} \tag{3.3.9}$$

$$\frac{\partial^2 c}{\partial z^2} = \frac{c_{i+1}^{j+1} - 2c_{i}^{j+1} + c_{i-1}^{j+1}}{h^2} \tag{3.3.10}$$

and taking the average, we have

$$\frac{\partial^2 c}{\partial z^2} = \frac{c_{i+1}^{j} + c_{i+1}^{j+1} - 2c_{i}^{j} - 2c_{i}^{j+1} + c_{i-1}^{j+1} + c_{i-1}^{j}}{2h^2}. \tag{3.3.11}$$

and thus, the scheme for the problem at hand is derived as follows

$$\begin{aligned} R\frac{c_{i}^{j+1} - c_{i}^{j}}{k} =& \frac{1}{Pe}\frac{c_{i+1}^{j+1} + c_{i+1}^{j} - 2c_{i}^{j+1} - 2c_{i}^{j} + c_{i-1}^{j+1} + c_{i-1}^{j}}{2h^2} \\ & - v\frac{c_{i+1}^{j+1} + c_{i+1}^{j} - c_{i-1}^{j+1} - c_{i-1}^{j}}{4h} - (\mu^* - \gamma^*)\, c_{i}^{j}. \end{aligned} \tag{3.3.12}$$

Multiplying both sides by $\frac{k}{R}$ and making c_i^{j+1} the subject gives,

$$
\begin{aligned}
c_i^{j+1} =& \frac{k}{2h^2 Pe\, R}\left(c_{i+1}^{j+1}+c_{i+1}^{j}-2c_i^{j+1}-2c_i^{j}+c_{i-1}^{j+1}+c_{i-1}^{j}\right)\\
&-\frac{k}{4hR}\left(c_{i+1}^{j+1}+c_{i+1}^{j}-c_{i-1}^{j+1}-c_{i-1}^{j}\right)+\left(1-\frac{k\,(\mu^*-\gamma^*)}{R}\right)c_i^j. \qquad (3.3.13)
\end{aligned}
$$

Setting

$$
\alpha=\frac{k}{2h^2R},\ \beta=\frac{k}{4hR},\ \lambda=1-\frac{k\,(\mu^*-\gamma^*)}{R},
$$

then

$$
\begin{aligned}
c_i^{j+1} &= \frac{\alpha}{Pe}\left(c_{i+1}^{j+1}+c_{i+1}^{j}-2c_i^{j+1}-2c_i^{j}+c_{i-1}^{j+1}+c_{i-1}^{j}\right)\\
&\quad -\beta\left(c_{i+1}^{j+1}+c_{i+1}^{j}-c_{i-1}^{j+1}-c_{i-1}^{j}\right)+\lambda c_i^j,\\
&= \frac{\alpha}{Pe}\left(c_{i+1}^{j+1}+c_{i+1}^{j}-2c_i^{j+1}-2c_i^{j}+c_{i-1}^{j+1}+c_{i-1}^{j}\right)\\
&\quad -\beta\left(c_{i+1}^{j+1}+c_{i+1}^{j}-c_{i-1}^{j+1}-c_{i-1}^{j}\right)+\lambda c_i^j, \qquad (3.3.14)
\end{aligned}
$$

and on rearranging,

$$
\begin{aligned}
&-\left(\frac{\alpha}{Pe}+\beta\right)c_{i-1}^{j+1}+\left(1+2\frac{\alpha}{Pe}\right)c_i^{j+1}-\left(\frac{\alpha}{Pe}-\beta\right)c_{i+1}^{j+1}\\
&\quad=\left(\frac{\alpha}{Pe}+\beta\right)c_{i-1}^{j}+\left(\lambda-2\frac{\alpha}{Pe}\right)c_i^{j}+\left(\frac{\alpha}{Pe}-\beta\right)c_{i+1}^{j}. \quad i=3,\cdots,N-1 \qquad (3.3.15)
\end{aligned}
$$

For $i=2$,

$$
\begin{aligned}
&-\left(\frac{\alpha}{Pe}+\beta\right)c_{1}^{j+1}+\left(1+2\frac{\alpha}{Pe}\right)c_2^{j+1}-\left(\frac{\alpha}{Pe}-\beta\right)c_{3}^{j+1}\\
&\quad=\left(\frac{\alpha}{Pe}+\beta\right)c_{1}^{j}+\left(\lambda-2\frac{\alpha}{Pe}\right)c_2^{j}+\left(\frac{\alpha}{Pe}-\beta\right)c_{3}^{j}, \qquad (3.3.16)
\end{aligned}
$$

and consequently,

$$
\begin{aligned}
&\left(1+\frac{2\alpha}{Pe}\right)c_2^{j+1}-\left(\frac{\alpha}{Pe}-\beta\right)c_{3}^{j+1}\\
&\quad=\left(\frac{\alpha}{Pe}+\beta\right)\left(c_{1}^{j}+c_1^{j+1}\right)+\left(\lambda-2\frac{\alpha}{Pe}\right)c_2^{j}+\left(\frac{\alpha}{Pe}-\beta\right)c_{3}^{j}. \qquad (3.3.17)
\end{aligned}
$$

For $i = N$,

$$-\left(\frac{\alpha}{Pe}+\beta\right)c_{N-1}^{j+1}+\left(1+\frac{2\alpha}{Pe}\right)c_{N}^{j+1}-\left(\frac{\alpha}{Pe}-\beta\right)c_{N+1}^{j+1}$$
$$=\left(\frac{\alpha}{Pe}+\beta\right)c_{N-1}^{j}+\left(\lambda-2\frac{\alpha}{Pe}\right)c_{N}^{j}+\left(\frac{\alpha}{Pe}-\beta\right)c_{N+1}^{j}, \qquad (3.3.18)$$

and consequently,

$$-\left(\frac{\alpha}{Pe}+\beta\right)c_{N-1}^{j+1}+\left(1+\frac{2\alpha}{Pe}\right)c_{N}^{j+1}$$
$$=\left(\frac{\alpha}{Pe}+\beta\right)c_{N-1}^{j}+\left(\lambda-\frac{2\alpha}{Pe}\right)c_{N}^{j}+\left(\frac{\alpha}{Pe}-\beta\right)\left(c_{N+1}^{j}+c_{N+1}^{j+1}\right). \qquad (3.3.19)$$

At each step (i.e. $j = 1, 2, \cdots M+1$),the system of $(N-1)\times(N-1)$ linear equations

$$AX = B \qquad (3.3.20)$$

is thus formed where

$$A=\begin{pmatrix} 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe} & 0 & 0 & 0 & \cdots & 0 & 0 & 0\\ -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe} & 0 & 0 & \cdots & 0 & 0 & 0\\ 0 & -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe} & 0 & \cdots & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe}\\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} \end{pmatrix} \qquad (3.3.21)$$

and

$$X = \begin{pmatrix} c_2^{j+1} \\ c_3^{j+1} \\ \vdots \\ c_{N-1}^{j+1} \\ c_N^{j+1} \end{pmatrix}, \quad B = \begin{pmatrix} \left(\frac{\alpha}{Pe}+\beta\right)\left(c_1^j + c_1^{j+1}\right) + \left(\lambda - 2\frac{\alpha}{Pe}\right)c_2^j + \left(\frac{\alpha}{Pe}-\beta\right)c_3^j \\ \vdots \\ \left(\frac{\alpha}{Pe}+\beta\right)c_{i-1}^j + \left(\lambda - 2\frac{\alpha}{Pe}\right)c_i^j + \left(\frac{\alpha}{Pe}-\beta\right)c_{i+1}^j \\ \vdots \\ \left(\frac{\alpha}{Pe}+\beta\right)c_{N-1}^j + \left(\lambda - \frac{2\alpha}{Pe}\right)c_N^j + \left(\frac{\alpha}{Pe}-\beta\right)\left(c_{N+1}^j + c_{N+1}^{j+1}\right) \end{pmatrix}. \tag{3.3.22}$$

A is an $(N-1)\times(N-1)$ matrix, X and B are $(N-1)\times 1$ column vectors. The diagram for the scheme is shown in figure (3.1)

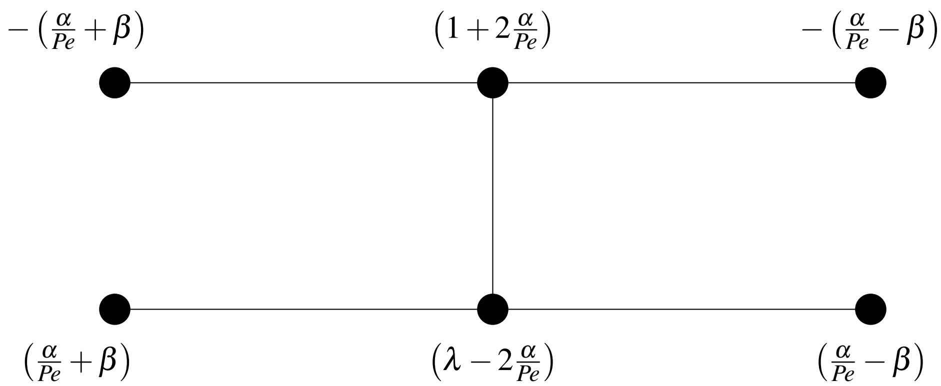

Figure 3.1: Schematic diagram

3.3.1 Initial conditions

The associated initial conditions are

$$c(0,t) = c_0,\ (t>0),\ c(z,0) = c^*,\ (0 \le z \le L),\ \frac{\partial c}{\partial z} = 0,\ (\text{ as } z \to \infty). \tag{3.3.23}$$

The first condition is discretized as

$$c(0,t) = c_0,\ t>0\ \Rightarrow c_1^j = c_0,\ j = 1,2,\cdots M+1. \tag{3.3.24}$$

The second condition is descritized as

$$c(z,0) = c^*,\ 0 \le z \le L\ \Rightarrow c_i^1 = c^*,\ i = 1,2,\cdots N+1. \tag{3.3.25}$$

The last condition is discretized as

$$\frac{\partial c}{\partial z} = 0,\ \text{ as } z \to \infty \Rightarrow \frac{\partial c}{\partial z} = \frac{c_{i+1}^{j+1} - c_{i-1}^{j+1} + c_{i+1}^{j} - c_{i-1}^{j}}{4h} = 0 \Rightarrow c_{N+1}^{j+1} = c_{N-1}^{j+1} - c_{N+1}^{j} + c_{N-1}^{j}. \tag{3.3.26}$$

Thus, the problem is reduced to solving the system of equations

$$AX = B \tag{3.3.27}$$

with the initial conditions

$$\left.\begin{aligned} c_1^j &= c_0,\ j = 1,2,\cdots M+1,\\ c_i^1 &= c^*,\ i = 1,2,\cdots N+1,\\ c_{N+1}^{j+1} &= c_{N-1}^{j+1} - c_{N+1}^{j} + c_{N-1}^{j},\ j = 1,2,\cdots M. \end{aligned}\right\} \tag{3.3.28}$$

where

$$A = \begin{pmatrix} 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe} & 0 & 0 & 0 & \cdots & 0 & 0 & 0\\ -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe} & 0 & 0 & \cdots & 0 & 0 & 0\\ 0 & -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe} & 0 & \cdots & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} & \beta-\frac{\alpha}{Pe}\\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & -\frac{\alpha}{Pe}-\beta & 1+\frac{2\alpha}{Pe} \end{pmatrix} \tag{3.3.29}$$

and

$$X=\begin{pmatrix} c_2^{j+1} \\ c_3^{j+1} \\ \vdots \\ c_{N-1}^{j+1} \\ c_N^{j+1} \end{pmatrix}, \quad B=\begin{pmatrix} \left(\frac{\alpha}{Pe}+\beta\right)\left(c_1^j+c_1^{j+1}\right)+\left(\lambda-2\frac{\alpha}{Pe}\right)c_2^j+\left(\frac{\alpha}{Pe}-\beta\right)c_3^j \\ \vdots \\ \left(\frac{\alpha}{Pe}+\beta\right)c_{i-1}^j+\left(\lambda-2\frac{\alpha}{Pe}\right)c_i^j+\left(\frac{\alpha}{Pe}-\beta\right)c_{i+1}^j \\ \vdots \\ \left(\frac{\alpha}{Pe}+\beta\right)c_{N-1}^j+\left(\lambda-\frac{2\alpha}{Pe}\right)c_N^j+\left(\frac{\alpha}{Pe}-\beta\right)\left(c_{N+1}^j+c_{N+1}^{j+1}\right) \end{pmatrix}. \tag{3.3.30}$$

A is an $(N-1)\times(N-1)$ matrix, X and B are $(N-1)\times 1$ column vectors.

Chapter 4

DISCUSSION OF RESULTS

The nondimensionalised transport equation (3.1.12) is discretised using the forward difference central difference (FDCD) scheme. The FDCD is presented following Crank Nicholson method of averaging the spatial discretization at two consecutive time step and the implicit schemes for the problem is obtained as a system of equations (3.3.27). The system of equations is solved at each time step and the parameters are set to default values $Pe = 2$, $R = 0.7$, $D = 0.1$, $v = 0.01$, $L = 10$, $\mu^* = -0.3$, $dx = 0.1$,$dt = 0.01$. The results are validated by comparing our present results with the results of Das *et al.* (2017) when $Pe = 0.7$, $D = 0.000015$, $v = 0.01$,$\mu^* = 0.0001$, $\gamma = 0$. Table (4.1) shows that there is a good agreement between the present results and existing literature.

Distance	**Das *et al.* (2017)**	**Present Results**
0.02	0.2852	0.285266
0.04	0.0418	0.041846
0.06	0.0169	0.016931
0.08	0.0177	0.017750
0.1	0.0182	0.018245

Table 4.1: Validation of the method

By varying the velocity, diffusivity and Peclet number, the dynamics of the transport problem are investigated and the results obtained are graphed as shown in figures (4.1 - 4.4) below.

Concentration of nitrogen is found to increase as diffusivity increases (see figure (4.1)). Diffusivity measures the rate of spread of mass and therefore as the rate increases, concentration is increased at all depths. The implication of this is that increase in diffusion rate will lead to quick contamination of the underground water. This explains why increase in the diffusivity leads to an increase in the concentration of nitrogen in the underground water flow. For this, water body contamination therefore increases rapidly down the ground. Peclet number measures the ratio of heat transfer by movement bulk fluid parcel (known as advection) to heat transfer by thermal conduction (known as diffusion). Increasing Peclet number indicates an increase in heat transfer by advection or a decrease in diffusion. This is explains why increase in Peclet number leads to a decrease in concentration as shown in figure (4.2). By increasing the Peclet number, the diffusion process reduces significantly, thereby reducing the rate of contamination. The nitrogen percolates slowly and thus, it reduces the rate of underground water contamination. Figure (4.3) shows that the longer the contaminated ground water stays on the ground, the higher the concentration goes. If the ground holds the contaminated water body for a longer time, the concentration of nitrogen in the underground water continues to rise significantly. Hence, increasing water-holding time of the soil leads to an increased contamination. It is also clear that as the flow velocity increases, the concentration increases also (figure (4.4)). Increase in velocity enhances percolation of the contaminated fluid down the ground. The contaminated water is able to burrow its way and reach the underground quickly.

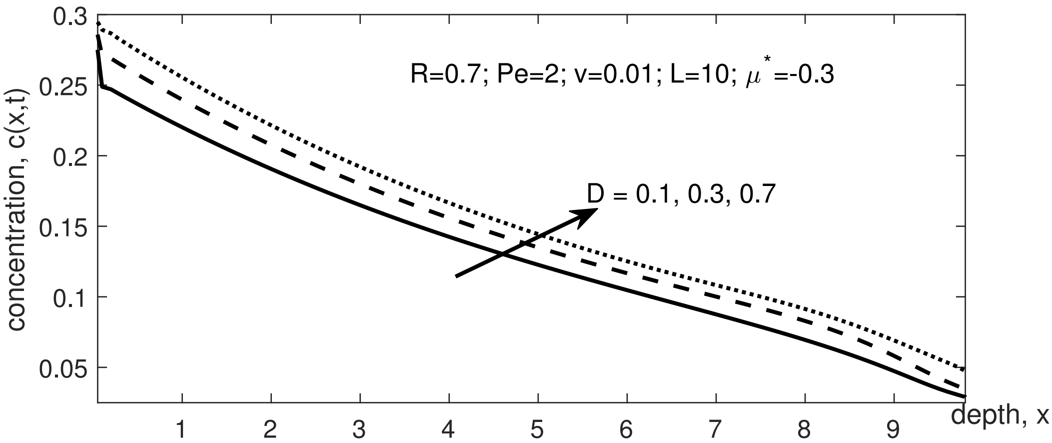

Figure 4.1: Effect of diffusivity on concentration

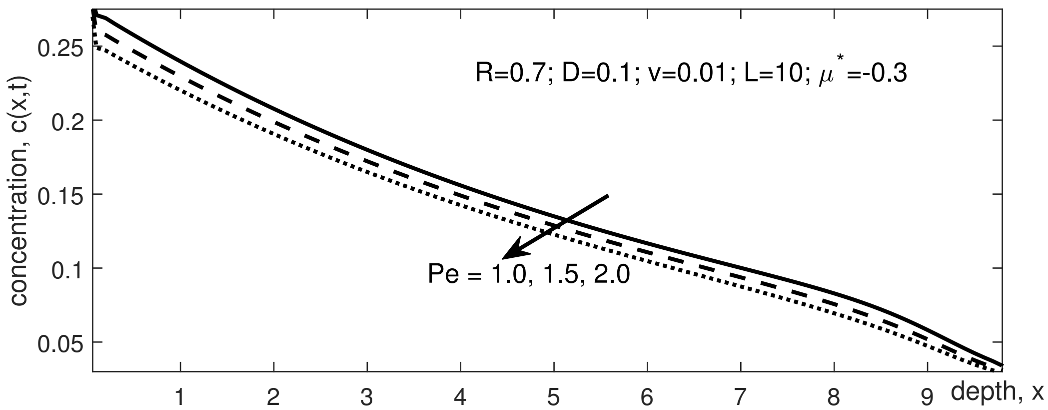

Figure 4.2: Effect of Peclet number on concentration

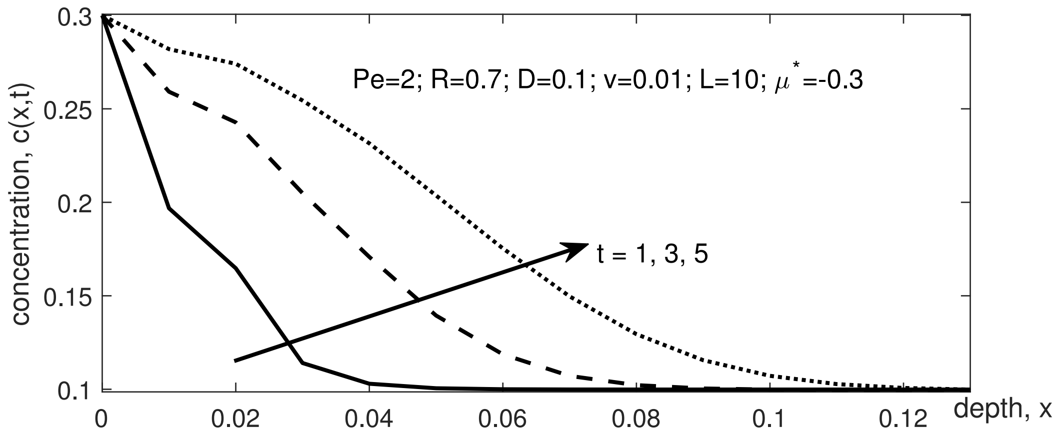

Figure 4.3: Variation of concentration with time

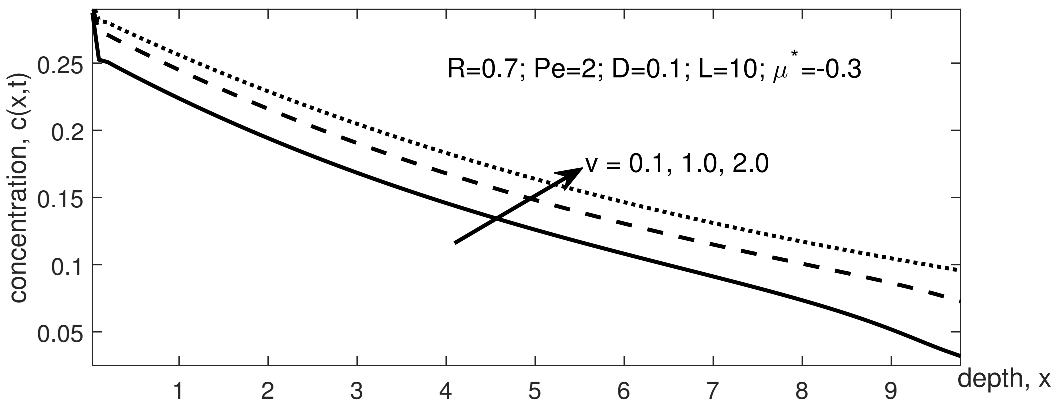

Figure 4.4: Effect of velocity on concentration

Chapter 5

CONCLUSION AND RECOMMENDATION

5.1 CONCLUSION

The equation for the transport of nitrogen as a contaminant in the underground water is formulated in this project. A linear source replaces the constant source that are often considered. The partial differential equation is rendered dimensionless by introducing some dimensionless variables. The dimensionless equation is solved using the The Forward-Time Central-Space (FDCD) finite difference scheme and the graphs are presented at various values of the parameters. The outcomes of the study indicates that

i. Concentration of nitrogen is found to increase as diffusivity increases.

ii. Increase in Peclet number leads to a decrease in concentration.

iii. The longer the contaminated groundwater stays on the ground surface, the more the underground water gets contaminated.

iv. Increase in velocity leads to an increase in concentration.

5.2 Recommendation

Based on the outcomes of this study, the following are recommended;

i. Erosion and flooding are major causes of increase in velocity. In order to reduce contamination of the underground water, drainages should be created to avoid erosion and flooding.

ii. The study reveals that if the contaminated water is allowed to stay for too long on the surface, then the underground water gets more contaminated. This can be avoided by prompt response to ground surface contamination. Prompt removal of contaminated water from the surface will reduce the rate of contamination that percolates into the underground water.

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APPENDICES

Appendix I: MATLAB codes for Model I

```
clc
Pe=2;R=0.7; D=0.1; v=0.01; L=10;
x0=0; xf=L; dx=0.1; N=(xf-x0)/dx;
mu=-0.3; gam = -0.2
t0=0; tf=1; dt=0.01; M=(tf-t0)/dt;
a=D*dt/(2*R*dx^2*Pe); b=v*dt/(4*dx*R);
lam=1-0.3*dt/R; c0=0.3; cN=0.0; ct0=0.1;
A = zeros(N-1,N-1); X = zeros(N-1,1); B = zeros(N-1,1);
c = zeros(M,N+1); c(1,N+1) = ct0;
LineNumber=0;
for D = [0.1,0.3,0.7]
   a=D*dt/(2*R*dx^2*Pe);
   for j=1:M+1
      c(j,1)=c0;
   end
   for j=2:N
      c(1,j)=ct0;
   end
   for j=1:M
      for i=1:N-1
         if i==1
            A(i,1) = 1+2*a;
            A(i,2) = b-a;
```

```
      B(i,1) = (a+b)*(c(j,1)+c(j+1,1))+...
             (lam-2*a)*c(j,2)+(a-b)*c(j,3);
    elseif i==N-1
      A(i,i-1)= -(a+b);
      A(i,i) = 1+2*a;
      B(i,1)= (a+b)*c(j,N-1)+(lam-2*a)*...
                 c(j,N)+(a-b)*(c(j,N+1)+c(j+1,N+1));
    else
      A(i,i-1) = -(a+b);
      A(i,i) = 1+2*a;
      A(i,i+1) = -(a-b);
      B(i,1) = (a+b)*c(j,i-1)+(lam-2*a)*...
                           c(j,i)+(a-b)*c(j,i+1);
    end
  end
  res = inv(A)*B;
  c(j+1,2:N)=res;
  c(j+1,N+1)=c(j+1,N-1)+c(j,N-1)-c(j,N+1);
end
x=0:dx:xf; t=0:dt:tf;
LineNumber=LineNumber+1
if LineNumber==1
  LineStyles = 'k-'
elseif LineNumber==2
  LineStyles = 'k--'
elseif LineNumber==3
  LineStyles = 'k:'
end
```

```
  figure(1);plot(x,c(M-3,:),LineStyles);
  xlabel('depth, x')
  ylabel('concentration, c(x,t)')
  hold on
end
```