

# **A NEW MODEL FOR GROUNDWATER TRANSPORT IN DUAL MEDIA**

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## DECLARATION

I, Mpafane Deyi, hereby declare that the dissertation hereby submitted by me to the Institute for Groundwater Studies in the Faculty of Natural and Agricultural Sciences at the University of Free State, in fulfilment of the degree Doctor of Philosophy, is my own independent work and I have not previously submitted it for a qualification at another institution of higher education. In addition, I declare that all sources cited have been acknowledge by means of a list of references.

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**In addition, the following articles has been submitted and is under review at an International Accredited Journal:**

- 1. Deyi, M. and Atangana, A., 2020. A new model for groundwater transport in dual media.**
- 2. Deyi, M. and Atangana, A., 2020. Groundwater transport model with fading memory property**
- 3. Deyi, M. and Atangana, A., 2020. A new groundwater transport in dual media with power law process.**
- 4. Deyi, M. and Atangana, A., 2020. New groundwater transport in dual media with the Atangana-Baleanu differential operators.**

## Abstract

The concept of differentiation has been the most used mathematical concept to express change of physical problems in time and space. The concept has been used in many disciplines in the last decades, for instance, in groundwater pollution problems. The movement of pollution within the subsurface have been a worry among researchers, as such has serious impact on health since many people of different background rely of subsurface water for commercial and domestic use. One of the breakout of the groundwater pollution is perhaps the Love Canal scenario that led to the loss of many lives of human beings and animals.

A Mathematical models that take into account the dispersion advection was introduced, used and modified with the aim to better depict such movement. However, this model and its modified versions were not able to replicate the anomalous movement of pollution as they were constructed with assumption that the geological formation is homogeneous. Another limitation of such models is to assume that the dispersion and advection coefficients are constant within and across the aquifer. However, it is worth noting that a mathematical model will accurately replicate the observed facts, if and only, the conversion from observation to mathematical formulas has taken into account of the main parameters of the real world problem. Additionally and more importantly, the advection dispersion equation does not provide us with transaction from matrix soil to fracture or the reverse. Neglection of such aspect could lead to incomplete and inaccurate model. Finally, the effect of variation of fracture aperture are not included into the mathematical model. Therefore such model can't really be used for aquifers with complex system.

In this thesis, an attempt to solve and extend the limitations of the classical advection dispersion equation is initiated. The new proposed model takes into account the transition of movement from matrix to fracture, this help to obtain a new mathematical model with variable dispersion and advection. The numerical simulations obtained from this model using classical differentiation with variable dispersion and advection let no doubt to believe that the variation of dispersion and advection coefficient play a crucial role to depict the effect of change in fracture aperture size. Beside, this new step forward, to capture the effect of elasticity of the geological formation, the well-known Caputo-Fabrizio fractional derivative was utilised to extend the classical model. Also to include the effect of fracture, a differential operator based on power law kernel was used to extend the classical advection dispersion equation with variable coefficient. Finally the Atangana-Baleanu differential operators was used to build a model with cross-over property. For each case a new numerical scheme was used to solve the model and numerical simulations were performed for different values of fractional orders

and variable coefficients. This new model will open new doors of investigations toward modeling the movement of subsurface water. Additionally, a new software better than FeFlow could be constructed.

**Key words:** diffusion, fracture, matrix dispersion, cross-over, power law, fractional differentiation

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## Table of Contents

<b>Abstract</b> .....	<b><i>i</i></b>
<b>Acknowledgements</b> .....	<b><i>iii</i></b>
<b>Nomenclature</b> .....	<b><i>vi</i></b>
<b>1 INTRODUCTION</b> .....	<b>1</b>
1.1 Groundwater Use.....	1
1.2 Groundwater Contamination.....	2
1.3 Groundwater Contamination Sources.....	3
1.4 Problem Identification.....	4
1.5 Motivation of the study.....	5
1.6 Limitations of the existing models.....	6
1.7 Research Objectives.....	7
1.8 Structure of this thesis.....	7
<b>2 LITERATURE REVIEW OF GROUNDWATER SYSTEMS</b> .....	<b>8</b>
2.1 Definitions of Groundwater Systems.....	8
2.1.1 Unconfined aquifer.....	9
2.1.2 Semi-confined aquifer.....	9
2.1.3 Fully Confined aquifer.....	10
2.1.4 Hard-rock aquifer.....	10
2.2 Properties of Aquifers.....	11
2.2.1 The structure of rock types.....	12
2.2.2 Heterogeneity.....	12
2.2.3 Hydraulic Conductivity.....	12
2.2.4 Aquifer Transmissivity.....	12
2.2.5 Porosity.....	13
2.2.6 Specific Storativity and the Yield.....	14
2.3 Characteristics of Fractured Media.....	14
2.3.1 Characteristics of a single fracture.....	15
2.3.2 Characteristics of Fracture Network.....	16
2.3.3 Types of fractures.....	16
2.3.4 Width of Hydraulic Fractures.....	17
2.4 Fundamental Equations in Groundwater Studies.....	17
2.4.1 Darcy's equation.....	17
2.4.2 Confined Aquifers.....	19
2.4.3 Permeability and groundwater.....	20
2.4.4 Isotropy and Homogeneity.....	20
2.5 Groundwater flow in dual media.....	21
2.5.1 Double or Dual Porosity Model.....	22
2.5.2 Impact of shape factor in a dual porosity model.....	23
2.5.3 Equivalent porous medium model.....	24
2.5.4 Discrete fracture network model.....	25
2.5.5 Introduction and application of fractional calculus.....	26
2.6 Groundwater Contamination Models.....	26
<b>3 Derivation of Equations and Numerical Analysis</b> .....	<b>28</b>
3.1 Groundwater Transport in Dual Media.....	28

3.1.1	Darcy's law equation .....	28
3.1.2	Relationship between hydraulic conductivity and intrinsic permeability .....	29
3.1.3	Hydrodynamic Dispersion .....	30
3.1.4	Retardation Factor .....	31
3.1.5	Groundwater transport in fracture .....	32
<b>3.2</b>	<b>Uniqueness of the proposed equations .....</b>	<b>34</b>
<b>3.3</b>	<b>Numerical Analysis of System of Equations.....</b>	<b>38</b>
3.3.1	Solving 1 dimension diffusion with advection for steady flow.....	38
3.3.2	Stability Analysis using von Neumann's method .....	40
<b>4</b>	<b><i>Introduction of fractional operators to the new equation .....</i></b>	<b>45</b>
<b>4.1</b>	<b>Diffusion Processes .....</b>	<b>45</b>
<b>4.2</b>	<b>New Proposed Equations.....</b>	<b>45</b>
<b>4.3</b>	<b>Fractional Differential Operators .....</b>	<b>46</b>
4.3.1	Riemann-Liouville Power-law .....	47
4.3.2	Caputo-Fabrizio Exponential decay law .....	47
4.3.3	Mittag-Leffler-Law .....	48
4.3.4	Atangana-Baleanu .....	49
4.3.5	One dimensional fractional diffusion equation and associated kernels .....	50
<b>4.4</b>	<b>Fractional Derivatives and Integrals.....</b>	<b>51</b>
4.4.1	Derivatives.....	51
4.4.2	Integrals.....	52
4.4.3	Laplace Transform.....	52
4.4.4	Applying Laplace transform technique to the integrals .....	55
4.4.5	Numerical Approximation .....	57
<b>4.5</b>	<b>Model with power-law process .....</b>	<b>66</b>
<b>4.6</b>	<b>Model with Caputo-Fabrizio .....</b>	<b>70</b>
<b>4.7</b>	<b>Model with Atangana-Baleanu .....</b>	<b>73</b>
<b>5</b>	<b><i>Simulations with the Classical Differentiation.....</i></b>	<b>84</b>
<b>5.1</b>	<b>Simulation with the Classical Diffusion Equation .....</b>	<b>84</b>
5.1.1	First Scenario for the Classical Differentiation Model .....	84
5.1.2	Second Scenario for the Classical Differentiation Model .....	86
5.1.3	The Third Scenario for Classical Differentiation Model .....	88
5.1.4	The Fourth Scenario for the for Classical Differentiation Model.....	91
<b>6</b>	<b><i>Summary Discussion .....</i></b>	<b>94</b>
<b>6.1</b>	<b>Diffusion-Advection Equation with Classical Differentiation.....</b>	<b>94</b>
<b>7</b>	<b><i>Conclusion.....</i></b>	<b>99</b>
<b>8</b>	<b><i>Conclusion.....</i></b>	<b>101</b>

## Nomenclature

Symbol	Description
Q	flow through a homogenous sand column
K	hydraulic conductivity
$k$	Intrinsic permeability
$K_{effective}$	the effective hydraulic conductivity
A	proportional to the cross-sectional area of the column
h	proportional to the difference in water level elevations
L	inversely proportional to the column's length
$\frac{dh}{dL}$	hydraulic gradient or change in hydraulic head (h) per change in distance (L) (dimensionless)
q	Specific discharge over an area
$\rho_{fluid}$	density of the fluid
$\mu_{fluid}$	viscosity of the fluid
$D_L$	is the longitudinal dispersivity or diffusion
$D_T$	is the transverse dispersivity or diffusion
$\phi$	water level
C	shape factor (dimensionless)
$d$	Average pore size between
$K_x, K_y, K_z$	coefficients of permeability in the different cartesian directions
$\rho$	density of fresh groundwater
$\omega$	Parameter relating fluid capacitance of the secondary porosity to that of the combined system. it is dimensionless
$t$	time
$D_h$	Hydrodynamic dispersion coefficient
$v_m$	advection Flux in the matrix
$v_f$	advection Flux in the fracture
$C_m$	Concentration in the matrix
$C_f$	Concentration in the fracture
$C'$	Concentration of contamination injected in the aquifer
$W$	the injection rate per unit area of aquifer
$\beta$	the maximum amount of solute that can be sorbed
$1 + \beta k_D$	the retardation factor

Symbol	Description
$K_f$	hydraulic conductivity for fracture
$K_m$	hydraulic conductivity for the soil matrix
$\Gamma_w$	Transfer term assumed to be proportional to the difference in pressure head between the fracture and matrix pore system
$w_f$	Volumetric weighting factor, it is dimensionless
$z$	Depth in the fracture and also in the soil matrix
$S_f$	the degree of fluid saturation
$L_x$	Matrix-block length
$L_y$	Matrix-block width
$L_z$	Matrix-block height
$\sigma$	Shape factor reflecting the geometry of the matrix elements; it controls the flow between the matrix and the fracture
$\delta$	aperture
$\lambda$	fracture density
$A_p$	aquifer parameter
$\gamma$	unit weight of water
$\mu$	dynamic viscosity
$v$	velocity
$n$	porosity of a fracture (dimensionless)

# 1 INTRODUCTION

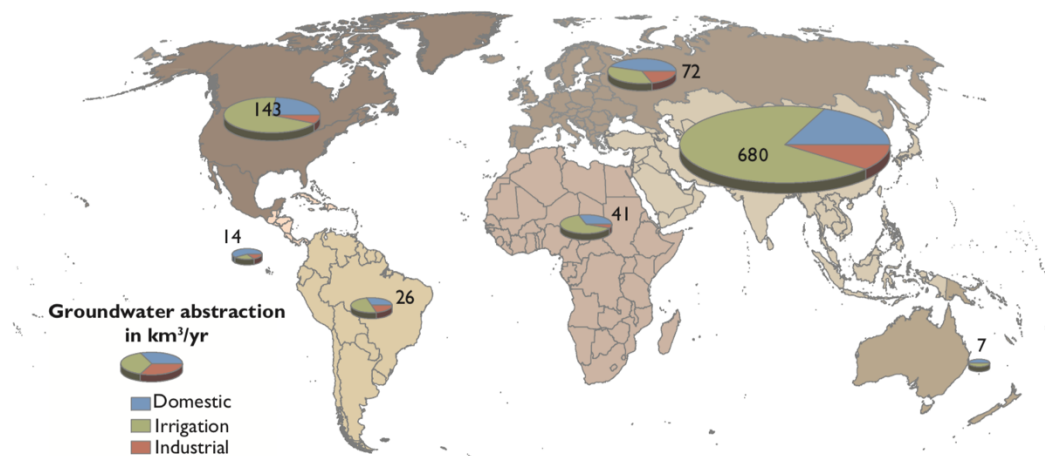
## 1.1 Groundwater Use

Groundwater has been considered to be and used as a reliable source for drinking water and irrigation in many places across the globe. In Egypt, wells were already being used in 3000 BC (Katko, 1997 in Sharma, 2001). The Bible is considered by many as a book of knowledge that describes the history of events, circumstances in which people lived and cultural heritage (Hillel, 2006). In the Bible we learn that wells were used as a reliable source of drinking water for both the people and livestock and that they were also considered when rivers were contaminated. In Exodus 7:24, it is stated that: “And all the Egyptians dug along the Nile to get drinking water, because they could not drink the water of the river”. Also in Genesis 26:18, it recorded, Isaac re-opened the wells which were dug during the lifetime of his father Abraham, which the Philistines had stopped using them after Abraham died. Isaac gave the wells the same names his father gave to them.

Groundwater is still regarded nowadays, as a reliable source of water for many people in different countries for different water uses ranging from domestic, irrigation and industrial. According to the study done by Margat & van der Gun in 2013: the worldwide groundwater use distribution based on the data collected from different countries is presented below:

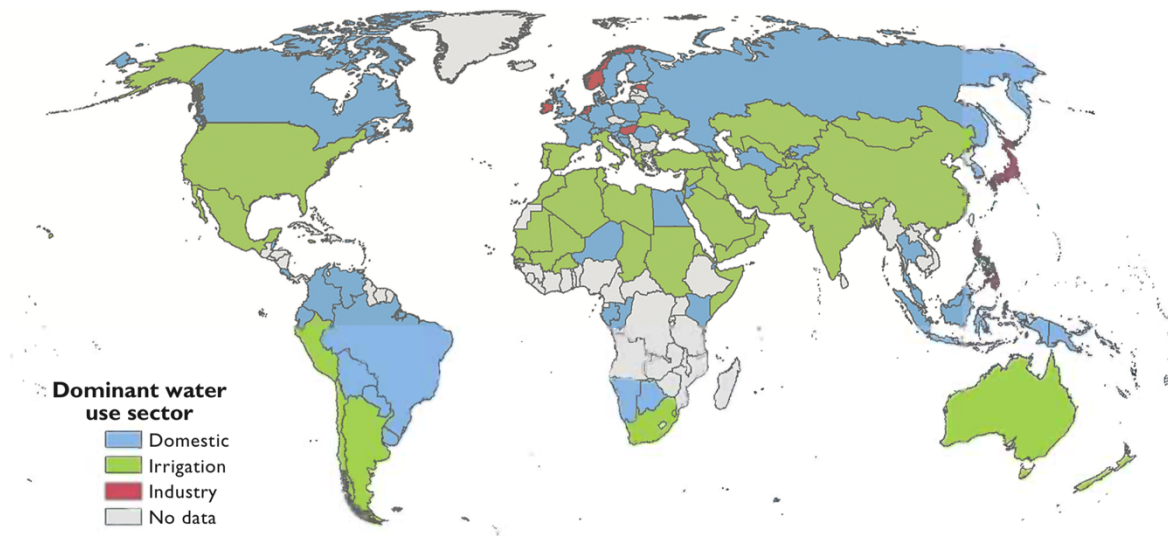
- groundwater abstraction for purposes of irrigation is reported to be at 70% across the world;
- approximately 21% of groundwater abstraction is for domestic use purposes; and
- approximately 9% of groundwater abstracted is intended/used for industrial and also for mining activities.

The groundwater abstraction/use percentages reported above, vary from continent to continent, this is presented below in figure 1-1.



**Figure 1-1:** Groundwater abstraction by continent (in km<sup>3</sup>/year) and the water-use breakdown by sector adapted from (Margat & van der Gun, 2013).

The dominant sector in terms of water use by country is shown in Figure 1-2.



*Figure 1-2: Dominant groundwater use by sector by country adapted from (Margat and van der Gun, 2013)*

By and large, groundwater is used the most for agricultural (irrigation) activities in many parts of the world. Contaminated groundwater may translate to a health risk for millions of people consuming produce from farmlands. On the other hand, irrigation activities may mobilise the transport of contaminants (chemicals and fertilizers) into the aquifers.

Heavy metals contamination in food produce is regarded as one of the major contaminating agents (Gholizadeh et al., 2009). Research has shown that, the most toxic and abundant metals in food are Lead and Cadmium. Chronic health conditions such as cardiovascular, bone, kidney, bone diseases to name but a few, are in the main, caused as a result of excessive accumulation of heavy metals in human bodies (Khan et al., 2009).

Incidents of arsenic in food have been studied and found to be in excessive concentrations in certain countries. Arsenic is well-known to be a highly toxic element, the consumption of food with arsenic is a cause for concern to the well-being of human beings and animals (Al Rmalli et al., 2005). Arsenic presence in groundwater has been reported as one of serious environmental health hazards in the globe. The consumption of food grown in fields irrigated with arsenic water is one of the serious health-risk to human beings (Das et al., 2004).

## **1.2 Groundwater Contamination**

Groundwater is deemed to have been stored and filtered through the soil matrix over long periods and therefore in most cases regarded as 'pure". Furthermore, groundwater is in often times available closer to where the demand is required and it requires less water treatment as compared to water sourced from the river.

Against these common advantages, it should be noted that groundwater is not immune to contamination by various anthropogenic activities like agricultural, domestic and industrial. Contrary to the popular impression and believe that the waters from the springs and wells are “pure”, patterns of pervasive pollution of groundwater are being uncovered (Sharma, 2001).

Groundwater contamination incidents have occurred in different places in the world and a wide range of materials identified as contaminants are found in groundwater. These include organic hydrocarbons, chemicals (organic and inorganic), inorganic cations, inorganic anions, pathogens, and radionuclides. Most of these materials are dissolved in water to a varying degree of concentration levels. Some of the organic compounds exist in both a dissolved form and as an insoluble non-aqueous phase, which can also migrate through the ground (Fetter et al. 2017).

Other emerging contaminants found in groundwater include pharmaceutical active compounds, personal care products, industrial chemicals and hormones such as endocrine disrupting compounds (Fetter et al. 2017, Meang, 2010).

### 1.3 Groundwater Contamination Sources

In literature, the groundwater contamination sources are grouped into five main categories and are provided in Table 1-1 below.

**Table 1-1:** Groundwater contamination sources adapted from (Fetter et al. 2017)

<b>Category</b>	<b>Sources</b>
Source Category I	<b>Infrastructure Designed and meant to Discharge Substance</b> <i>e.g. septic tanks and cesspools, injection wells and land application</i>
Source Category II	<b>Infrastructure Designed to Store, Treat and/or Dispose of Substances</b> <i>Landfills, Open dumps, Residential disposal, Surface impoundments, Mine wastes, Material stockpiles, Graveyards, Animal burials, Above-ground storage tanks, Underground storage tanks, Containers storing chemicals, Open incineration and detonation sites, Radioactive-waste-disposal sites</i>
Source Category III	<b>Infrastructure Designed to Retain Substances During Transport</b> <ul style="list-style-type: none"> <li>• <i>Sewer lines conveying sewerage, petroleum, natural gas</i></li> <li>• <i>Material transport and transfer</i></li> </ul>
Source Category IV	<b>Infrastructure Discharging Substances as a Consequence of Other Planned Activities</b> <i>Irrigation, Pesticide applications, Fertilizer application, Farm animal wastes, Salt application for highway deicing, Home water softeners, Urban runoff, Percolation of atmospheric pollutants, Mine drainage and excursions and Fracking fluids.</i>
Source Category V	<b>Infrastructure Providing a Conduit for Contaminated Water to Enter Aquifers</b> <i>Production wells, Monitoring wells and exploration borings, Infiltration galleries and dry wells, Construction excavations</i>
Source Category VI	<b>Naturally Occurring Sources Whose Discharge is created and/or exacerbated by human activities</b> <i>Groundwater-surface-water interactions, Natural leaching, Saltwater intrusion</i>

Groundwater contamination can have long-time effects as it may take long time to recover the contaminated site or aquifer. Atangana, (2013) identified two challenges that hamper the restoration of polluted aquifers at a large-scale. The first one, is that, groundwater is as a result of runoff which has infiltrated the soil surface at one time or another and therefore could contain possible large quantities of dissolved solids that are potentially hazardous to living organisms, human beings and animals. The second one is that, groundwater is, with the exception of natural springs and other seepage faces, is invisible. It is thus not always easy to detect and control groundwater contamination.

This issue is further complicated by the fact that there are different geological formations underground that have different behaviour depending on the contamination load they are subjected to. Recovering and cleaning a groundwater contaminated site can take a very long-time and could require a lot of money. In the year 2011, the China State Council made available a budget to a tune of \$5.5 billion over a period of 10 years to prevent and treat groundwater contamination (Qiu, 2011). Recovering a contaminated groundwater is a difficult challenge which may in some cases not be an achievable goal (MacDonald & Kavanaugh, 2008; Travis and Doty, 2003).

#### **1.4 Problem Identification**

Groundwater is not visible to the eye as compared to other water resources such as rivers, streams, rainwater harvested and the ocean. Furthermore, groundwater processes are not visible to the naked eye, they include groundwater transport (flow), water quality transformation, physical (filtration), geochemical and biological processes to name but a few.

The above mentioned processes require a deeper understanding of processes involved and 'rules' that govern the following phenomenon i.e. physical, mechanical, hydraulics, surface and groundwater interaction, geological formation characteristics. Edelman, (1972) summarised this thinking into "we have no everyday experience with groundwater, as we have with mechanical phenomena; the best way to get acquainted with the nature of the phenomena is to solve, as an exercise, a series of elementary problems".

Mathematical models have many advantages compared with other methods of solving complex problems. They have capabilities of reflecting complex physical structures and irregular geometric shapes of an aquifer system; furthermore they are convenient and flexible to use and easy to calibrate where there is reliable input data; and they can describe not only the phenomena of water flow in porous media but also the mass and energy transports and other complex physical-chemical-biological phenomena in porous media (Sun, 1996).

Groundwater is abstracted from different types of aquifer systems, these systems are predominantly characterised by geological formation, surface-water-and-groundwater interactions. In a nutshell, aquifer systems can generally be grouped into: - confined aquifers, semi-confined aquifers and unconfined aquifers. There is still a knowledge gap on understanding the mathematical rules that govern the behaviour of different aquifer systems as these systems are complex in nature. There is still a need to solve groundwater problems numerically considering the complexities of aquifer systems, i.e. groundwater hydraulics, transport, water quality, geological formation and properties.

The hard-rock aquifer systems are of particular interest, in their nature, they are controlled, by and large, by fracturing or a network of fractures and thus render them to be anisotropic and heterogeneous media. The hydrogeology of hard-fractured rocks is still not fully understood as a result there are ongoing studies.

Fracture networks or reservoirs are deemed to be the principal pathways of contamination transport in groundwater systems.

Various research interests include:

- Contamination migration from one type of medium to the other or from one area to the other e.g. the quantification of the movement of contamination through fracture.
- Contamination transport in dual media i.e. contamination transport between the network of fractures and soil matrix blocks or soil aggregates.
- Modelling of contamination transport in space and time and capturing of the memory.
- Transformation of contaminated groundwater linked to preferential movement and hydraulic flow regimes (transient and steady flow).

Furthermore, the groundwater transport and interaction between a fracture network and the porous matrix blocks or soil aggregates is not fully understood.

## **1.5 Motivation of the study**

Groundwater is often preferred because it requires less treatment, in many cases the only treatment step done is the disinfection. Furthermore, groundwater is deemed to have a better bacteriological quality as it has been filtered through the soil matrix over a long time and this which helps to minimise the spread of waterborne diseases like cholera (Appelo and Postma 2004). It is observed in literature that groundwater is regarded as the most important source of water for domestic use and for the irrigation of fruits and vegetables in farmlands.

Understanding of travel time of contamination and transformation of groundwater is very important especially in cases of dual media.

An interest in understanding and modelling the exchange between fracture networks and porous matrix blocks or soil aggregates is a long standing challenge and still not fully understood, a complete set of equations are still outstanding to explain this phenomenon.

To develop knowledge on this subject the following progress has been achieved in the over the years:

- Beranblatt et al., 1960 introduced a concept of modeling exchange between a fracture network and the matrix. They assumed that the flow occurs at steady state between fracture and matrix. Furthermore, in their model they assumed that a porous medium is made up of two separate but connected continua;
- Double-priority type models to estimate the flow of water in a fractured reservoir are reported in literature (Warren and Root, 1963; Duguid and Lee, 1977; Moench, 1984);
- Kazemi et al. (1976) introduced an extension of the dual porosity model which was proposed by Warren and Root (1960) to a two-phase flow which could account for fluid movement, the effects of gravity, and variation in formation properties; and
- Thomas et al. (1983) developed a three-dimensional and a three-phase model for simulation the flow of water, oil, and gas in fractured systems.

A fair amount of effort has been invested towards the development of an understanding of groundwater flow in dual media, however, this can't be said for contamination transport in dual media and there is less research done on this topic thus far.

This study adds value by developing new knowledge and introducing a new model for contamination transport in dual media. Understanding contamination transport in dual media is very important as groundwater contamination is so serious as its long-term impacts. Contaminated groundwater may take a long time to be discovered and decades to recover or clean the aquifer. It may take decades to discover a groundwater contaminated site as the accumulation and transport of contaminants would have occurred over very long periods.

## **1.6 Limitations of the existing models**

Limitations of the existing proposed models are presented below:

- The existing models model large-scale flow through which are naturally connected fractured system and have been proven to be beneficial in many settings.

- Notwithstanding the benefits, these models require a number of approximations which are not always suitable e.g. fracture characteristics and the corresponding dual-porosity properties are not always established. Furthermore, these models assume that the pressure is constant throughout the matrix.
- The models do not model concentrations variation and changes within a network of fractures and soil matrix blocks or soil aggregates.
- The existing models lack the ability to describe the memory effects in the aquifer.

## 1.7 Research Objectives

The ultimate goal of this study was to develop a new model for contamination transport in dual media. The specific objectives of the study to achieve this goal, are as follows:-

- To conduct a detailed literature review on existing mathematical models for groundwater transport in single and dual media,
- To investigate and reveal limitations of the existing models,
- To derive a system of equations for contamination transport in dual media,
- To build a new model using local differentiation, solve it numerically and test it with simulation modelling,
- To build a new model using fractional differentiation and perform numerical analysis.

## 1.8 Structure of this thesis

<b>Chapter 1</b>	Covers the background on groundwater, groundwater contamination and sources of groundwater contamination, problem identification, motivation of this study and research objectives.
<b>Chapter 2</b>	Cover a detailed literature review of hydrogeology and contamination models
<b>Chapter 3</b>	Covers the derivation of equations and numerical analysis
<b>Chapter 4</b>	Covers the introduction of fractional operators to the transport equation
<b>Chapter 5</b>	Covers the simulation of contamination transport in dual media with fractional models with interpretation
<b>Chapter 6</b>	Covers summary discussion of the simulation results of the models.
<b>Chapter 7</b>	Covers the conclusion of the study
<b>Chapter 8</b>	Lists the Bibliography

## 2 LITERATURE REVIEW OF GROUNDWATER SYSTEMS

Groundwater, is sometimes referred to as sub-surface water, a term which is used to describe all water not seen on the earth surrounding and can only be found beneath the ground but near to the surface. Groundwater flows through different types of porous medium e.g. the soil matrix, natural fractures and induced fractures by means of drilling. As discussed briefly above, this water is contained and abstracted from different groundwater systems, they are defined in this chapter.

### 2.1 Definitions of Groundwater Systems

Groundwater systems are in general described and classified by rock types based on their permeability properties (Nonner, 2002). The following terminology is described below; Aquifer, Aquitard, Aquiclude and last but not the least Aquifuge.

#### **An Aquifer:**

Todd (1959) in Bear and Cheng (2010), traced the term 'aquifer' to its origin in Latin: *aqui* comes from *aqua*, which means "water", and *fer*, from *ferre*, which means "to bear". Therefore, an aquifer is a term used to define a porous medium or a geological formation which (1) is fully saturated by water through the pores and (2) allows the movement of water through its pores under normal field conditions. An aquifer may also be considered to be an underground storage reservoirs that are replenished naturally by precipitation and influent streams or through wells and other artificial recharge methods (Bear, 1972). Groundwater naturally leaves an aquifer through faults (in a form of springs) or streams and sometimes through artificially induced methods such as abstraction through pumps installed in wells.

In literature, other terms are used to define an aquifer, they include groundwater reservoir, groundwater basin and sometimes called water bearing zone, however, in this thesis, aquifer is the only term used. The definitions for the types or aquifers presented below are found in Nonner, 2002 and Bear, 1972.

#### **An Aquitard:**

An *aquitard* is a semi-pervious geological formation or rock type with a low permeability as it allows water transmitted at a very slow rate as compared to other rock types in the aquifer. The rock only allows the movement of groundwater in small volumes that may be significant over time and when the total flow in a groundwater system is considered, for example, over a large-horizontal area it may allow the passage of large amounts of water between the neighbouring aquifers. An *aquitard* is commonly referred to in literature as a *leaky formation*.

**An Aquiclude:**

An *aquiclude* is an impervious formation with a very low permeability and it may contain water. This formation hardly transmits any groundwater under ordinary field conditions even though it can contain large volumes of water for example in the case of a clay layer.

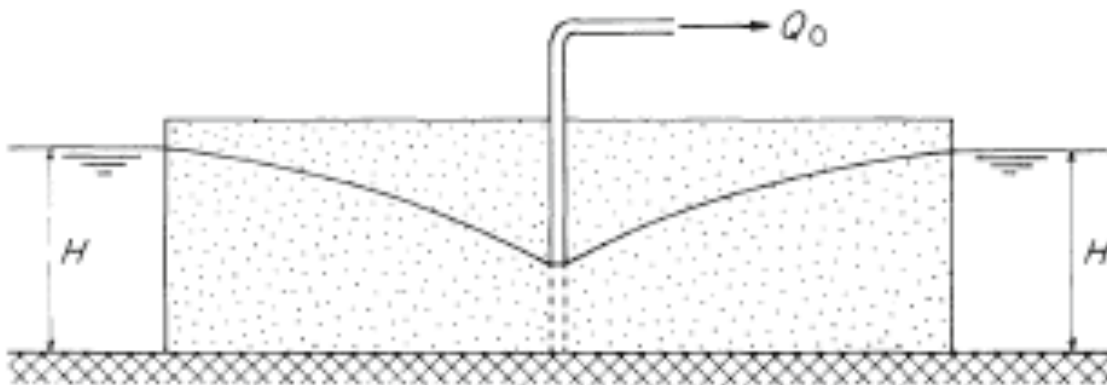
**An Aquifuge:**

An *aquifuge* is an impervious formation with an insignificant permeability and porosity, furthermore, an aquifuge does not transmit any water at all; also it does not contain any groundwater.

Aquifers can also be classified based on their location in the groundwater system. The following terminology is commonly used to define the aquifers; they include unconfined, semi-confined, fully confined and hard-rock aquifers depending on the physical evidence of the presence or absence of a water table.

**2.1.1 Unconfined aquifer**

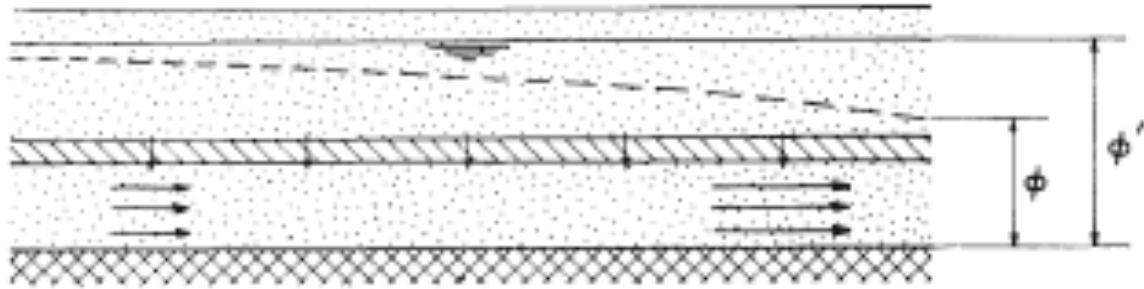
Unconfined aquifers (shown in figure 2-1), are aquifers which contain groundwater and that the groundwater is in direct contact with the atmosphere. In various places, unconfined aquifers are referred to as the uppermost aquifers (Nonner, 2002).



**Figure 2-1:** Unconfined aquifer adapted from (Verruijt, 1970)

**2.1.2 Semi-confined aquifer**

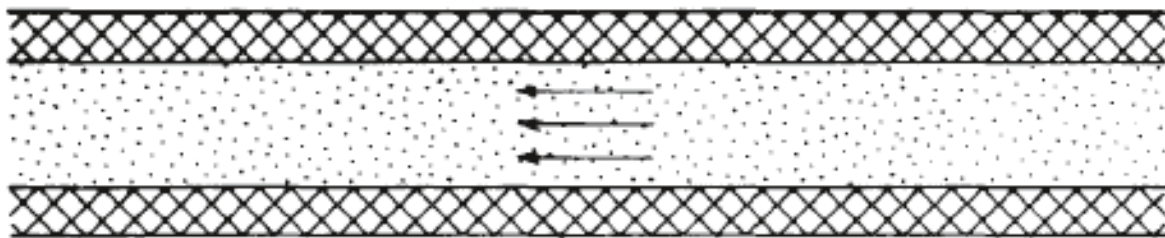
Semi-confined aquifers (shown in figure 2-2), for this type of aquifers, the groundwater filling the aquifer has not direct contact with the atmosphere. By and large, these type of aquifers are overlain by aquitards. One of the unique characteristic of semi-confined aquifer is that the inflow or outflow of groundwater is mostly through the overlying or underlying aquitards (Nonner, 2002).



**Figure 2-2:** Semi-confined aquifer adapted from (Verruijt 1970)

### 2.1.3 Fully Confined aquifer

Fully confined aquifers (shown in figure 2-3) are characterised by groundwater which is not in direct contact with the atmosphere, in some books they are also referred to as a *pressure aquifers* as the groundwater is enveloped by impervious formations above and below groundwater. These type of aquifers are positioned below aquicludes. The groundwater inflow and outflow in a vertical direction is not possible in a fully confined aquifer (Nonner, 2002 and Bear 1972).



**Figure 2-3:** Confined aquifer adapted from (Verruijt 1970)

### 2.1.4 Hard-rock aquifer

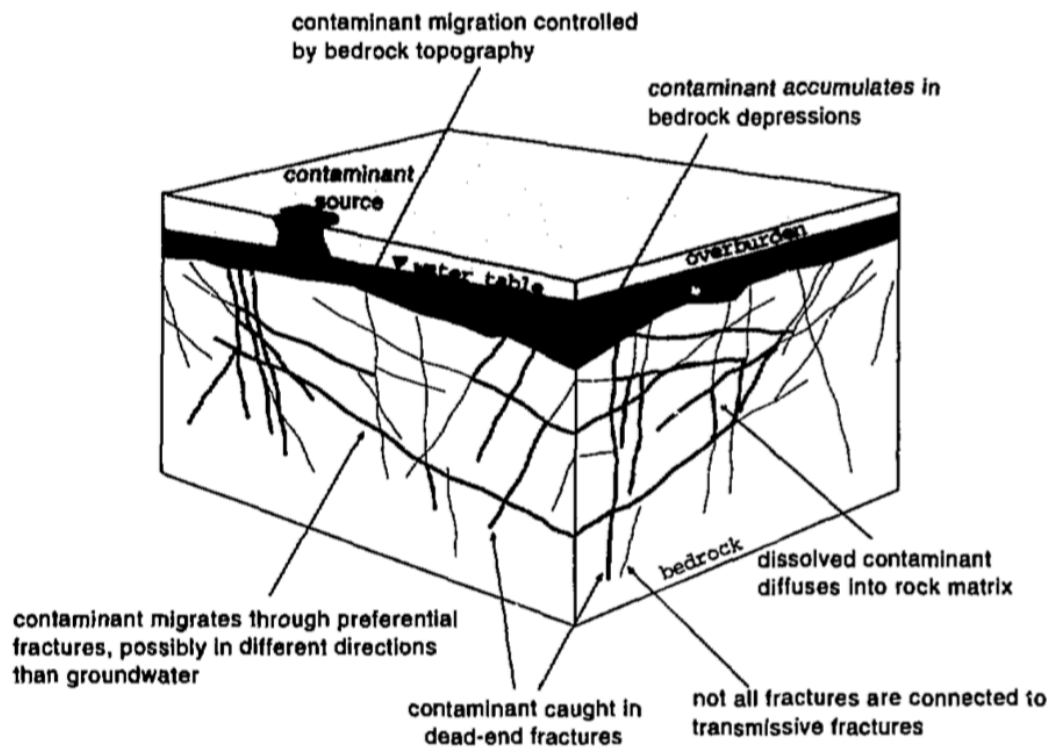
Ahmed et al. (2008) offers a concise description of hard-rock aquifers. The term hard rock aquifer was originally contrived by explorers to indicate poor ability to drill or 'drillability' of some rocky surfaces. The hard rock aquifers are characterised by their dominant property which is the negligible permeability. The permeability in hard-rock is categories in two types of porosity (1) primary (inter-granular) porosity (2) primary permeability. The hydraulic features of these rocks are in the main determined by the type and extent of fracturing, in some text they are referred to as fractured rocks. The hard rocks by their formation and nature are classified as anisotropic and heterogeneous media unlike the sedimentary rocks.

Hard rocks in the past were not considered to be a possible source of groundwater, either for domestic or irrigation purposes. The main reason was that they are expected to have relatively low permeability and the cost of drilling and resources required were expected to be high.

In the recent years, hydrogeological studies have revealed that some rocks could yield good results especially for oil and gas commodities.

Fluid mechanics and contamination transport in fractures have received little attention when compared to the study of fluid flow in other formations for example soil matrix (Parrish, 1963).

Problematic factors of contaminant behaviour associated with hard rock aquifers are presented in Figure 2-4 below.



*Figure 2-4: Problematic factors of contamination behaviour in fractured formations adapted from Cohen, 1995*

Hard rocks have various types of rock discontinuities, the discontinuities vary in size and degree from few millimetres (mm) size joints to major faults zones and lineaments. The main known rock discontinuities are fractures, faults, foliation and lineaments.

## 2.2 Properties of Aquifers

Properties governing the ability of an aquifer to receive, transmit, yield and store water are discussed in this section. Brief descriptions of these properties are presented to enunciate salient variables influencing the behaviour of the above defined aquifers.

### 2.2.1 The structure of rock types

Groundwater systems are made up of a composition of rock types (soil matrix) containing water. Physical features of rock types include; hardness, shape, mineral and chemical composition, arrangements (packing or sorting) e.g. well-sorted, well rounded, poorly sorted, angular shape, cubic packing etc. (Nonner, 2002).

Rocks in general may be classified into two rock types namely: consolidated and unconsolidated rocks. The consolidated rocks are commonly referred to as hard rocks. Hard rocks are composed of solid material where the different minerals are cemented together and cannot easily be separated from each other even by mechanical means. The unconsolidated rock types often termed soft rocks are composed of loose material, typically consisting of separated minerals (Nonner, 2002).

### 2.2.2 Heterogeneity

Heterogeneity is a term used to define the porous characteristic-nature of the subsurface. A porous medium domain is said to be homogeneous if its permeability is the same at all its points across the area of concern. Otherwise, the domain is said to be heterogeneous or inhomogeneous. Most sub-surface domains are known to be highly heterogeneous and said to be anisotropic (Bear and Cheng 2010).

### 2.2.3 Hydraulic Conductivity

Hydraulic conductivity is the measure of the ability of the aquifer material to transmit water through its body under hydraulic gradients (Bear, 1972 and Fetter et al., 2017). The aquifer material maybe in the form of a porous media (soil matrix) or fracture. In literature, hydraulic conductivity is also known as the coefficient of permeability (Nonner, 2002).

Hydraulic conductivity can have different values, depending on the direction the water flowing is taking through a porous media or fracture. In such a case the medium is said to be **anisotropic**. The value of the hydraulic conductivity can be measured in three directions,  $K_x$ ,  $K_y$  and  $K_z$ , when the hydraulic conductivity is similar in all directions, then  $K_x = K_y = K_z = K$  and the medium is said to be isotropic (Fetter et al., 2017).

### 2.2.4 Aquifer Transmissivity

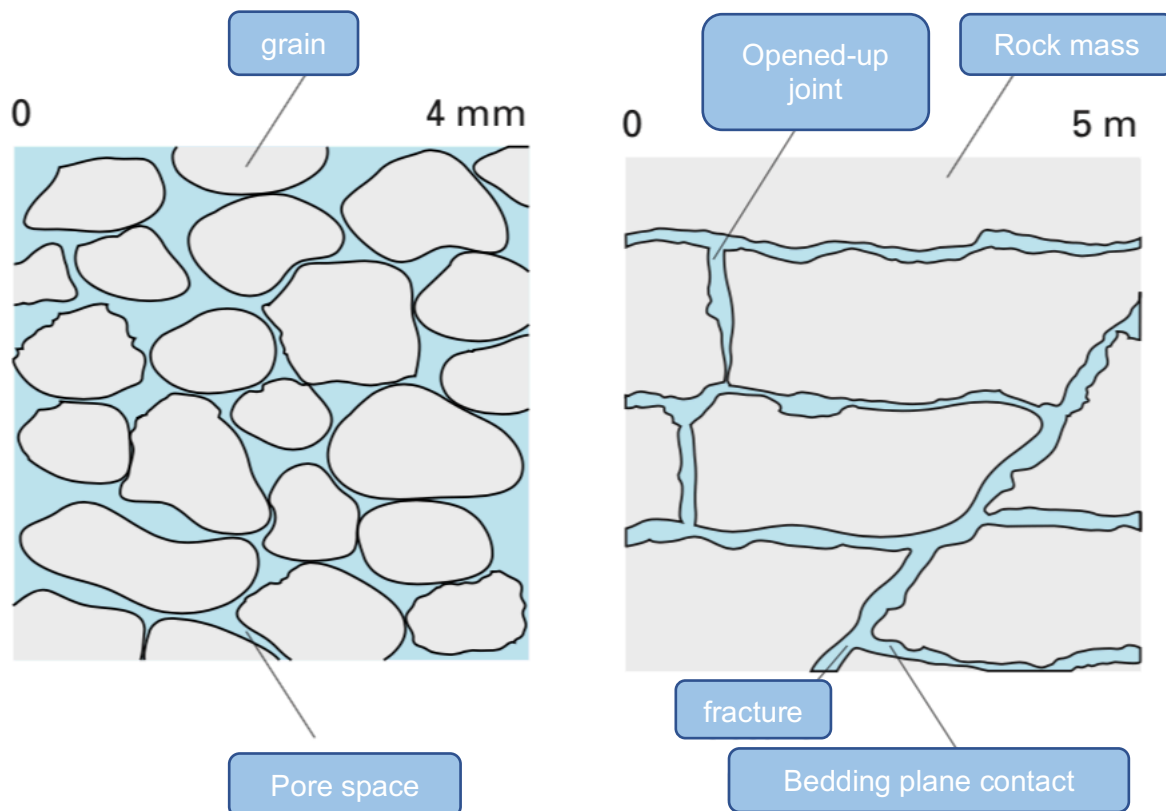
Transmissivity is related to the available pore space for the fluid to flow and the connectivity of fracture network with the thickness of an aperture for example. It is one of the bulk water and contamination transport characteristics of an aquifer. In mathematical terms,

transmissivity is the product of a hydraulic conductivity together with aquifer thickness. Most aquifers are not homogeneous in nature and therefore large differences in hydraulic conductivity can be expected. The distribution of flowlines in an aquifer can be calculated by proportioning the volume of flow according to the transmissivity difference (Appelo and Postma, 2004).

### 2.2.5 Porosity

Porosity can be defined as pores or voids within the all geological materials, it can be presented as a percentage of voids in the entire matrix volume. Uliana, (2012) differentiates and draws a distinction between the two main porosity types found in geological materials and they are primary and secondary porosity.

**Primary Porosity:** is the void space that is formed inside the rock during deposition and diagenesis for example the empty space in-between sand grains in a sandstone. Primary porosity allows in general, greater storage but less flow for example in the case of clay. An illustration of primary porosity in an unconsolidated soil matrix and secondary porosity in a consolidated rock type is show in figure 2-5.



**Figure 2-5:** Unconsolidated soil matrix (left) and consolidated rock type (right) adapted from Nonner, 2002

**Secondary Porosity:** the void space that is formed post diagenesis. e.g. fractures, dissolution features. Secondary porosity allows for less storage but higher flow by comparison to the primary porosity.

**Effective Porosity:** the void space available for fluid flow and storage.

Materials with available void space but low effective porosity include:

- Clay, it has a lot of saturated void volume, however, the volume of water cannot move.
- Vesicular basalts, have pore volume space, however, the spore spaces are not connected to aid the flow of the fluid.

### 2.2.6 Specific Storativity and the Yield

The storativity or storage in an aquifer is a function of the compressibility volume of the water and the elastic property of the soil matrix (Chiang and Kinzelbach, 2001). It is known as a measure of the amount of water a confined aquifer will give up for a certain change in a pressure-head (Atangana, 2016).

Specific storativity is the volume of water which an unconfined aquifer lets out from storage per unit surface-area of an aquifer per unit decline in the water table (Chiang & Kinzelbach, 2001).

## 2.3 Characteristics of Fractured Media

The study of flow in fractures can be traced back to the petroleum industry. According to Duguid and Lee (1997), the study of flow in a fractured media was first developed in the petroleum industry early in the 1940's. This work stemmed from the observation that production of a well could substantially be increased by inducing fracture on the medium near the well.

Fractured geological formations are of interest in a number of disciplines, contexts and various fields including: (1) groundwater exploration for water supply; (2) contamination from point and non-point sources; (3) petroleum reservoir exploration; (4) geothermal exploration and heat storage; (5) mineralisation and mining processes; (6) geotechnical investigations and applications; and (7) ocean floor hydrothermal venting and earthquakes (Berkowitz, 2002).

Fractures are very important in the context of hydrogeology, especially when considering the volumes of groundwater that could be abstracted, on the other hand, it also means that a huge volume of contamination could be transported in space over a very short time span.

The type of a fracture set is characterised by various factors, they include the orientation and the extent of the stresses responsible for the fracturing, the number of overlying, different stress regimes and events, the thickness of bedding, and the rock properties of the fractured strata (Lorenz et al., 1996).

Due to the nature of a fractured media, especially, natural fractures, they tend to have small fracture openings which may range in size from a hairline to widths greater than 0,5 mm, it can therefore be expected that the majoring of the groundwater flow regime to be laminar with a lower Reynolds number. According to Verruijt (1982), the known establish critical value of Reynolds number for groundwater flow systems is of the order of magnitude of 10.

One crack in a rock or one length of a natural fracture may be worth a thousand pores and therefore this renders fractures to play a very important role in investigating contamination transport and also for deciding on recovery method to be used for water and or oil (Sangree, 1967).

### 2.3.1 Characteristics of a single fracture

Characteristics of a single fracture are discussed below, it is critical to gain an understanding of the most important properties deemed salient for this research. A summary of properties of fractures are presented below:

**Table 2-1:** Characteristics of a single fracture

<b>Properties of a single fracture</b>	
<b>Aperture</b>	Aperture is the an important property of a single fracture as it controls groundwater and flow properties (Sahimi, 2011).
<b>Contact Area</b>	The permeability of a fracture depends on the available contact-area, it also depends on the character of the asperities (Tsenn, 2012 and Zimmerman et al., 1992)
<b>Surface Height</b>	The key variable when modelling a single fracture is the surface height $h(x, y)$ , the surface height controls the fracture aperture (Sahimi, 2011)
<b>Surface Roughness</b>	Surface roughness dictates the preferential flow paths and shear-flow behaviour and has a notable impact on the hydraulic, thermal, mechanical and transport behaviour of a single fractures (Huang et al., 2018; Luo et al., 2016)

### 2.3.2 Characteristics of Fracture Network

A fracture network can be distinguished, statistically by the distributions of six prominent properties of its fractures configuration and they include (1) aperture distribution; (2) density; (3) orientation; (4) length; (5) connectivity, and (6) displacement. Research reveal that most rock fractures properties follow power-law statistics (Zimmerman et al., 1992).

### 2.3.3 Types of fractures

There are essentially two types of fracture which are found in the field, they include natural fractures and induced fractures by means of drilling (for oil or petroleum exploration), this study focusing only on natural fractures. It is worth noting that, even though most fractures may have similar properties they are not always equal in aperture size, length, height and permeability even if they are formed under similar stress regimes and geological conditions (Lorenz et al., 1996).

Brief descriptions for different types of fractures are provided in the table 2-2.

**Table 2-2:** *Types of fractures and descriptions adapted from (Sangree, 1967)*

Type of Fracture	Description
Fracture	Any break in a rock
Fissure	An open fracture
Joint	One of a group of parallel fracture which has no detectable displacement parallel to the fracture surfaces.
Fault	A fracture with detectable displacement parallel to the fracture surfaces, frequently slickensided (friction grooved)
Gash Fracture	Generally a short fracture with a relatively wide opening, closely allied to joints;

Natural fractures are also classified as tectonic fractures. In Aguilera (1998), tectonic fractures are described as those whose origin can, on the basis of distribution, distribution, and morphology, be associated with, a local tectonic event. Tectonic events are the principal factors that control fracture development in many settings (Zeng et al., 2013).

There are two different types of measurement of a fracture used, they are fracture and aperture width. Based on the previous studies, evidence points that most deeper fractures are by and large vertical (Dysart and Whitsitt, 1967).

### 2.3.4 Width of Hydraulic Fractures

The geometry of natural created fractures remains a complex problem as it may vary with varying degrees from one area to the area. One question of practical importance is the width of fracture under dynamic condition, i.e. while the fracture is being created and extended (Perkins & Kern, 1961). The width is a very important feature to use when estimating the area of a fracture and an extent of contamination storage and transport.

Fracture width is the original width of the fracture opening prior to mineral filling. Fracture widths are classified as described in Table 2-3.

*Table 2-3: Fracture width and description adapted from Sangree, 1967*

Fracture width	Description
Hairline	: appears only as hairline trace or core surface
Visible	: width is visible but less than 0.5mm
Width greater than 0.5mm	: record maximum width

It is very important to note that in many settings, different fracture intensities and patterns may be produced and therefore fractures in the same matrix or reservoir may have varying differences in length, aperture and height even if they were formed in the same stress regime (Lorenz et al., 1996).

Aperture width, is the width of the fracture opening in the core. Fracture transmissivity is related to aperture width. Equally, fracture connectivity ultimately determines if a fracture is significant hydrologically since a fracture is only transmissive if it is connected to other transmissive fractures.

## 2.4 Fundamental Equations in Groundwater Studies

In this section, mathematical models are discussed without delving into finer details. Fundamental principles of groundwater transport are shared in this section.

### 2.4.1 Darcy's equation

The roots of the Darcy equation can be traced back to the year 1856, in which the City Engineer of Dijon, Henri Darcy, published a set of results of an investigation that he had conducted for the design of water transport and distribution system based on subsurface water conveyed to the valley in which Dijon in the southern part of France is located, by permeable layers of soil, and supplied by rainfall on the surroundings (Verruijt, 1970).

Darcy did his investigation on homogeneous, vertical and saturated sand filters to establish the flow of water in the vertical direction for the city's water fountains (Bear, 2010). Since that time the hydraulics of groundwater movement and fluid mechanics of pressurised water distribution carry his name.

In principle, Darcy's Law is the essential equation used to model the flow of a fluid at different heights through a porous media including groundwater. Its application is wide in various fields including engineering and science disciplines including water science and engineering, hydrology, hydro-informatics, hydrogeology, petroleum, soil science and chemical engineering. It has been applied for over 160 years (Chery and de Marsily 2007). The application of Darcy's equation is only limited to flows with low Reynold's-number i.e. laminar flows (Sahimi, 2011). Darcy's equation is given as:

$$Q = KA \frac{h^{(1)} - h^{(2)}}{L} \quad (2.1)$$

Where:

- Q = flow through a homogenous sand column (m<sup>3</sup>/day)
- K = Hydraulic conductivity (m/day)
- A = proportional to cross-sectional area of the column (m<sup>2</sup>)
- h = proportional to difference in water level elevations, h<sup>(1)</sup> and h<sup>(2)</sup>, at the inflow and outflow reservoirs of the column, respectively, and (m)
- L = inversely proportional to the column's length (m)

The specific discharge over a specific area can be determined using Darcy's equation below:

$$q = \frac{Q}{A} \quad (2.2)$$

- Q = flow through a homogenous sand column (m<sup>3</sup>/day)
- q = Specific discharge over an area (m/day)
- A = Area proportional to cross-sectional area of the column (m<sup>2</sup>)

The specific discharge in equation (2.2) above expressed differently can be rewritten as:

$$q = K \frac{h_{inflow} - h_{outflow}}{L} \quad (2.3)$$

It is worth noting that, the properties and the pore space play a very big role in terms of permeability of the soil matrix.

### 2.4.2 Confined Aquifers

In a confined aquifer, two relevant components with regard to specific discharge are the following:

Darcy equation for x direction

$$q_x = -K_x \frac{\partial \phi}{\partial x} \quad (2.4)$$

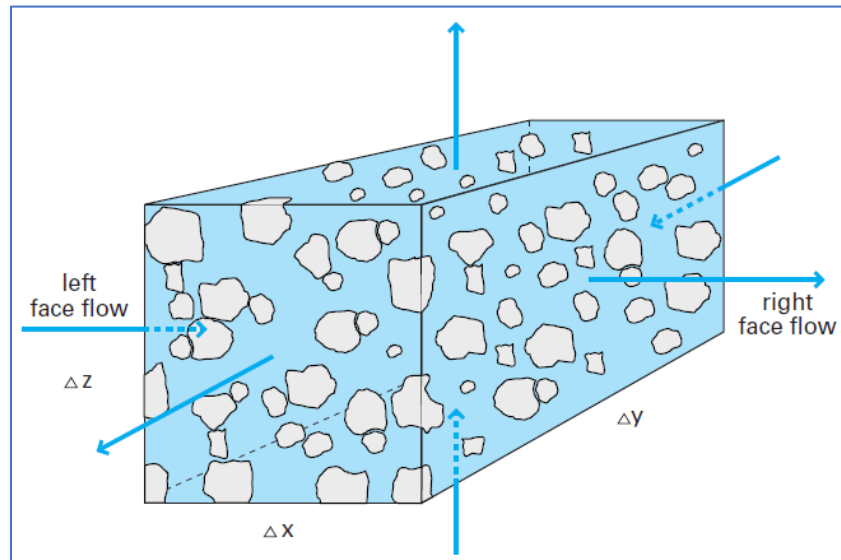
Darcy equation for y direction

$$q_y = -K_y \frac{\partial \phi}{\partial y} \quad (2.5)$$

Darcy equation for z direction

$$q_z = -K_z \frac{\partial \phi}{\partial z} \quad (2.6)$$

In a confined aquifer (see figure 2-3), it is assumed that there can be no flow in the vertical direction i.e. through the upper and lower boundaries. In a nutshell, meaning that the flow can be considered in the cartesian plain i.e. x, y and z direction as shown in Figure 2-6 below.



**Figure 2-6:** Cartesian showing x, y and z direction (adapted from Nonner, 2002)

When applying the continuity equation to solve groundwater flow problems. The following general mass flow rate equation is applied:

$$-\left[ \frac{\partial(\rho q_x)}{\partial x} + \frac{\partial(\rho q_y)}{\partial y} + \frac{\partial(\rho q_z)}{\partial z} \right] \Delta x \Delta y \Delta z = \frac{\partial(\Delta M)}{\partial t} \quad (2.7)$$

### 2.4.3 Permeability and groundwater

Permeability plays a critical role in groundwater movement and transport. Different coefficients of permeability are considered for isotropy and homogeneity conditions of the soil matrix in different cartesian directions and are known as  $K_x$ ,  $K_y$  and  $K_z$ . The general equation for the coefficient of permeability is provided below:

$$k = Cd^2 \quad \begin{array}{l} C = \text{is the shape factor and it is dimensionless} \\ d = \text{is the average pore size between grains (m)} \end{array} \quad (2.8)$$

### 2.4.4 Isotropy and Homogeneity

The coefficients of permeability ( $K_x$ ,  $K_y$  and  $K_z$ ) may be the same in all direction, when this happen, the rock is said to be *isotropic*. On the contrary, when the coefficients are not the same, the rock is said to be *anisotropic*. This can happen when there are different layers of material for example, coarse and finer sands (Nonner, 2002).

In other cases, there could be a series of rock types with same coefficients of permeability. Different rock types, even at different location can be considered to have similar coefficients of permeability ( $K_x$ ,  $K_y$  and  $K_z$ ), if this is the case rock are referred to as a homogeneous rock. In a case where coefficients of permeability ( $K_x$ ,  $K_y$  and  $K_z$ ) for the same rock differ, this phenomenon is regarded to be inhomogeneous (Nonner, 2002).

Previous studies have been done in hydrogeology with a particular focus on the characteristics of porous and hard (fractured) aquifers. The distinction between granular and fractured hard rock aquifers are shown in Table 2-1. As it can be observed in Table 2-1 that Darcy's law may not be applicable on fractured rock aquifer as this type of groundwater requires different thinking and approach altogether. Fractures are important geological structures from the hydrogeology point of view as they play a big role on the groundwater flow and storage.

**Table 2-4:** Distinction between granular and fractured rock aquifers adapted from (Ahmed et al., 2008)

<b>Aquifer Characteristics</b>	<b>Aquifer Type</b>	
	<i>Granular Rock</i>	<i>Fractured Rock</i>
Effective porosity	Mostly primary	Mostly secondary through joints, fractures etc
Isotropy	More isotropic	Mostly anisotropic
Homogeneity	More homogeneous	Less homogeneous
Flow	Laminar	Possibly rapid and turbulent
Flow predictions	Darcy's law usually applies	Darcy's law may not apply, cubic law applicable
Recharge	Dispersed	Primary dispersed with some point recharge
Temporary head variation	Minimal variation	Moderate variation

<b>Aquifer Characteristics</b>	<b>Aquifer Type</b>	
	<i>Granular Rock</i>	<i>Fractured Rock</i>
Water quality variation	Minimal variation	Greater variation

In the next section, groundwater transport in dual media is discussed. Other discontinuities affecting groundwater movement such as faults and dykes will not be explored as they act as barriers of groundwater transport (Ahmed, Jayakumar et al. 2008).

## 2.5 Groundwater flow in dual media

Groundwater transport patterns in fractured media are complex in nature, therefore difficult to understand. Other areas of interest include but not limited to the following:

- Groundwater storage and water balance;
- Continuous geological dynamics such as weathering, joints expansion etc.;
- Water quality aspects to name but a few.

Some of the existing models describing groundwater flow in fractured medium as discussed by Ahmed, Jayakumar et al. (2008) and are presented below:

- Double or dual porosity model: this is concerned with studying how a fractured aquifer behaves in a regional groundwater investigation. There are three types of matrix blocks which are considered and they include the following:  
1) spherical blocks, 2) cubes and 3) horizontal slabs.
- Equivalent porous medium model: is considered where a large volume of groundwater transport is assumed to be the same with that of a porous medium chiefly in cases where fracture density is deemed to be high.
- Discrete fracture network model: this model is used to evaluate groundwater flow in fracture settings with variable distribution, spacing, orientations and dimensions and the model incorporates various surface flows, roughness, mixing and channelling phenomena at fracture convergence.

It is worth noting that the above mentioned models, in general, require extensive knowledge about characteristic unique features of an individual fracture and capture the impact of heterogeneity.

### 2.5.1 Double or Dual Porosity Model

The flow of groundwater and transportation of contamination in dual media through preferential paths is phenomena which cannot be avoided in real-life physical problems in the catchments and aquifers. It is against this background that in this section we examine the existing models in dual porous media. The transport of contamination and groundwater flow in porous media are frequently explained by the use of double-porosity (or dual) models.

Porous media often reveal a wide variety of heterogeneities, for example: cracks, interaggregate pore, fissure and fractures and in certain cases can reveal dynamic instabilities of the wetting front during infiltration (Gerke & Genuchten, 1993; Vafai, 2015).

Warren & Root (1963) studied how naturally fractured reservoirs behave with an intention of developing an idealised model for the purposes of studying the characteristic nature and behaviour of a permeable medium which is expected to contribute considerably to the volume of pores in the system but contribute insignificantly to the flow capacity i.e. a natural fracture.

In their study, they found out that two salient variables are adequate to characterise the deviation of the behaviour of a medium with double porosity (primary and secondary) from that of a homogenous porous medium. One of the variables,  $\omega$ , is a measure of the ability of a fluid to manoeuvre within the secondary porosity and the other,  $\lambda$ , is related to the extent of the heterogeneity occurring in the system. These variables are often assessed by analysing the pressure build-up data obtained from suitably designed tests (Warren & Root, 1963).

Gerke and Genuchten (1993) in their model considered a dual-porosity approach where they assumed that the matrix is divided by different pore systems, which are considered as homogeneous media with unique hydraulic and solute transport properties.

The following one-dimensional Darcy-type equations were considered in both fracture and matrix pore system. Vertical flow in the fracture pore system is represented by this equation:

$$C_f \frac{\partial h_f}{\partial t} = \frac{\partial}{\partial z} \left( K_f \frac{\partial h_f}{\partial z} - K_f \right) - \frac{\Gamma_w}{w_f} - S_f \quad (2.9)$$

Vertical flow in the matrix pore system is represented by this equation:

$$C_m \frac{\partial h_m}{\partial t} = \frac{\partial}{\partial z} \left( K_m \frac{\partial h_m}{\partial z} - K_m \right) - \frac{\Gamma_w}{1 - w_f} - S_m \quad (2.10)$$

At any depth ( $z$ ), the transfer term  $\Gamma_w$  is estimated to be corresponding to the pressure-head difference between the fracture and matrix pore system as following:

$$\Gamma_w = \alpha_w (h_f - h_m) \quad (2.11)$$

The formulation from the above equations lead to the development of two coupled systems of nonlinear partial differential equations which were solved using the Galerkin finite element approach. The model was able to simulate various degrees of non-equilibrium at the macroscopic level by choosing appropriate model variables. However, the model requires estimates of hydraulic, transport, and the transfer term variables which are not easy to measure experimentally.

### 2.5.2 Impact of shape factor in a dual porosity model

The 'transfer term' or the matrix-to-fracture transfer in dual porosity model is influenced, by and large, by a shape factor. The role that the shape factor plays is the leakage term between the matrix and fracture channels. Different shape factors are reported in the literature, this is due to the fact that different assumption of porosity are assumed, this yields to different leakage or transfer term.

The influence of various shape factors based on different geometric assumptions on their matrix-fracture transfer rate has been studied by (Lai & Pao, 2013). In their study they compared and evaluated different equations proposed for the shape factor, few models are presented below.

Waren and Root (1963) proposed the following equation for a rectangular shape factor:

$$\sigma = \frac{4n(n+2)}{L_e^2} \quad (2.12)$$

Wherein 'n' refers to the fracture sets present and:

$$n = 1; L_e = L_x \quad (2.13)$$

$$n = 2; L_e = \frac{2L_x L_y}{(L_x + L_y)} \quad (2.14)$$

$$n = 3; L_e = \frac{3L_x L_y L_z}{L_x L_y + L_x L_z + L_y L_z} \quad (2.15)$$

Kazemi et al. (1976) proposed a shape factor for rectangular geometry as:

$$\sigma = 4 \left( \frac{1}{L_x^2} + \frac{1}{L_y^2} + \frac{1}{L_z^2} \right) \quad (2.16)$$

Other researchers concluded that the proposed equation by Kazemi must be multiplied by a factor of 2 or 3 to get more realistic results of the pressure distributions (Lai & Pao, 2013).

Another form of a shape factor was proposed by Coats (1989) for rectangular geometry as:

$$\sigma = 8 \left( \frac{1}{L_x^2} + \frac{1}{L_y^2} + \frac{1}{L_z^2} \right) \quad (2.17)$$

Lai and Pao (2013) concluded that after they performed a dimensionless analysis and comparison, they found out that there different flow behaviours for different shape factors.

### 2.5.3 Equivalent porous medium model

According to Long et al., (1982), a fractured rock is considered to behave like an equivalent porous medium (EPM) when it meets the following conditions, that: (1) there is an insignificant change in the value of the equivalent permeability with a small addition or subtraction to the test volume and (2) an equivalent permeability tensor exists which predicts the correct flux when the direction of a constant gradient is changed. The EPM model is often considered if the surrounding matrix have porosity which allowed contamination diffusion into the matrix towards to the fracture. Furthermore, when the rate of diffusion is faster when compared to the velocity of groundwater in the fracture, the impact of transport could be predicted by regarding the system to be an EPM (Pankow et al., 1986).

Applications of the EPM model are found, for example, in the studies of contamination migration and studies of flow dynamics in karst aquifers (Abusaada & Sauter, 2013; Pankow et al., 1986).

The equivalent porous medium was applied to model contamination migration in fracture porous soil in two sites namely: Alkali Lake, Oregon and Burlington, Ontario. In the findings of their study, it was concluded that the application of the EPM approach does not guarantee that the transport modelling will be a straight forward process in a particular given system. However, the EPM approach describes the contamination transport well (Pankow et al., 1986).

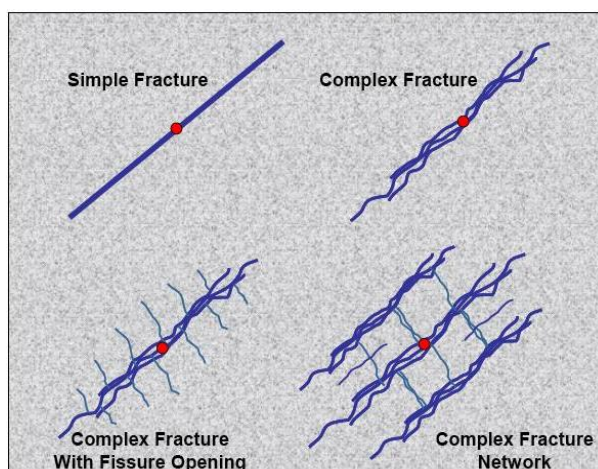
The EPM model was chosen and used in Israel and West-Bank at the Western Mountain Aquifer Basin which is shared by both countries. The EPM model was selected to model groundwater flow because of the complex nature of karst aquifers as they have the highest

degree of heterogeneity, which impact on the hydraulic variables and discharge behaviour. The discharge behaviour is associated with the hydraulic conductivity of the karst conduits and also the delayed drainage of the low-permeability fractured matrix after recharge events. The EPM model was chosen to achieve the following: (1) to validate the recharge estimation of the aquifer taking into account the high variation in spatial and temporal distributions of rainfall (2), to study the aquifer's response's under different historical climatic and management conditions and (3) finally, to predict the aquifer safe yield for different management scenarios under different climate change scenarios (Abusaada & Sauter, 2013).

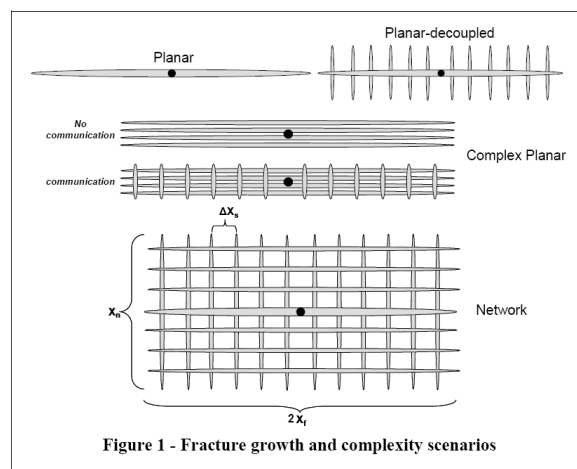
The application of the EPM model showed that it can be applied to simulate karst systems which in nature can be regarded as porous medium despite their large contrast in hydraulic conductivities (Abusaada & Sauter, 2013).

#### 2.5.4 Discrete fracture network model

Discrete fracture network model is used to analyse flow in different sets of fracture with distribution which are caused by either hydraulic fracturing and horizontal drilling. The following figures presents typical fracture growth and complex scenarios.



**Figure 2-7:** Complex fracture growth and scenarios in (Meyer & Bazan, 2011)



**Figure 2-8:** Complex fracture growth and scenarios in (Meyer & Bazan, 2011)

The discrete fracture network (DFN) model has also been applied to the modelling of flow distribution of groundwater with field data. The application of the DFN model made it attainable to explain the irregular flow distribution, furthermore, the analysis of the migration experiment demonstrate that the DFN concept is a beneficial method to illustrate flow in fractured rock (Dverstorp & Andersson, 1989).

### 2.5.5 Introduction and application of fractional calculus

Fractional calculus is a field of mathematics study that grows out of the traditional definitions of calculus integral and derivative operators in much the same way fractional exponents in an outgrowth of exponents with inter value (Rahimy, 2010).

In the recent years, fractional calculus has been applied in different disciplines such as engineering (electrical & mechanical), sciences (chemistry & biology) as well as in the field of economics, notably control theory, and signal and image processing (Atangana & Secer, 2013). As an example of its relevance and application to the groundwater studies. Atangana and Alkahtani (2015) developed new model of groundwater flow within a confined aquifer in the Caputo-Fabrizio derivative sense, the advantage of this fractional derivative is that it is able to capture and replicate the memory effect. Furthermore, their derivative is able to take into account the effect of the porosity with small permeable media. This derivative was found to be able to describe diffusion of material at different and variable scales.

## 2.6 Groundwater Contamination Models

In recent years, the quality of groundwater has been elevated and received the attention it deserves. For example, in certain situations, where aquifers are subjected to great exposure to sewage contamination and while on the other hand they are also used as sources of domestic water supply (Sun, 1996). An equation suggested by Sun:

The governing equation of water quality for this problem (Sun, 1996).

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} + \frac{C'W}{bn} \quad (2.18)$$

where  $C'$  is the concentration of contamination injected, where  $W$  is the injection rate per unit area of aquifer,  $b$  is the thickness of the aquifer, and the  $n$  is the effective porosity.

The one-dimensional advection-dispersion equation in its simplest form is:

$$\frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = 0 \quad (2.19)$$

Appelo & Postma, (2004) presents a one dimensional model to model the fate of chemicals that leach from solid waste management sites and appear to vanish in the invisible groundwater environment.

The one-dimensional model presented by Appelo and Postma is presented below:

$$\left(\frac{\partial C}{\partial t}\right)_x = -v\left(\frac{\partial C}{\partial x}\right)_t - \left(\frac{\partial q}{\partial t}\right)_x + D_L\left(\frac{\partial^2 C}{\partial x^2}\right)_t \quad (2.20)$$

where  $C$  is the solute concentration (mol/L),  $v$  is pore water flow velocity (m/s),  $D_L$  is hydrodynamic dispersion coefficient (m<sup>2</sup>/s) and  $q$  is the concentration in the solid (mol/L of pore water).

Now when considering the retardation factor and when  $q$  is considered to be a linear function of  $C$  then the equation is as shown below.

$$(1 + K_d)\left(\frac{\partial C}{\partial t}\right)_x = -v\left(\frac{\partial C}{\partial x}\right)_t + D_L\left(\frac{\partial^2 C}{\partial x^2}\right)_t \quad (2.21)$$

where  $(1 + K_d)$  is a retardation factor and  $K_d$  is the distribution coefficient.

In the next following chapters we present the derivation of the proposed equation and numerical analysis of the system of equations of contamination transport in dual media.

### 3 Derivation of Equations and Numerical Analysis

Mathematical equations have been extensively used to explain natural, physical, chemical biological and mechanical processes taking place during groundwater transport. Edelman, (1972) summarised his thoughts into “we have no everyday experience with groundwater, as we have with mechanical phenomena; the best way to get acquainted with the nature of the phenomena is to solve, as an exercise, a series of elementary problems”.

In this chapter, different set of equations are developed as a way of contributing to the existing body of knowledge. The first set of equations discussed hereunder seek to address groundwater contamination transport in dual media.

The concept of modeling exchange between fracture network and the matrix was first introduced by Beranblatt et al., 1960. They assumed that the flow happen at steady state between the fracture and matrix. They also assumed in their model that a porous medium is composed of separate but connected continua. Kazemi et al. (1976) introduced an extension to the dual porosity model Warren and Root (1960) to a two-phase flow which accounts for relative gravitational effects, fluid mobilities and variation of the formation properties. Even though they have been major efforts have been devoted to the development of realistic theoretical models that seek to explain processes taking place, predictive answers related to real fractured media remain severely limited (Berkowitz and Scher 1997).

#### 3.1 Groundwater Transport in Dual Media

##### 3.1.1 Darcy's law equation

We begin the derivation of the equation from the ancient Darcy's law equation.

$$Q = A * K * \frac{dh}{dL} \quad (3.1)$$

where :

$Q$  = discharge [ $m^3/hr$ ]

$A$  = cross sectional area [ $m^2$ ]

$K$  = hydraulic conductivity [ $m/hr$ ]

$\frac{dh}{dL}$  = hydraulic gradient or change in hydraulic head (h) per change in distance (L)

Now deriving a darcian velocity or Flux [ $m^3 hr^{-1}/m^2$ ], where we divide the flow rate by cross-sectional area, therefore the volumetric discharge reduces down to a 1-dimensional discharge (q).

$$\frac{Q}{A} = K * \frac{dh}{dL} \quad (3.2)$$

Therefore the darcian velocity (q) is:

$$q = K * \frac{dh}{dL} \quad (3.3)$$

It must be noted that mentioned above is the flow rate and darcian velocity of water. When dealing with different types of liquids with varying densities or viscosity, an **intrinsic permeability** ( $k$ ) must be determined.  $k$  is a value that characterises the ease with which any fluid flows through porous media.

$$Q = A * k \frac{\rho_{fluid} * g}{\mu_{fluid}} * \frac{dh}{dL} \quad (3.4)$$

$Q$  = discharge [ $m^3/s$ ]

$A$  = cross sectional area [ $m^2$ ]

$k$  = intrinsic permeability [ $m^2$ ]

$\rho_{fluid}$  = density of the fluid [ $kg/m^3$ ]

$\mu_{fluid}$  = viscosity of the fluid [ $kg/m*hr$ ]

$g$  = gravitational constant [ $m/s^2$ ]

$\frac{dh}{dL}$  = hydraulic gradient or change in hydraulic head (h) per change in distance (L)

### 3.1.2 Relationship between hydraulic conductivity and intrinsic permeability

A relationship between **hydraulic conductivity** ( $K$ ) and **intrinsic permeability** ( $k$ ) is demonstrated below:

$$k = K \frac{\mu_{fluid}}{\rho_{fluid} * g} \quad (3.5)$$

**Deriving an advection** equation, advection is nothing else but the movement of a volume of a chemical or biological solute or dissolved over an area at a particular time. It is considered to be the main process that drives transport mechanism called advective transport .

Deriving an advection equation in one dimension from Darcy's law, it is basically the flux, or the advection Flux and can be written as:

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} \quad (3.6)$$

The above equation can also be written as

$$\frac{\partial C}{\partial t} = -K * \frac{dh}{dL} * \left( \frac{\partial C}{\partial x} \right) \quad (3.6a)$$

We must note that due to the heterogeneity of geologic materials, advective transport in different strata can result in solute fronts spreading at different rates in each stratum (Fetter et al., 2017).

### 3.1.3 Hydrodynamic Dispersion

Hydrodynamic dispersion can be defined as the spread of solute involving mixing with native groundwater. Dutta (2013) defines the hydrodynamic dispersion as the stretching of a solute band in the flow direction during its transport by an advecting fluid. Hydrodynamic dispersion coefficient is:

$$D_{hydrodynamic} = D_{mechanical} + D_{molecular} \quad (3.7)$$

$$D_h = D_{mech.} + D_{molec}$$

Molecular diffusion is the spread of the solute molecules due to thermal motions.

Given by Fick's first law:

$$F_{diff} = -D_{molec} \frac{\partial C}{\partial x} \quad (3.8)$$

The negative sign indicates that the movement is from areas of greater concentration to those of lesser concentration (Fetter, et al, 2017).

Where  $\frac{dC}{dx}$  = the concentration gradient.

Therefore the diffusion Flux is Fick's 1<sup>st</sup> Law

$$Diffusion_{flux} = -D_{molec} * \frac{dC}{dx} \quad (3.9)$$

$$\frac{\partial C}{\partial t} = -D_{molec} \frac{\partial^2 C}{\partial x^2} \quad (3.10)$$

Therefore the total flux (F) is:

1 Dimension Flux:

$$\frac{\partial C}{\partial t} = -v * \frac{\partial C}{\partial x} + D_h \left( \frac{\partial^2 C}{\partial x^2} \right) \quad (3.11)$$

2 Dimension Flux:

$$\frac{\partial C}{\partial t} = -v * \frac{\partial C}{\partial x} + D_L \left( \frac{\partial^2 C}{\partial x^2} \right) + D_T \left( \frac{\partial^2 C}{\partial y^2} \right) \quad (3.12)$$

$D_L$  = is the longitudinal dispersivity or diffusion

$D_T$  = is the transverse dispersivity or diffusion

### 3.1.4 Retardation Factor

Chemical reactions or transformation processes during transport are described briefly below. According to Berkowitz (2002) sorption reactions in groundwater systems involve many kinds of chemical constituents and different physical and chemical processes. Chemical sorption onto colloids is usually governed by a slow kinetic process. Highly mobile colloids can propagate quickly through an interconnected network of fractures and thus enhance significantly the rate of contaminant migration. The added difficulty associated with measuring colloid movement (and estimating, e.g., colloid filtration coefficients) and colloid-chemical interactions at the field scale serves to further increase model and prediction uncertainty.

According to Fetter et al., (2017) sorption processes include adsorption, chemisorption, absorption, and ion exchange. **Adsorption** includes the processes by which a solute clings to a solid surface. **Chemisorption** occurs when the solute is incorporated on a sediment, soil, or rock surface by a chemical reaction. **Absorption** occurs when the aquifer particles are porous so that the solute can diffuse into the particle and be sorbed onto interior surfaces.

Equilibrium surface reaction isotherm is basically a relationship that is not a function of time showing the concentration in solution ( $C$ ) versus that absorbed ( $S$ ) on the solid surface.

Shown below is a transport equation has two variables,  $C$  and  $S$ .

$$\frac{\partial C}{\partial t} + \beta \frac{\partial S}{\partial t} = D_h \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (3.13)$$

where:

$\beta$  = is the maximum amount of solute that can be sorbed.

Replacing  $S$  with  $K_D C$

$$\frac{\partial C}{\partial t} + \beta \frac{\partial k_D C}{\partial t} = D_h \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (3.14)$$

Now simplifying the above the above equation:

$$(1 + \beta k_D) \frac{\partial C}{\partial t} = D_h \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (3.15)$$

where:

$(1 + \beta k_D)$  = is the retardation factor

Therefore the equation to model transport in the matrix is:

$$(1 + \beta k_D) \frac{\partial C}{\partial t} = D_h \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (3.16)$$

### 3.1.5 Groundwater transport in fracture

Now deriving an equation for groundwater transport in fracture, we first bring an understanding of the movement of water through soil as a steady flow and can be best described with Darcy's equation:

$$q = K * \frac{dh}{dL} \quad (3.17)$$

Now defining the effective  $K$  as:

$$K_{effective} = -\delta^3 \lambda \frac{\gamma}{12 \mu} \quad (3.18)$$

where:

$\delta$  = aperture [L]

$\lambda$  = fracture density [ $L^2/L^3$ ] or [ $L/L^2$ ] or [ $1/L$ ]

$\gamma$  = unit weight of water

$\mu$  = dynamic viscosity

$v$  = velocity

$\rho$  = density [ $M/L^3$ ]

$n$  = porosity of a fracture [dimension less]

now replacing  $K$  in equation (3.17) we get:

$$q = -\delta^3 \lambda \frac{\gamma}{12 \mu} \frac{dh}{dL} \quad (3.19)$$

The above equation represent Darcy's law with the effective hydraulic conductivity  $K_{effective}$  and  $q$  being the effective Flux.

#### 3.1.5.1 Solving for an aperture

Now solving for an effective aperture we get:

$$\delta = \left( \frac{K 12 \mu}{\lambda \gamma} \right)^{1/3} \quad (3.20)$$

Please note that the above equation does not consider things like infilling and fluid pressure as both have an impact on an aperture. The average velocity through fracture:

$$v_x = \frac{q}{n} = \frac{-K}{n} \frac{dh}{dx} \quad (3.21)$$

The average porosity in a fracture is expressed as :

$$porosity = n = \delta\lambda \quad (3.22)$$

Now substituting  $n$  by  $\delta\lambda$  we get:

$$v_x = \frac{q}{n} = \frac{-K}{\delta\lambda} \frac{dh}{dx} \quad (3.23)$$

Substituting with the effective aperture in the equation as expressed in equation (3.23) above.

$$v_x = -K^{2/3} \left(12\lambda^2 \frac{\mu}{\gamma}\right)^{-1/3} \frac{dh}{dx} \quad (3.24)$$

Now going back to the one dimension advection diffusion/dispersion equation derived above for matrix.

$$\frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D_L \left(\frac{\partial^2 C}{\partial x^2}\right) + D_T \left(\frac{\partial^2 C}{\partial y^2}\right) \quad (3.25)$$

Now replacing  $v_x$  in equation (3.25) to make it advection diffusion/dispersion equation for a fracture:

$$\frac{\partial C_f}{\partial t} = \left(-K^{2/3} \left(12\lambda^2 \frac{\mu}{\gamma}\right)^{-1/3} \frac{dh}{dx}\right) \frac{\partial C_f}{\partial x} + D_L \left(\frac{\partial^2 C_f}{\partial x^2}\right) + D_T \left(\frac{\partial^2 C_f}{\partial y^2}\right) \quad (3.26)$$

Transverse diffusion ( $D_T$ ) is negligible because it is expected to be very small, we can therefore regard that term as zero, and therefore the advection diffusion equation for a fracture is.

$$\frac{\partial C_f}{\partial t} = \left(-K^{2/3} \left(12\lambda^2 \frac{\mu}{\gamma}\right)^{-1/3} \frac{dh}{dx}\right) \frac{\partial C_f}{\partial x} + D_L \left(\frac{\partial^2 C_f}{\partial x^2}\right) \quad (3.27)$$

Now we have two sets of equations for matrix and fracture:

Matrix:

$$(1 + \beta k_D) \frac{\partial C}{\partial t} = D_h \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (3.28)$$

Fracture when considering retardation effect:

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = \left(-K^{2/3} \left(12\lambda^2 \frac{\mu}{\gamma}\right)^{-1/3} \frac{dh}{dx}\right) \frac{\partial C_f}{\partial x} + D_h \left(\frac{\partial^2 C_f}{\partial x^2}\right) \quad (3.28)$$

A comparison between the matrix and fracture is presented in the table below.

**Table 3-1: Matrix versus Fracture Properties**

	Matrix	Fracture
Primary Porosity	Dominating	
Secondary Porosity		Dominating
Permeability	Low by comparison	Higher
Travel time (velocity)	Generally slow	Faster

### 3.2 Uniqueness of the proposed equations

In this section, the Picard-Lindelöf theorem is used to prove the uniqueness of the proposed system of equations for the matrix and fracture network. The Picard-Lindelöf theorem is a well-known and an important theorem on existence and uniqueness of solutions to first-order differential equations with given initial conditions (Nevanlinna, 1989).

Now in this section we are considering the proposed equations:

For the soil matrix:

$$(1 + \beta k_D) \frac{\partial C_m}{\partial t} = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (3.29)$$

For the fracture:

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = \left( -K^{2/3} \left( 12 \lambda^2 \frac{\mu}{\gamma} \right)^{-1/3} \frac{dh}{dx} \right) \frac{\partial C_f}{\partial x} + D_h \left( \frac{\partial^2 C_f}{\partial x^2} \right) \quad (3.29)$$

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = D_h \left( \frac{\partial^2 C_f}{\partial x^2} \right) - (v_f) \frac{\partial C_f}{\partial x} \quad (3.30)$$

Now replacing the retardation factor  $(1 + \beta k_D)$  with R in both equations we get the following:

For matrix:

$$R \frac{\partial C_m}{\partial t} = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (3.31)$$

For fracture:

$$R \frac{\partial C_f}{\partial t} = D_h \left( \frac{\partial^2 C_f}{\partial x^2} \right) - (v_f) \frac{\partial C_f}{\partial x} \quad (3.32)$$

Now taking into account the transfer term we add the transfer term. A *transfer term* determines the communication between fracture and matrix domain. The transfer term is the most relevant feature in a dual porosity model as it governs the flow between matrix and fracture.

Adopting the definition of Warren & Root (1963) and change the pressure differential to between the matrix and fracture to concentration difference.

$$R \frac{\partial C_f}{\partial t} = D_h \left( \frac{\partial^2 C_f}{\partial x^2} \right) - (v_f) \frac{\partial C_f}{\partial x} + \sigma \frac{k_m}{\mu} (C_m - C_f) \quad (3.33)$$

Now to simplify the equations we divide the above set of equations by the retardation factor.

$$\frac{\partial C_m}{\partial t} = \frac{D_h}{R} \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (3.34)$$

$$\frac{\partial C_f}{\partial t} = \frac{D_h}{R} \left( \frac{\partial^2 C_f}{\partial x^2} \right) - \frac{v_f}{R} \frac{\partial C_f}{\partial x} + \frac{\sigma k_m}{R \mu} (C_m - C_f) \quad (3.35)$$

for simplicity we let:

$$\frac{\partial C_m}{\partial t} = F(x, t, C_m, C_f) \quad (3.36)$$

$$\frac{\partial C_f}{\partial t} = H(x, t, C_m, C_f) \quad (3.37)$$

then applying the integral on both sides we get :

For matrix

$$C_m(x, t) - C_m(x, 0) = \int_0^t F(x, \tau, C_m(x, \tau), C_f(x, \tau)) \quad (3.38)$$

$$C_m(x, t) = C_m(x, 0) + \int_0^t F(x, \tau, C_m(x, \tau), C_f(x, \tau)) \quad (3.39)$$

For fracture

$$C_f(x, t) - C_f(x, 0) = \int_0^t H(x, \tau, C_m(x, \tau), C_f(x, \tau)) \quad (3.40)$$

$$C_f(x, t) = C_f(x, 0) + \int_0^t H(x, \tau, C_m(x, \tau), C_f(x, \tau)) \quad (3.41)$$

Then we define:

$$C(x, t) = C(x, 0) + \int_0^t \pi(x, \tau, C(x, \tau)) d\tau \quad (3.42)$$

$$C(x, t) = [C_m(x, t), C_f(x, t)] \quad (3.43)$$

$$C(x, 0) = [C_m(x, 0), C_f(x, 0)] \quad (3.44)$$

where:

$$\begin{aligned} \pi(x, t, C(x, t)) = & F(x, t, C_m(x, t), C_f(x, t)) \\ & H(x, t, C_m(x, t), C_f(x, t)) \end{aligned} \quad (3.45)$$

Now defining Aquifer Parameter ( $A_p$ )

$$A_p = T_{t_{max}}(t_0) X_{C_0}(b) \quad (3.46)$$

$$T_{t_{max}}(t_0) = [t_{max} - t_0, t_0 + t_{max}] \quad (3.47)$$

$$X_{C_0}(b) = [C_0 - b, C_0 + b] \quad (3.48)$$

$$\|F(x, t, C_{m1}, C_f)\| < M_1 \quad (3.49)$$

$$\|H(x, t, C_{m2}, C_f)\| < M_2 \quad (3.50)$$

$$\|\pi(x, t, C_m, C_f)\| < M_\pi \quad (3.51)$$

We define a contraction mapping ( $\Upsilon$ ) as:

$$\Upsilon \bigvee(x, t) = C(x, 0) + \int_0^t \pi(x, \tau, C(x, \tau)) d\tau \quad (3.52)$$

The supremum infimum is define below as:

$$\|V\| = \sup_{t \in T_{t_{max}}(t_0)} |V(x, t)| \quad (3.53)$$

$$\|V\| = \sup_{x \in X_{C_0}(b)} |V(x, t)| \quad (3.54)$$

$$\|Y \sqrt{V(x, t) - C(x, o)}\| = \int_0^t \pi(x, \tau, C(x, \tau)) d\tau \quad (3.55)$$

$$\begin{aligned} \|Y \sqrt{V(x, t) - C(x, o)}\| &= \int_0^t \pi(x, \tau, C(x, \tau)) d\tau \quad (3.56) \\ &= \left\| \int_0^t \pi(x, \tau, C(x, \tau)) d\tau \right\| \\ &\leq \int_0^t \|\pi(x, \tau, C(x, \tau))\| d\tau \\ &< \int_0^t M_\pi d\tau \\ &< M_\pi t_{max} < b \\ t_{max} &< \frac{b}{M_\pi} \end{aligned}$$

$$\|Y \sqrt{V(x, t) - Y U(x, t)}\| < K \|v(x, t) - U(x, t)\| \quad (3.57)$$

To prove the above we must first check that:

$$\|F(x, t, C_m, C_f) - F(x, t, C'_m, C'_f)\| < K \|C_m - C'_m\| \quad (3.58)$$

$$F(x, t, C_m, C_f) - F(x, t, C'_m, C'_f) = \frac{D_h}{R} \frac{\partial^2}{\partial x^2} [(C_m - C'_m)] - v \frac{\partial}{\partial x} [(C_m - C'_m)] \quad (3.59)$$

$$\|F(x, t, C_m, C_f) - F(x, t, C'_m, C'_f)\| \leq \frac{D_h}{R} \quad (3.60)$$

$$\begin{aligned} \left\| \frac{\partial^2}{\partial x^2} [C_m - C'_m] \right\| + \frac{v}{R} \left\| \frac{\partial}{\partial x} [C_m - C'_m] \right\| &\leq \frac{D_h}{R} \theta_2^2 \|C_m - C'_m\| + \frac{v}{R} \theta_1 \|C_m - C'_m\| \quad (3.61) \\ &\leq \left( \frac{D_h}{R} \theta_2^2 + \frac{v}{R} \theta_1 \right) \|C_m - C'_m\| \\ &\leq L \|C_m - C'_m\| \end{aligned}$$

In a similar way we show that:

$$\|H(x, t, C_m, C_f) - H(x, t, C'_m, C'_f)\| \leq L \|C_m - C'_m\| \quad (3.62)$$

and

$$\|H(x, t, C_m, C_f) - H(x, t, C'_m, C'_f)\| \leq L_2 \|C_f - C'_f\| \quad (3.63)$$

### 3.3 Numerical Analysis of System of Equations

In this chapter, the derived equations above are evaluated and solved numerically using different methods proposed in earlier literature. The first method considered is Crank–Nicolson method, it is a finite difference method used for numerically solving the heat equation and similar partial differential equations (Cebeci & Bradshaw, 2012). The Crank-Nicolson method is considered to be an unconditionally stable, implicit numerical scheme with second-order accuracy in both time and space (Sun & Trueman, 2003).

The second method considered to do the stability analysis on the proposed equations is von Neumann's. The von Neumann's stability analysis method has been applicable to non-stationary convection-diffusion equations and also on the investigation into the transient behaviour of viscoelastic pipelines (Wesseling, 1996 and Zecchin et al., 2008).

#### 3.3.1 Solving 1 dimension diffusion with advection for steady flow

The previously derived equations considered include one for the matrix equation (3.16) and one for the fracture equation (3.28).

##### Equation for the soil matrix

$$(1 + \beta k_D) \frac{\partial C_m}{\partial t} = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (3.64)$$

Concentration defined on a spatial interval is shown below:

$$\begin{aligned} \frac{C_{im}^{j+1} - C_{im}^j}{\Delta t} = & D_h \frac{1}{2(\Delta x)^2} \left( (C_{im}^{j+1} - 2C_{im}^{j+1} + C_{im-1}^{j+1}) + (C_{im+1}^j - 2C_{im}^j + C_{im-1}^j) \right) - \\ & v_m \frac{1}{2} \left( \left( \frac{C_{im+1}^{j+1} - C_{im-1}^{j+1}}{2\Delta x} \right) + \left( \frac{C_{im+1}^j + C_{im-1}^j}{2\Delta x} \right) \right) \end{aligned} \quad (3.65)$$

Now looking at the equation for fracture:

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = \left( -K^{2/3} \left( 12\lambda^2 \frac{\mu}{\gamma} \right)^{-1/3} \frac{dh}{dx} \right) \frac{\partial C_f}{\partial x} + D_h \left( \frac{\partial^2 C_f}{\partial x^2} \right) \quad (3.66)$$

Now replacing the term  $-K^{2/3} \left( 12\lambda^2 \frac{\mu}{\gamma} \right)^{-1/3} \frac{dh}{dx}$  with  $v_f$  we get:

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = D_h \left( \frac{\partial^2 C_f}{\partial x^2} \right) - (v_f) \frac{\partial C_f}{\partial x} \quad (3.67)$$

Applying and solving the first equation (3.64) numerically using the Crank-Nicolson method where  $i$  represent the position (in-space) and  $j$  represent the time in space.

**For the soil matrix:**

$$(1 + \beta k_D) \frac{\partial C_m}{\partial t} = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (3.68)$$

For simplicity on the an analysis, we consider splitting the equation into three terms for the ease of the analysis and presentation, then we have:

$$(1 + \beta k_D) \frac{\partial C_m}{\partial t}; D_h \frac{\partial^2 C_m}{\partial x^2}; -v_m \frac{\partial C_m}{\partial x} \quad (3.69)$$

Then we present and analyse each term as follow:

$$(1 + \beta k_D) \frac{\partial C_m}{\partial t} = (1 + \beta k_D) \frac{C_{i,m}^{j+1} - C_{i,m}^j}{\Delta t} \quad (3.70)$$

$$D_h \frac{\partial^2 C_m}{\partial x^2} = D_h \frac{1}{2(\Delta x)^2} \left( (C_{i+1,m}^{j+1} - 2C_{i,m}^{j+1} + C_{i-1,m}^{j+1}) + (C_{i+1,m}^j - 2C_{i,m}^j + C_{i-1,m}^j) \right) \quad (3.71)$$

$$-v_m \frac{\partial C_m}{\partial x} = -v_m \frac{1}{2} \left( \left( \frac{C_{i+1,m}^{j+1} - C_{i-1,m}^{j+1}}{2\Delta x} \right) + \left( \frac{C_{i+1,m}^j - C_{i-1,m}^j}{2\Delta x} \right) \right) \quad (3.72)$$

**Therefore** the discretised equation for the matrix is shown below:

$$(1 + \beta k_D) \frac{C_{i,m}^{j+1} - C_{i,m}^j}{\Delta t} = D_h \frac{1}{2(\Delta x)^2} \left( (C_{i+1,m}^{j+1} - 2C_{i,m}^{j+1} + C_{i-1,m}^{j+1}) + (C_{i+1,m}^j - 2C_{i,m}^j + C_{i-1,m}^j) \right) - v_m \frac{1}{2} \left( \left( \frac{C_{i+1,m}^{j+1} - C_{i-1,m}^{j+1}}{2\Delta x} \right) + \left( \frac{C_{i+1,m}^j - C_{i-1,m}^j}{2\Delta x} \right) \right) \quad (3.73)$$

**For the Fracture:**

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = D_h \frac{\partial^2 C_f}{\partial x^2} - v_f \frac{\partial C_f}{\partial x} \quad (3.74)$$

Splitting the equation into three terms for the ease of the analysis and presentation we have:

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t}; D_h \frac{\partial^2 C_f}{\partial x^2}; -v_f \frac{\partial C_f}{\partial x} \quad (3.75)$$

Then we present and analyse each term as follow:

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = (1 + \beta k_D) \frac{C_{i,f}^{j+1} - C_{i,f}^j}{\Delta t} \quad (3.76)$$

$$D_h \frac{\partial^2 C_f}{\partial x^2} = D_h \frac{1}{2(\Delta x)^2} \left( (C_{i+1,f}^{j+1} - 2C_{i,f}^{j+1} + C_{i-1,f}^{j+1}) + (C_{i+1,f}^j - 2C_{i,f}^j + C_{i-1,f}^j) \right) \quad (3.77)$$

$$-v_f \frac{\partial C_f}{\partial x} = -v_f \frac{1}{2} \left( \left( \frac{C_{i+1,f}^{j+1} - C_{i-1,f}^{j+1}}{2\Delta x} \right) + \left( \frac{C_{i+1,f}^j - C_{i-1,f}^j}{2\Delta x} \right) \right) \quad (3.78)$$

Therefore the discretised equation for the fracture is displayed below:

$$(1 + \beta k_D) \frac{\partial C_f}{\partial t} = D_h \left( \frac{\partial^2 C_f}{\partial x^2} \right) - (v_f) \frac{\partial C_f}{\partial x} \quad (3.79)$$

Then we have:

$$\begin{aligned} (1 + \beta k_D) \frac{C_{i,f}^{j+1} - C_{i,f}^j}{\Delta t} &= D_h \frac{1}{2(\Delta x)^2} \left( (C_{i+1,f}^{j+1} - 2C_{i,f}^{j+1} + C_{i-1,f}^{j+1}) \right. \\ &+ \left. (C_{i+1,f}^j - 2C_{i,f}^j + C_{i-1,f}^j) \right) - v_f \frac{1}{2} \left( \left( \frac{C_{i+1,f}^{j+1} - C_{i-1,f}^{j+1}}{2\Delta x} \right) \right. \\ &\left. + \left( \frac{C_{i+1,f}^j - C_{i-1,f}^j}{2\Delta x} \right) \right) \end{aligned} \quad (3.80)$$

In the next section we consider the stability analysis using von Neumann method.

### 3.3.2 Stability Analysis using von Neumann's method

In this section, equation (3.73) and (3.80) are analysed numerically using von Neumann method to establish the stability of the two equations. Von Neumann's method has been applied in groundwater problems, particularly, on the derivation of new models to test the stability of equations numerically. Bethke (1985) developed new numerical method which allows for the solving of compaction-driven groundwater flow and associated heat transfer in evolving sedimentary basins and used von Neumann's method to test the stability of the new model.

Ramotsho & Atangana (2018) used the von Neumann's method to assess the stability of the numerical solution of a groundwater flow model within leaky and self-similar aquifers, on a model they had derived.

#### Assessing the stability of the equation for the matrix

$$\begin{aligned} (1 + \beta k_D) \frac{C_{i,m}^{j+1} - C_{i,m}^j}{\Delta t} &= D_h \frac{1}{2(\Delta x)^2} \left( (C_{i+1,m}^{j+1} - 2C_{i,m}^{j+1} + C_{i-1,m}^{j+1}) + (C_{i+1,m}^j - 2C_{i,m}^j + \right. \\ &\left. C_{i-1,m}^j) \right) - v_m \frac{1}{2} \left( \left( \frac{C_{i+1,m}^{j+1} - C_{i-1,m}^{j+1}}{2\Delta x} \right) + \left( \frac{C_{i+1,m}^j - C_{i-1,m}^j}{2\Delta x} \right) \right) \end{aligned} \quad (3.81)$$

Now replacing  $(1 + \beta k_D)$  with  $R_m$  then we have:

$$R_m \frac{C_{i,m}^{j+1} - C_{i,m}^j}{\Delta t} = D_h \frac{1}{2(\Delta x)^2} \left( (C_{i+1,m}^{j+1} - 2C_{i,m}^{j+1} + C_{i-1,m}^{j+1}) + (C_{i+1,m}^j - 2C_{i,m}^j + C_{i-1,m}^j) \right) - v_m \frac{1}{2} \left( \left( \frac{C_{i+1,m}^{j+1} - C_{i-1,m}^{j+1}}{2\Delta x} \right) + \left( \frac{C_{i+1,m}^j - C_{i-1,m}^j}{2\Delta x} \right) \right) \quad (3.82)$$

Multiplying by  $\Delta t$  on both sides and dividing by  $R_m$

$$(C_{i,m}^{j+1} - C_{i,m}^j) = \frac{D_h \Delta t}{R_m 2(\Delta x)^2} \left( (C_{i+1,m}^{j+1} - 2C_{i,m}^{j+1} + C_{i-1,m}^{j+1}) + (C_{i+1,m}^j - 2C_{i,m}^j + C_{i-1,m}^j) \right) - \frac{\Delta t v_m}{R_m} \frac{1}{2} \left( \left( \frac{C_{i+1,m}^{j+1} - C_{i-1,m}^{j+1}}{2\Delta x} \right) + \left( \frac{C_{i+1,m}^j - C_{i-1,m}^j}{2\Delta x} \right) \right) \quad (3.83)$$

Now let  $\frac{D_h \Delta t}{R_m 2(\Delta x)^2} = A$  and let  $\frac{v_m \Delta t}{R_m 2 \cdot 2\Delta x} = B$

Therefore equation (3.81) becomes:

$$(C_{i,m}^{j+1} - C_{i,m}^j) = A \left( (C_{i+1,m}^{j+1} - 2C_{i,m}^{j+1} + C_{i-1,m}^{j+1}) + (C_{i+1,m}^j - 2C_{i,m}^j + C_{i-1,m}^j) \right) - B \left( (C_{i+1,m}^{j+1} - C_{i-1,m}^{j+1}) + (C_{i+1,m}^j - C_{i-1,m}^j) \right) \quad (3.84)$$

Multiplying in by A and B we get:

$$(C_{i,m}^{j+1} - C_{i,m}^j) = \left( (AC_{i+1,m}^{j+1} - 2AC_{i,m}^{j+1} + AC_{i-1,m}^{j+1}) + (AC_{i+1,m}^j - 2AC_{i,m}^j + AC_{i-1,m}^j) \right) - \left( (BC_{i+1,m}^{j+1} - BC_{i-1,m}^{j+1}) + (BC_{i+1,m}^j - BC_{i-1,m}^j) \right) \quad (3.85)$$

Now solving the equation:

$$C_{i,m}^{j+1} - C_{i,m}^j = AC_{i+1,m}^{j+1} - 2AC_{i,m}^{j+1} + AC_{i-1,m}^{j+1} + AC_{i+1,m}^j - 2AC_{i,m}^j + AC_{i-1,m}^j - BC_{i+1,m}^{j+1} + BC_{i-1,m}^{j+1} - BC_{i+1,m}^j + BC_{i-1,m}^j \quad (3.86)$$

$$C_{i,m}^{j+1} + 2AC_{i,m}^{j+1} = C_{i,m}^j + AC_{i+1,m}^{j+1} + AC_{i-1,m}^{j+1} + AC_{i+1,m}^j - 2AC_{i,m}^j + AC_{i-1,m}^j - BC_{i+1,m}^{j+1} + BC_{i-1,m}^{j+1} - BC_{i+1,m}^j + BC_{i-1,m}^j \quad (3.87)$$

Now simplifying the equation:

$$C_{i,m}^{j+1}(1 + 2A) = C_{i,m}^j - 2AC_{i,m}^j + AC_{i+1,m}^{j+1} - BC_{i+1,m}^{j+1} + AC_{i-1,m}^{j+1} + BC_{i-1,m}^{j+1} + AC_{i+1,m}^j - BC_{i+1,m}^j + AC_{i-1,m}^j + BC_{i-1,m}^j \quad (3.88)$$

And when simplifying the equation further we get:

$$C_{i,m}^{j+1}(1+2A) = C_{i,m}^j(1-2A) + C_{i+1,m}^{j+1}(A-B) + C_{i-1,m}^{j+1}(A+B) + C_{i+1,m}^j(A-B) + C_{i-1,m}^j(A+B) \quad (3.89)$$

Furthermore we get:

$$\begin{aligned} \zeta_{j+1,m}e^{ibmx}(1+2A) &= \zeta_{j,m}e^{ibmx}(1-2A) + \zeta_{j+1,m}e^{ibm(x+\Delta x)}(A-B) \\ &+ \zeta_{j+1,m}e^{ibm(x-\Delta x)}(A+B) + \zeta_{j,m}e^{ibm(x+\Delta x)}(A-B) + \zeta_{j,m}e^{ibm(x-\Delta x)}(A+B) \end{aligned} \quad (3.90)$$

$$\begin{aligned} \zeta_{j+1,m}(1+2A) &= \zeta_{j,m}(1-2A) + \zeta_{j+1,m}e^{ibm\Delta x}(A-B) + \zeta_{j+1,m}e^{-ibm\Delta x}(A+B) + \\ &\zeta_{j,m}e^{ibm(\Delta x)}(A-B) + \zeta_{j,m}e^{-ibm(\Delta x)}(A+B) \end{aligned} \quad (3.91)$$

$$\begin{aligned} \zeta_{j+1,m}(1+2A) + \zeta_{j+1,m}e^{ibm\Delta x}(A-B) + \zeta_{j+1,m}e^{-ibm\Delta x}(A+B) &= \zeta_{j,m}(1-2A) + \\ &+ \zeta_{j,m}e^{ibm(\Delta x)}(A-B) + \zeta_{j,m}e^{-ibm(\Delta x)}(A+B) \end{aligned} \quad (3.92)$$

$$\begin{aligned} \zeta_{j+1,m}(1+2A) + \zeta_{j+1,m}e^{ibm\Delta x}(A-B) + \zeta_{j+1,m}e^{-ibm\Delta x}(A+B) &= \zeta_{j,m}(1-2A) + \\ &+ \zeta_{j,m}e^{ibm(\Delta x)}(A-B) + \zeta_{j,m}e^{-ibm(\Delta x)}(A+B) \end{aligned} \quad (3.93)$$

$$\left| \frac{\zeta_{j+1,m}}{\zeta_{j,m}} \right| < \left| \frac{(1-2A) + e^{ibm(\Delta x)}(A-B) + e^{-ibm(\Delta x)}(A+B)}{(1+2A) - e^{ibm\Delta x}(A-B) - e^{-ibm\Delta x}(A+B)} \right| \quad (3.94)$$

Since we know that  $e^{ibm\Delta x} = \cos(km\Delta x) + i \sin(km\Delta x)$ , therefore, the above equation become:

$$\begin{aligned} & \left| \frac{\zeta_{j+1,m}}{\zeta_{j,m}} \right| \\ & < \left| \frac{(1-2A) + (A-B)[\cos(km\Delta x) + i \sin(km\Delta x)] + (A+B)[\cos(km\Delta x) - i \sin(km\Delta x)]}{(1+2A) - (A-B)[\cos(km\Delta x) + i \sin(km\Delta x)] - (A+B)[\cos(km\Delta x) - i \sin(km\Delta x)]} \right| \end{aligned} \quad (3.95)$$

Therefore:

(3.96)

$$\left| \frac{\zeta_{j+1,m}}{\zeta_{j,m}} \right| < \left| \frac{(1 - 2A) + (A - B) [\cos(km\Delta x) + i \sin(km\Delta x)] + (A + B) [\cos(km\Delta x) - i \sin(km\Delta x)]}{(1 + 2A) - (A - B) [\cos(km\Delta x) + i \sin(km\Delta x)] - (A + B) [\cos(km\Delta x) - i \sin(km\Delta x)]} \right|$$

Then equation (3.96) becomes:

$$\left| \frac{\zeta_{j+1,m}}{\zeta_{j,m}} \right| < \left| \frac{(1 - 2A) + 2A \cos(km\Delta x) - 2Bi \sin(km\Delta x)}{(1 + 2A) - 2A \cos(km\Delta x) + 2Bi \sin(km\Delta x)} \right| \quad (3.97)$$

knowing that:

$$|a + ib| = \sqrt{a^2 + b^2} \quad (3.98)$$

Then we get:

$$\left| \frac{\zeta_{j+1,m}}{\zeta_{j,m}} \right| < \left| \frac{((1 - 2A + 2A \cos(km\Delta x))^2 + (2B \sin(km\Delta x))^2)}{((1 + 2A - 2A \cos(km\Delta x))^2 + (2B \sin(km\Delta x))^2)} \right| \quad (3.99)$$

$$\frac{(1 - 2A + 2A \cos(km\Delta x))^2 + (2B \sin(km\Delta x))^2}{(1 + 2A - 2A \cos(km\Delta x))^2 + (2B \sin(km\Delta x))^2} < 1 \quad (3.100)$$

$$\begin{aligned} & (1 - 2A + 2A \cos(km\Delta x))^2 + (2B \sin(km\Delta x))^2 \\ & < (1 + 2A - 2A \cos(km\Delta x))^2 + (2B \sin(km\Delta x))^2 \end{aligned} \quad (3.101)$$

$$4A \cos(km\Delta x) < 4A \quad (3.102)$$

$$\cos(km\Delta x) < 1 \quad (3.103)$$

Therefore we conclude that the equation is stable. The same condition is expected for fracture as variables are similar.

In this chapter we have proposed an equation to model the fate of contamination transport between soil matrix and fracture. Picard-Lindelöf theorem was used to prove the uniqueness

of the proposed system of equations for the matrix and fracture and the equation was found to be unique.

Two methods were used to conduct numerical and stability analysis. The two methods are Crank–Nicolson and von Neumann’s stability analysis method.

## 4 Introduction of fractional operators to the new equation

### 4.1 Diffusion Processes

Diffusion processes have been studied and diffusion equations have been used to model the movement of many particles in different environments or mediums. The objects or particles can be as small as basic particles in physics, bacteria, molecules, cells, or very large objects like animals, plants, or certain types of events like epidemics. Thus, diffusion processes are important in many applications in science and engineering fields (Ibe, 2013).

Of particular interest to us are diffusion processes during contamination transport in dual media or matrix-fracture contamination transport. In groundwater, molecular diffusion is defined as the concentration difference between two points, a process driven by the random Brownian movement of molecules (Appelo and Postma, 2004). The molecules diffuse away from their original source because molecules always diffuse along their concentration gradient. This means that they diffuse from where they are in high concentration to where they are in low concentration (Ibe, 2013).

The discretized diffusion equation from the previous chapter are presented in this chapter.

### 4.2 New Proposed Equations

In the previous chapter we showed that the proposed equations: equation (4.1) and (4.2) for matrix and fracture can be discretized and it was proven that the equations are stable after conducting the von Nuemann's method of analysis.

Proposed equation for the matrix:

$$(1 + \beta k_D) \frac{\partial c_m}{\partial t} = D_h \frac{\partial^2 c_m}{\partial x^2} - v_m \frac{\partial c_m}{\partial x} \quad (4.1)$$

Proposed equation for the fracture:

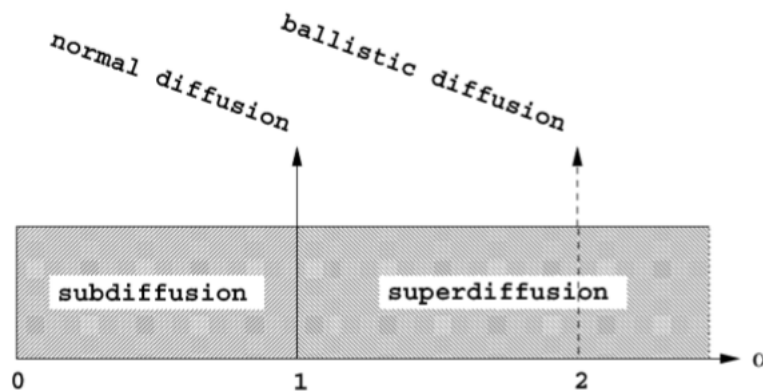
$$(1 + \beta k_D) \frac{\partial c_f}{\partial t} = D_h \frac{\partial^2 c_f}{\partial x^2} - v_m \frac{\partial c_f}{\partial x} \quad (4.2)$$

In the next section fractional differential operators are discussed and presented. Fractional differential operators are deemed to be the one of the most used mathematical tools to construct mathematical models is perhaps differential operators (Owolabi & Atangana, 2019).

### 4.3 Fractional Differential Operators

In recent decades, fractional calculus is one of the most powerful mathematical tools used to model real-world problems in many fields of science, technology and engineering (Atangana and Gómez-Aguilar 2018). Furthermore, the fractional calculus provides a suitable framework to deal with complex systems such as fracture networks (Tateishi et al., 2017). The strength of the application of fractional differentiation is that it offers the ability to describe the memory effect (Atangana and Gómez-Aguilar, 2018; Caputo, 1967).

The nature of contamination transport in the geological environments of the Earth's subsurface is often observed to be anomalous (Berkowitz and Scher 1997). Metzler and Klafter (2000) provides a detailed approach for the development and the description of a fractional dynamics approach for anomalous diffusion. Different domains or regimes of anomalous diffusion are presented in figure 4-1 below.



**Figure 4-1:** Different domains of anomalous diffusion, defined through the mean squared displacement, parameterised by the anomalous diffusion exponent  $\alpha$ : (a) sub-diffusion for  $0 < \alpha < 1$ , (b) super-diffusion for  $\alpha > 1$ . ballistic diffusion corresponds to  $\alpha = 2$ , whereas  $\alpha > 2$  corresponds to super-ballistic motion. Adapted from (Metzler and Klafter 2000 and Sandev et al. 2019).

One of the main ideas behind the use of fractional differentiation is its ability to describe the memory effect (Atangana and Gómez-Aguilar 2018).

Tateishi, et.al (2017), did a comprehensive study and analysis of the existing fractional operators and they have shown that the general diffusion equations with fractional order derivatives are efficient in describing diffusion in complex systems. It is against these basis that fractional operators are considered for the proposed Matrix-Fracture diffusion equations.

Different fractional operators which have been recently proposed are presented in the next section with their statistical properties, they include the Riemann-Liouville, Caputo-Fabrizio and Atangana-Beleanu.

Atangana and Bonyah (2019) describes the sole mathematical properties of the proposed fractional operators, the differential equations have different constant coefficients, where the differential operators can be: local (rate of change, conformable derivative, and fractal derivative), non-local with a singular kernel (Riemann-Liouville, Caputo, and modified versions), local with a non-singular kernel (Caputo-Fabrizio derivatives), and finally, non-local and non-singular (Atangana- Baleanu derivatives).

#### 4.3.1 Riemann-Liouville Power-law

The Riemann-Liouville power-law differential operator is regarded to be the only mathematical tool to replicate all physical problems. Atangana and Gómez-Aguilar (2018) in their paper argue that not all physical problems follow the power-law distribution.

Due to the fact the power law cannot be used to model all the physical problems, Caputo and Fabrizio have suggested as an alternative, the concept of differentiation using the exponential-decay as kernel instead of the power-law (Atangana and Gómez-Aguilar 2018).

Graphs presented in literature by different scholars show that the power-law kernel does not provide or present a good memory and has Non-Gaussian probability distribution characteristics (Atangana and Gómez-Aguilar, 2018; Tateishi et. al, 2017).

#### 4.3.2 Caputo-Fabrizio Exponential decay law

Caputo (1967) introduced a differential operator as an imperial formula. Some applied mathematicians suggested that the Caputo is suitable for real-world problem due to the fact that it allows usual initial conditions when playing with integral transform for instance Laplace transform (Atangana and Gómez-Aguilar 2018). The Caputo derivative is shown below in equation (4.3).

$${}^c_0D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) (t-\tau)^{-\alpha} d\tau \quad (4.3)$$

Caputo and Fabrizio (2015) presented a new definition of fractional derivative with a smooth kernel which takes on two different representations for the temporal and spatial variable. The interest for this new approach with a regular kernel was born from the prospect that there is a class of non-local systems, which have the ability to describe the material heterogeneities and the fluctuations of different scales, which cannot be well described by classical local theories or by fractional models with singular kernel. Properties of Caputo-Fabrizio fractional derivative were analysed in classical and distributional settings by (Atanacković, et. al, 2018).

The Caputo-Fabrizio derivate is shown below in equation 4.4.

$${}^{CF}D_t^\alpha f(t) = \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) \exp\left[-\frac{\alpha}{1-\alpha}(t-\tau)\right] d\tau \quad (4.4)$$

Some applications of the Caputo-Fabrizio derivative are presented in the work of Caputo and Fabrizio (2016) and Tateishi et. al, (2017).

Various researchers have shown interest on the Caputo-Fabrizio properties and investigated them with a view of extending the derivation, findings are discussed by (Baleanu, Mousalou, and Rezapour, 2018; Atanacković et al., 2018 and Alqahtani, 2016).

In previous studies it has been established that, fractional operators modify the behaviour of the waiting time distribution in the context of fractional diffusion. Caputo-Fabrizio can be related to a well-defined physical quantity (resetting rate) (Tateishi, Ribeiro, and Lenzi 2017).

Exponential kernels suggested by Caputo and Fabrizio have been applied on real world problems in various fields (Atangana and Gómez-Aguilar 2018).

Atangana and Gómez-Aguilar (2018) show in their paper after running simulation for different values of  $\alpha$  that, the memory is consistent from the beginning to the end is fading. This is an improvement by comparison to the previously discussed power-law kernel which proved to have an incomplete memory.

### 4.3.3 Mittag-Leffler-Law

Gösta Magnus Mittag-Leffler a Swedish Mathematician discovered and introduced special functions in 1903. The Mittag-Leffler function arises naturally in the solution of fractional order integral equations or fractional order differential equations, and especially in the investigations of the fractional generalization of the kinetic equation, random walks, Levy flights, super-diffusive transport and in the study of complex systems (Haubold et al., 2011). Shown below is the function which was named after Gösta Magnus Mittag-Leffler (1846–1927).

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}, \quad \alpha \in \mathbb{C}, \operatorname{Re} \alpha > 0, \quad (4.5)$$

There has been a growing interest on the application of Mittag-Leffler function in physical, biological and earth sciences including engineering disciplines (Haubold et al., 2011). The recent growing interest on this function is mainly due to its close relation to the Fractional Calculus and especially to fractional problems which come from applications (Gorenflo et al. 2014).

The Mittag-Leffler function has been applied across many disciplines, for instance: anomalous diffusion applications, biochemical transport kinetics, molecular transport, information processing in neural networks, viscoelasticity in polymer networks, heat conduction, scaling behaviour in human travel and signal processing among many others (Owolabi & Atangana, 2019).

Due to the limitation faced by the power-law, a new derivative with fractional order base on the concept of the Mittag-Leffler-law was suggested by Atangana and Baleanu (Atangana and Gómez-Aguilar 2018).

Atangana and Gómez-Aguilar (2018) show in their paper after running simulation for different values of  $\alpha$  that, the Mittag-Leffler kernel shows an exponential decay memory partially and also power-law memory. Furthermore, it proves that the Mittag-Leffler kernel has excellent memory by comparison to the previously discussed kernels and it has properties of both power-law and exponential-law.

#### 4.3.4 Atangana-Baleanu

The Mittag-Leffler kernel was used to construct the Atangana-Baleanu fractional derivative. Atangana and Baleanu introduced new fractional derivatives in Riemann–Liouville and Caputo sense.

The kernel Atangana–Baleanu fractional derivative (ABFD) shown in equation (4.6) is based on the generalized Mittag–Leffler function without singularity and locality (Atangana & Baleanu, 2016). ABFD is suitable to describe the physical and real-world phenomena. The non-singularity and non-locality of the kernel gives a better description of the memory within the structure with different scale. Furthermore, the Atangana–Baleanu operators satisfy all the mathematical principles under the scope of fractional calculus (Saqib, Khan, and Shafie 2018).

$${}^{ABC}D_t^\alpha f(t) = \frac{B(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) E_\alpha \left[ -\alpha \frac{(t-r)^\alpha}{1-\alpha} \right] d\tau \quad (4.6)$$

Saqid et al., (2018) applied the Atangana–Baleanu derivative fractional in Caputo sense to convective flow of Carboxy–Methyl–Cellulose (CMC) based Carbon nanotubes (CNT's) nanofluid in a vertical microchannel. The kernel was used in the mathematical formulation to get the time fractional governing equations subject to physical initial and boundary conditions.

Tateishi et al., (2017) when applying the Atangana–Baleanu operator, found a crossover from stretched exponential to power-law between the two diffusive regimes; a usual for smaller

times and a sub-diffusive for long times, a feature observed in several empirical systems. Furthermore, they found that the operator can be associated with a fractional diffusion equation with derivatives of distributed order.

The probability distribution of the operator crossover from Gaussian to non-Gaussian. The Atangana-Baleanu fractional derivative has proven to be helpful in the analysis of real world problems and it is favourable when using the Laplace transform to solve many physical problems with initial conditions.

#### 4.3.5 One dimensional fractional diffusion equation and associated kernels

In this section we consider the one dimensional fractional diffusive equation and the associated differential operators. The diffusion equation (4.7) below is expressed in the Riemann-Liouville sense is presented.

$$\frac{\partial}{\partial t} \rho(x, t) = D \mathcal{F}_t^\alpha \left( \frac{\partial^2}{\partial x^2} \rho(x, t) \right) \quad (4.7)$$

The fractional operator of the above equation is shown below:

$$\mathcal{F}_t^\alpha \rho(x, t) = \frac{\partial}{\partial t} \int_0^t \rho(x, t') \mathcal{K}(t - t') dt' \quad (4.8)$$

Now considering the Riemann–Liouville fractional operator. First we know that  $\mathcal{K}(t) = \delta(t)$  therefore the Riemann–Liouville kernel is:

$$\mathcal{K}(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)} \quad (4.9)$$

$$RL\mathcal{K}(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)} \quad (4.10)$$

This kernel corresponds to the Caputo-Fabrizio fractional operator in Caputo and Riemann form.

$$\mathcal{K}(t) = b \exp\left(-\frac{\alpha t}{1-\alpha}\right) \quad (4.11)$$

$$CF\mathcal{K}(t) = b \exp\left(-\frac{\alpha t}{1-\alpha}\right) \quad (4.12)$$

This kernel corresponds to the Atangana-Baleanu fractional operator, where  $E_\alpha$  is the Mittag-Leffler function.

$$\mathcal{K}(t) = b E_\alpha \left( -\frac{\alpha t^\alpha}{1-\alpha} \right) \quad (4.13)$$

The kernel shown in equation (4.14) corresponds to the Atangana and Baleanu fractional operator.

$$AB\mathcal{K}(t) = b E_{\alpha} \left( -\frac{\alpha t^{\alpha}}{1-\alpha} \right) \quad (4.14)$$

It is worth noting that the Riemann–Liouville operator has a singularity at the origin where ( $t = 0$ ), while the recently-proposed Caputo-Fabrizio and Atangana-Baleanu are non-singular operators (Tateishi et al., 2017).

## 4.4 Fractional Derivatives and Integrals

Various fractional derivatives reported in literature and applied to solve and explain the natural phenomenon are discussed in this section, and they are; Caputo, Caputo Fabrizio, Atangana-Baleanu and Fractal Fractional with power-law.

### 4.4.1 Derivatives

The derivatives of the above-mentioned equations are presented below from equation (4.15) to (4.18), they are different expressions of the fractional derivatives.

A Caputo derivative is shown in equation (4.15) below adapted from Caputo (1967).

$${}^c_0D_t^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) (t-\tau)^{-\alpha} d\tau \quad \text{Caputo derivative} \quad (4.15)$$

A Caputo-Fabrizio derivative is shown in equation 4.16 below adapted from Atanacković et al., (2018).

$${}^{CF}_0D_t^{\alpha} f(t) = \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) \exp \left[ -\frac{\alpha}{1-\alpha} (t-\tau) \right] d\tau \quad \text{Caputo-Fabrizio derivative} \quad (4.16)$$

Atangana-Baleanu derivative is shown in equation (4.17) below adapted from (Tateishi et al., 2017).

$${}^{ABC}_0D_t^{\alpha} f(t) = \frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) E_{\alpha} \left( -\frac{\alpha}{1-\alpha} (t-\tau)^{\alpha} \right) d\tau \quad \text{Atangana-Baleanu derivative} \quad (4.17)$$

Fractal Fractional derivative is shown in equation (4.18) below adapted from (Atangana, 2017).

$${}^{FFP}_0D_t^{\alpha,\beta} f(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt^{\beta}} \int_0^t f(\tau) (t-\tau)^{-\alpha} d\tau \quad \text{Fractal Fractional derivative} \quad (4.18)$$

#### 4.4.2 Integrals

There are different definitions of the fractional integro-differentials. Each of the derivatives has its advantages and limitations and the choice depends, in the main, on the purpose and area of application (Ibe, 2013). The fractional integral associated to the above listed fractional derivatives equations in section 4.4.1 are provided below.

An integral of Caputo derivative is provided:

$${}_0^C J_t^\alpha f(t) = f(0) + \frac{1}{\Gamma(\alpha)} \int_0^t f(\tau) (t - \tau)^{\alpha-1} d\tau \quad (4.19)$$

An integral of Caputo-Fabrizio derivative is provided:

$${}_0^{CF} J_t^\alpha f(t) = f(0) + \frac{1 - \alpha}{M(\alpha)} f(t) + \frac{\alpha}{M(\alpha)} \int_0^t f(\tau) d\tau \quad (4.20)$$

An integral of Atangana-Baleanu derivative is provided:

$${}_{0}^{ABC} J_t^\alpha f(t) = f(0) + \frac{1 - \alpha}{AB(\alpha)} f(t) + \frac{\alpha}{\Gamma(\alpha)AB(\alpha)} \int_0^t f(\tau) (t - \tau)^{\alpha-1} d\tau \quad (4.21)$$

An integral of Fractal Fractional derivative is provided:

$${}_{0}^{FFPC} J_t^{\alpha,\beta} f(t) = \frac{\beta}{\Gamma(\alpha)} \int_0^t \tau^{\beta-1} (t - \tau)^{\alpha-1} f(\tau) d\tau \quad (4.22)$$

#### 4.4.3 Laplace Transform

The Laplace transform function can be used to derive exact solutions of linear ordinary and partial differential equations. With the Laplace transform, it is often possible to avoid working with equations of differential order directly by translating the equation into a domain where the solution presents itself algebraically. The usual definition of the Laplace transform is defined as:

$$\mathcal{L}\{f(t)\} = \int_0^\infty e^{-st} f(t) dt = \bar{f}(s) \quad (4.23)$$

If equation (4.23) is a convergent integral, then we say that the Laplace transform of the function  $f(t)$  exists.

Applying Laplace transform to transform a function of time  $f(t)$  into a new function  $S$  in order to be able to solve the equations.

## Caputo Derivative

The Caputo derivative from equation (4.15) is brought forward and simplified.

$${}^c_0D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) (t-\tau)^{-\alpha} d\tau \quad (4.19)$$

Now re-arranging the equation, we get:

$${}^c_0D_t^\alpha f(t) = \int_0^t \frac{d}{d\tau} f(\tau) \frac{(t-\tau)^{-\alpha}}{\Gamma(1-\alpha)} d\tau \quad (4.20)$$

$${}^c_0D_t^\alpha f(t) = \frac{df(t)}{dt} * \frac{(t)^{-\alpha}}{\Gamma(1-\alpha)} \quad (4.21)$$

Now finding the Laplace transform for equation (4.21), the purpose of using the Laplace transform technique is to establish an equation we could use to find the exact analytical solution from.

$$\mathcal{L}\left({}^c_0D_t^\alpha f(t)\right) = \mathcal{L}\left(\frac{df(t)}{dt}\right) \mathcal{L}\left(\frac{t^{-\alpha}}{\Gamma(1-\alpha)}\right) \quad (4.22)$$

$$\mathcal{L}\left({}^c_0D_t^\alpha f(t)\right) = \left(S\tilde{f}(s) - f(0)\right) S^{\alpha-1} \quad (4.23)$$

then we have:

$$\mathcal{L}\left({}^c_0D_t^\alpha f(t)\right) = S^\alpha \tilde{f}(s) - S^{\alpha-1} f(0) \quad (4.24)$$

## Caputo-Fabrizio

The Caputo-Fabrizio derivative from equation (4.16) is brought forward:

$${}^{CF}_0D_t^\alpha f(t) = \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) \exp\left[-\frac{\alpha}{1-\alpha}(t-\tau)\right] d\tau \quad (4.25)$$

Now re-writing the equation, we get:

$${}^{CF}_0D_t^\alpha f(t) = \int_0^t \frac{d}{d\tau} f(\tau) \exp\left[-\frac{(t-\tau)\alpha}{1-\alpha}\right] \frac{M(\alpha)}{1-\alpha} d\tau \quad (4.26)$$

Then finally we have:

$${}^{CF}_0D_t^\alpha f(t) = \frac{d}{d(t)} f(t) \exp\left[-\frac{\alpha t}{1-\alpha}\right] \quad (4.27)$$

Now finding the Laplace transform for equation (4.27).

$$\mathcal{L}\left({}^{CF}_0D_t^\alpha f(t)\right) = \mathcal{L}\left(\frac{df(t)}{dt} \frac{M(\alpha)}{1-\alpha} \exp\left[-\frac{\alpha}{1-\alpha}t\right]\right) \quad (4.28)$$

$$\mathcal{L}\left({}^{CF}_0D_t^\alpha f(t)\right) = \mathcal{L}\left(\frac{df(t)}{dt}\right) \frac{M(\alpha)}{1-\alpha} \mathcal{L}\left(\exp\left[-\frac{\alpha}{1-\alpha}t\right]\right) \quad (4.29)$$

$$\mathcal{L}\left({}^{CF}_0D_t^\alpha f(t)\right) = [S\tilde{f}(s) - f(0)] \frac{M(\alpha)}{1-\alpha} \frac{1}{S + \frac{\alpha}{1-\alpha}} \quad (4.30)$$

Then finally we have:

$$\mathcal{L}\left({}^{CF}_0D_t^\alpha f(t)\right) = \frac{S\tilde{f}(s) - f(0)}{S + \frac{\alpha}{1-\alpha}} M(\alpha) \quad (4.31)$$

### Atangana-Baleanu

Now the Atangana-Baleanu derivative from equation (4.17) is also brought forward.

$${}^{ABC}_0D_t^\alpha f(t) = \frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) E_\alpha\left(-\frac{\alpha}{1-\alpha}(t-\tau)^\alpha\right) d\tau \quad (4.32)$$

Now re-arranging the equation, we get:

$${}^{ABC}_0D_t^\alpha f(t) = \int_0^t \frac{d}{d\tau} f(\tau) \frac{AB(\alpha)}{(1-\alpha)} E_\alpha\left(-\frac{\alpha}{1-\alpha}(t-\tau)^\alpha\right) d\tau \quad (4.33)$$

Then we have:

$${}^{ABC}_0D_t^\alpha f(t) = \frac{d}{dt} f(t) * \frac{AB(\alpha)}{(1-\alpha)} E_\alpha\left(-\frac{\alpha}{1-\alpha}t^\alpha\right) \quad (4.34)$$

Now finding the Laplace transform for equation (4.34).

$$\mathcal{L}\left({}^{ABC}_0D_t^\alpha f(t)\right) = \mathcal{L}\left(\frac{d}{dt} f(t) \frac{AB(\alpha)}{1-\alpha} E_\alpha\left[-\frac{\alpha}{1-\alpha}t^\alpha\right]\right) \quad (4.35)$$

$$\mathcal{L}\left({}^{ABC}_0D_t^\alpha f(t)\right) = \mathcal{L}\left(\frac{d}{dt} f(t) \frac{AB(\alpha)}{1-\alpha}\right) \mathcal{L}\left(E_\alpha\left[-\frac{\alpha}{1-\alpha}t^\alpha\right]\right) \quad (4.36)$$

$$\mathcal{L}\left({}^{ABC}_0D_t^\alpha f(t)\right) = [S\tilde{f}(s) - f(0)] \frac{AB(\alpha)}{1-\alpha} \frac{S^{\alpha-1}}{S^\alpha + \frac{\alpha}{1-\alpha}} \quad (4.37)$$

Then finally we have:

$$\mathcal{L}\left({}^{ABC}_0D_t^\alpha f(t)\right) = \frac{S^\alpha \tilde{f}(s) - S^{\alpha-1} f(0)}{S^\alpha + \frac{\alpha}{1-\alpha}} AB(\alpha) \quad (4.38)$$

## Fractal Fractional derivative

Now the Fractal Fractional derivative from equation (4.18) is also brought forward.

$${}^{FFP}D_t^{\alpha,\beta} f(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt^\beta} \int_0^t f(\tau) (t-\tau)^{-\alpha} d\tau \quad (4.39)$$

Now re-arranging the equation we get:

$${}^{FFP}D_t^{\alpha,\beta} f(t) = \int_0^t \frac{d}{dt^\beta} f(\tau) \frac{(t-\tau)^{-\alpha}}{\Gamma(1-\alpha)} d\tau \quad (4.40)$$

and finally we have:

$${}^{FFP}D_t^{\alpha,\beta} f(t) = \frac{d}{dt^\beta} f(t) * \frac{t^{-\alpha}}{\Gamma(1-\alpha)} \quad (4.41)$$

Now finding the Laplace transform for equation (4.41).

$$\mathcal{L}\left({}^{FFP}D_t^{\alpha,\beta} f(t)\right) = \mathcal{L}\left(\frac{d}{dt^\beta} f(t) * \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\right) \quad (4.42)$$

$$\mathcal{L}\left({}^{FFP}D_t^{\alpha,\beta} f(t)\right) = \mathcal{L}\left(\frac{d}{dt^\beta} f(t)\right) \mathcal{L}\left(\frac{t^{-\alpha}}{\Gamma(1-\alpha)}\right) \quad (4.43)$$

The Laplace Transform for the above derivative could not be found because of the fractal derivative.

### 4.4.4 Applying Laplace transform technique to the integrals

In this section we are applying the Laplace transform technique on the integrals in (4.4.2).

#### Caputo Derivative Integral

An integral of Caputo derivative is brought forward from equation (4.19).

$${}^C J_t^\alpha f(t) = f(0) + \frac{1}{\Gamma(\alpha)} \int_0^t f(\tau) (t-\tau)^{\alpha-1} d\tau \quad (4.44)$$

Now re-writing the integral we get:

$${}^C J_t^\alpha f(t) = f(0) + \int_0^t f(\tau) \frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)} d\tau \quad (4.45)$$

Then we have the following:

$${}^C J_t^\alpha f(t) = f(0) + f(t) * \frac{t^{\alpha-1}}{\Gamma(\alpha)} \quad (4.46)$$

Now applying the Laplace transform technique:

$$\mathcal{L}\left({}^C J_t^\alpha f(t)\right) = \mathcal{L}(f(0)) + \mathcal{L}(f(t)) \mathcal{L}\left(\frac{t^{\alpha-1}}{\Gamma(\alpha)}\right) \quad (4.47)$$

$$\mathcal{L}\left({}^C J_t^\alpha f(t)\right) = \frac{f(0)}{s} + \tilde{f}(s) s^{-\alpha} \quad (4.48)$$

$$\mathcal{L}\left({}^C J_t^\alpha f(t)\right) = \frac{f(0)}{s} + \frac{\tilde{f}(s)}{s^\alpha} \quad (4.49)$$

### Caputo-Fabrizio Derivative Integral

An integral of Caputo-Fabrizio derivative is brought forward from equation (4.20).

$${}^{CF}J_t^\alpha f(t) = f(0) + \frac{1-\alpha}{M(\alpha)}f(t) + \frac{\alpha}{M(\alpha)}\int_0^t f(\tau)d\tau \quad (4.50)$$

Now applying the Laplace transform technique.

$$\mathcal{L}\left({}^{CF}J_t^\alpha f(t)\right) = \mathcal{L}(f(0)) + \mathcal{L}\left(\frac{1-\alpha}{M(\alpha)}f(t)\right) + \mathcal{L}\left(\frac{\alpha}{M(\alpha)}\int_0^t f(\tau)d\tau\right) \quad (4.51)$$

Then we have:

$$\mathcal{L}\left({}^{CF}J_t^\alpha f(t)\right) = f(0) + \frac{1-\alpha}{M(\alpha)}\tilde{f}(s) + \frac{\alpha}{M(\alpha)}\frac{\tilde{f}(s)}{s} \quad (4.52)$$

### Atangana-Baleanu Derivative Integral

An integral of Atangana-Baleanu derivative is brought forward from equation (4.21).

$${}^{ABC}J_t^\alpha f(t) = f(0) + \frac{1-\alpha}{AB(\alpha)}f(t) + \frac{\alpha}{\Gamma(\alpha)AB(\alpha)}\int_0^t f(\tau)(t-\tau)^{\alpha-1}d\tau \quad (4.53)$$

Now re-writing the integral we get:

$${}^{ABC}J_t^\alpha f(t) = f(0) + \frac{1-\alpha}{AB(\alpha)}f(t) + \int_0^t f(\tau)\frac{\alpha(t-\tau)^{\alpha-1}}{\Gamma(\alpha)AB(\alpha)}d\tau \quad (4.54)$$

Now applying the Laplace transform technique to equation (4.54).

$$\mathcal{L}\left({}^{ABC}J_t^\alpha f(t)\right) = \mathcal{L}(f(0)) + \mathcal{L}\left(\frac{1-\alpha}{AB(\alpha)}f(t)\right) + \mathcal{L}\left(\int_0^t f(\tau)\frac{\alpha(t-\tau)^{\alpha-1}}{\Gamma(\alpha)AB(\alpha)}d\tau\right) \quad (4.55)$$

$$\mathcal{L}\left({}^{ABC}J_t^\alpha f(t)\right) = \frac{f(0)}{s} + \frac{1-\alpha}{AB(\alpha)}\tilde{f}(s) + \mathcal{L}(f(s))\mathcal{L}\left(\frac{\alpha(t-\tau)^{\alpha-1}}{\Gamma(\alpha)AB(\alpha)}\right) \quad (4.56)$$

Then finally we have:

$$\mathcal{L}\left({}^{ABC}J_t^\alpha f(t)\right) = \frac{f(0)}{s} + \frac{1-\alpha}{AB(\alpha)}\tilde{f}(s) + \frac{\tilde{f}(s)}{s^\alpha}\frac{\alpha}{AB(\alpha)} \quad (4.57)$$

#### 4.4.5 Numerical Approximation

Numerical approximation and discretisation of derivatives and integrals presented above in sections 4.4.1) and 4.4.2. Numerical approximation of partial differential equations is regarded as an important branch of Numerical Analysis (Quarteroni & Valli, 2008). Furthermore, Numerical approximation or schemes have been recognized as powerful mathematical tools to solve non-linear ordinary differential equations with local and non-local operators. In the main, they are normally used when all the applied analytical methods fail (Toufik and Atangana, 2017).

##### 4.4.5.1 Numerical Approximation of Derivatives

The purpose of numerical approximation is to calculate accurate approximation to the derivatives. Numerical approximation of derivatives have been applied by many scholars when solving numerical schemes and they include (Eckhoff & Wasberg, 1995; Quarteroni & Valli, 2008; Toufik and Atangana, 2017).

We start a numerical approximation and the discretisation of the **Caputo Derivative**.

$${}^c_0D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) (t-\tau)^{-\alpha} d\tau \quad (4.58)$$

Now doing partial differentiation of the equation (4.58)

$${}^c_0D_t^\alpha f(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{d\tau} f(x, \tau) (t-\tau)^{-\alpha} d\tau \quad (4.59)$$

At  $(x_i, t_{n+1})$  we present the numerical approximation as follows:

$${}^c_0D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{n+1}} \frac{d}{d\tau} f(x_i, \tau) (t_{n+1}-\tau)^{-\alpha} d\tau \quad (4.60)$$

$${}^c_0D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{n+1}} \frac{dt}{dr} (x_i, \tau) (t_{n+1}-\tau)^{-\alpha} d\tau \quad (4.61)$$

$${}^c_0D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} \frac{dt}{dr} (x_i, \tau) (t_{n+1}-\tau)^{-\alpha} d\tau \quad (4.62)$$

$${}^c_0D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} \left( \frac{f(x_i, t_{j+1}) - f(x_i, t_j)}{\Delta t} \right) (t_{n+1}-\tau)^{-\alpha} d\tau \quad (4.63)$$

$${}^c_0D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \int_{t_i}^{t_{j+1}} (t_{n+1}-\tau)^{-\alpha} d\tau \quad (4.64)$$

Now if we let  $y = t_{n+1} - \tau$ , where  $\tau = t_j$ ,  $y = t_{n+1} - t_j$

Now let us let  $\tau = t_j + 1$ ,  $y = t_{n+1} - t_{j+1}$   $dy = -d\tau$  therefore  $d\tau = -dy$

$${}_0^C D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \int_{t_i}^{t_{n+1}-t_{j+1}} y^{-\alpha} (-dy) \quad (4.65)$$

Since we know that  $-\int_a^b = \int_b^a$  and that

$$(1-\alpha)\Gamma(1-\alpha) = \Gamma(2-\alpha)$$

Since we also know that:

$$\int_{t_{n+1}-t_{j+1}}^{t_{n+1}-t_j} y^{-\alpha} = \frac{y^{1-\alpha}}{(1-\alpha)} \Big|_{t_{n+1}-t_{j+1}}^{t_{n+1}-t_j} \quad (4.66)$$

Therefore we have:

$${}_0^C D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \frac{y^{1-\alpha}}{(1-\alpha)} \Big|_{t_{n+1}-t_{j+1}}^{t_{n+1}-t_j} \quad (4.67)$$

$${}_0^C D_t^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left\{ \frac{(t_{n+1} - t_j)^{1-\alpha}}{1-\alpha} - \frac{(t_{n+1} - t_{j+1})^{1-\alpha}}{1-\alpha} \right\} \quad (4.68)$$

$$= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \{ ((n+1)\Delta t - j\Delta t)^{1-\alpha} - ((n+1)\Delta t - (j+1)\Delta t)^{1-\alpha} \} \quad (4.69)$$

Therefore the discretised derivative for Caputo is shown below:

$${}_0^C D_t^\alpha f(x_i, t_{n+1}) = \frac{(\Delta t) - \alpha}{\Gamma(1-\alpha)} \sum_{j=0}^n (f_i^{j+1} - f_i^j) \{ (n+1-\alpha)^{1-\alpha} - (n-j)^{1-\alpha} \} \quad (4.70)$$

Now we do the numerical approximation and the discretisation of **Caputo-Fabrizio Derivative**.

$${}_0^{CF} D_t^\alpha f(t) = \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) \exp \left[ -\frac{\alpha}{1-\alpha} (t-\tau) \right] d\tau \quad (4.71)$$

At  $(x_i, t_{n+1})$  we present the numerical approximation as follows:

$${}_0^{CF} D_t^\alpha f(x_i, t_{n+1}) = \frac{M(\alpha)}{(1-\alpha)} \int_0^{t_{n+1}} \frac{df(x_i, r)}{dr} \exp \left[ \frac{-\alpha(t_{n+1}-r)}{1-\alpha} \right] dr \quad (4.72)$$

$${}_0^{CF} D_t^\alpha f(x_i, t_{n+1}) = \frac{M(\alpha)}{(1-\alpha)} \int_{t_j}^{t_{j+1}} \frac{df(x_i, r)}{dr} \exp \left[ \frac{-\alpha(t_{n+1}-r)}{1-\alpha} \right] dr \quad (4.73)$$

$${}^{CF}_0 D_t^\alpha f(x_i, t_{n+1}) = \frac{M(\alpha)}{(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \int_{t_j}^{t_{j+1}} \exp\left(\frac{-\alpha(t_{n+1}-r)}{1-\alpha}\right) dr \quad (4.74)$$

$$\begin{aligned} & {}^{CF}_0 D_t^\alpha f(x_i, t_{n+1}) \\ &= \frac{M(\alpha)}{(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \int_{t_j}^{t_{j+1}} \left[ \exp\left(\frac{-\alpha(t_{n+1}-t_{j+1})}{1-\alpha}\right) \frac{1}{1-\alpha} \right. \\ & \quad \left. - \exp\left(\frac{-\alpha(t_{n+1}-t_j)}{1-\alpha}\right) \right] \end{aligned} \quad (4.75)$$

Therefore the discretised derivative for Caputo-Fabrizio is shown below:

$${}^{CF}_0 D_t^\alpha f(t) = \frac{M(\alpha)}{\alpha} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left[ \exp\left(\frac{-\alpha(n-j)\Delta t}{1-\alpha}\right) - \exp\left(\frac{-\alpha(n-j+1)\Delta t}{1-\alpha}\right) \right] \quad (4.76)$$

Now we do the numerical approximation and the discretisation of **Atangana-Baleanu Derivative**.

$${}^{ABC}_0 D_t^\alpha f(t) = \frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) E_\alpha\left(-\frac{\alpha}{1-\alpha}(t-\tau)^\alpha\right) d\tau \quad (4.77)$$

$${}^{ABC}_0 D_t^\alpha f(x, t) = \frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} f(x, r) E_\alpha\left(-\frac{\alpha(t-\tau)^\alpha}{1-\alpha}\right) d\tau \quad (4.78)$$

At  $(x_i, t_{n+1})$  we present the numerical approximation as follows:

$${}^{ABC}_0 D_t^\alpha f(t) = \frac{AB(\alpha)}{(1-\alpha)} \int_0^{t_{n+1}} \frac{d}{d\tau} f(x_i, r) E_\alpha\left(-\frac{\alpha(t_{n+1}-\tau)^\alpha}{1-\alpha}\right) d\tau \quad (4.79)$$

$${}^{ABC}_0 D_t^\alpha f(t) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \int_{t_j}^{t_{j+1}} E_\alpha\left(-\frac{\alpha(t_{n+1}-\tau)^\alpha}{1-\alpha}\right) d\tau \quad (4.80)$$

$${}^{ABC}_0 D_t^\alpha f(t) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \int_{t_j}^{t_{j+1}} \sum_{k=0}^{\infty} \frac{\left[\frac{-\alpha(t_{n+1}-\tau)^\alpha}{1-\alpha}\right]^k}{\Gamma(\alpha k + 1)} d\tau \quad (4.81)$$

$${}^{ABC}_0 D_t^\alpha f(t) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \sum_{k=0}^{\infty} \frac{\left(\frac{-\alpha}{1-\alpha}\right)^k}{\Gamma(\alpha k + 1)} \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha k} d\tau \quad (4.82)$$

$$= \frac{AB(\alpha)}{(1-\alpha)} \sum_0^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \sum_{k=0}^{\infty} \frac{\left(\frac{-\alpha}{1-\alpha}\right)^k}{\Gamma(\alpha k + 1)} (\Delta t)^{\alpha k + 1} [(n-j+1)^{\alpha k + 1} - (n-j)^{\alpha k + 1}] \quad (4.83)$$

$$= \frac{AB(\alpha)}{(1-\alpha)} \sum_0^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left[ \sum_{k=0}^{\infty} \left(\frac{-\alpha}{1-\alpha}\right)^k ((n-j+1)\Delta t)^{\alpha k + 1} - \sum_{k=0}^{\infty} \frac{\left(\frac{-\alpha}{1-\alpha}\right)^k ((n-j)\Delta t)^{\alpha k + 1}}{\Gamma(\alpha k + 2)} \right] \quad (4.84)$$

$$= \frac{AB(\alpha)}{(1-\alpha)} \sum_0^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left[ (n-j+1)\Delta t \sum_{k=0}^{\infty} \frac{\left(\frac{(-\alpha(n-j+1)\Delta t)^{\alpha}}{1-\alpha}\right)^k}{\Gamma(\alpha k + 2)} - (n-j)\Delta t \sum_{k=0}^{\infty} \frac{\left(\frac{(-\alpha(n-j)\Delta t)^{\alpha}}{1-\alpha}\right)^k}{\Gamma(\alpha k + 2)} \right] \quad (4.85)$$

$$= \frac{AB(\alpha)}{(1-\alpha)} \sum_0^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left[ (n-j+1)\Delta t E_{\alpha,2} \left[ \frac{(-\alpha(n-j+1)\Delta t)^{\alpha}}{1-\alpha} \right] - (n-j)\Delta t E_{\alpha,2} \left[ \frac{(-\alpha(n-j)\Delta t)^{\alpha}}{1-\alpha} \right] \right] \quad (4.86)$$

Therefore the discretised derivative for **Atangana-Baleanu Derivative** is shown below:

$${}^{ABC}_0 D_t^{\alpha} f(t) = \frac{AB(\alpha)}{(1-\alpha)} \sum_0^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left[ (n-j+1)\Delta t E_{\alpha,2} \left[ \frac{(-\alpha(n-j+1)\Delta t)^{\alpha}}{1-\alpha} \right] - (n-j)\Delta t E_{\alpha,2} \left[ \frac{(-\alpha(n-j)\Delta t)^{\alpha}}{1-\alpha} \right] \right] \quad (4.87)$$

In this section we have performed numerical approximation of three derivatives namely: the Caputo, Caputo-Fabrizio and Atangana-Baleanu.

In the next section we will do numerical approximation of the integral presentation in section 4.4.2 above.

#### 4.4.5.2 Numerical Approximation of Integrals

Numerical approximation of integrals is considered when analytical integration are difficult to evaluate analytically (Odibat, 2006). According to (Kumar et al., (2019) Numerical integrations for the fractional integrals also become important in developing the algorithms for solving applied problems defined using fractional derivatives.

#### Riemann–Liouville

We start the numerical approximation with **Riemann–Liouville** approach.

$$J_0^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t f(\tau)(t - \tau)^{\alpha-1} d\tau \quad (4.88)$$

$$J_0^\alpha f(x, t) = \frac{1}{\Gamma(\alpha)} \int_0^t f(x, \tau)(t - \tau)^{\alpha-1} d\tau \quad (4.89)$$

At  $(x_i, t_{n+1})$  we present the numerical approximation as follows:

$$J_0^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} f(x_i, \tau) (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.90)$$

$$J_0^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_{t_j}^{t_{j+1}} f(x_i, \tau) (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.91)$$

$$J_0^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\tau} \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.92)$$

$$J_0^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left( \frac{(t_{n+1} - \tau)^{\alpha-1+1}}{-\alpha + 1 - 1} \Big|_{t_j}^{t_{j+1}} \right) \quad (4.92)$$

$$J_0^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \left( \frac{(t_{n+1} - t_j)^\alpha}{\alpha} - \frac{(t_{n+1} - t_{j+1})^\alpha}{\alpha} \right) \quad (4.93)$$

$$J_0^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} \frac{1}{\alpha} \left( ((n - j + 1)\Delta t)^\alpha - ((n - j)\Delta t)^\alpha \right) \quad (4.94)$$

Then, finally we have:

$$J_0^\alpha f(x_i, t_{n+1}) = \frac{1}{\Gamma(\alpha + 1)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{\Delta t} (\Delta t)^\alpha ((n - j + 1)^\alpha - (n - j)^\alpha) \quad (4.95)$$

Now we do numerical approximation for the **Caputo integral**.

$${}^c J_t^\alpha f(t) = f(0) + \frac{1}{\Gamma(\alpha)} \int_0^t f(\tau) (t - \tau)^{\alpha-1} d\tau \quad (4.96)$$

At  $f(x_i, 0)$  we present the numerical approximation as follows:

$${}^c J_t^\alpha f(t) = f(x_i, 0) + \frac{1}{\Gamma(\alpha)} \int_0^t f(x_i, \tau) (t - \tau)^{\alpha-1} d\tau \quad (4.97)$$

$${}^c J_t^\alpha f(t) = f(x_i, 0) + \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} f(x_i, \tau) (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.98)$$

$${}^c J_t^\alpha f(t) = f(x_i, 0) + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \int_0^{t_{j+1}} f(x_i, \tau) (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.99)$$

$${}^c J_t^\alpha f(t) = f(x_i, 0) + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{\Delta t} \int_0^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.100)$$

$${}^c J_t^\alpha f(t) = f(x_i, 0) + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{\Delta t} \left( \frac{(t_{n+1} - t_j)^\alpha \Delta t^\alpha}{\alpha} - \frac{(t_{n+1} - t_{j+1})^\alpha \Delta t^\alpha}{\alpha} \right) \quad (4.101)$$

$$\begin{aligned} &= f(x_i, 0) + \frac{1 - \alpha}{\Gamma(\alpha + 1)} \left( \frac{f_i^{n+1} - f_i^n}{2} \right) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} - f_i^j}{2} \left[ \frac{(t_{n+1} - t_j)^\alpha}{\alpha} - \frac{(t_{n+1} - t_{j+1})^\alpha}{\alpha} \right] \end{aligned} \quad (4.102)$$

$${}^c J_t^\alpha f(t) = f(x_i, 0) + \frac{1}{\Gamma(\alpha + 1)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{\Delta t} \Delta t^\alpha ((n - j + 1)^\alpha - (n - j)^\alpha) \quad (4.103)$$

Then, finally we have:

$${}^c J_t^\alpha f(t) = f(x_i, 0) + \frac{1}{\Gamma(\alpha + 1)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{\Delta t} \Delta t^\alpha ((n - j + 1)^\alpha - (n - j)^\alpha) \quad (4.104)$$

Now we do numerical approximation for the **Caputo-Fabrizio integral**.

$${}^{CF}J_t^\alpha f(t) = f(0) + \frac{1-\alpha}{M(\alpha)} f(t) + \frac{\alpha}{M(\alpha)} \int_0^t f(\tau) d\tau \quad (4.105)$$

At  $(x_i, t_{n+1})$  we present the numerical approximation as follows:

$${}^{CF}J_t^\alpha f(t) = f(x_i, 0) + \frac{1-\alpha}{M(\alpha)} f(x_i, t_{n+1}) + \frac{\alpha}{M(\alpha)} \int_0^t f(x_i, t_{n+1}) dt \quad (4.106)$$

$${}^{CF}J_t^\alpha f(t) = f(x_i, 0) + \frac{1-\alpha}{M(\alpha)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) + \frac{\alpha}{M(\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} f(x_i, t_{n+1}) dt \quad (4.107)$$

$${}^{CF}J_t^\alpha f(t) = f(x_i, 0) + \frac{1-\alpha}{M(\alpha)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) + \frac{\alpha}{M(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{2} (t|_{t_j}^{t_{j+1}}) \quad (4.108)$$

$${}^{CF}J_t^\alpha f(t) = f(x_i, 0) + \frac{1-\alpha}{M(\alpha)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) + \frac{\alpha}{M(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{2} (t_{j+1} - t_j) \quad (4.109)$$

Then, finally we have:

$${}^{CF}J_t^\alpha f(t) = f(x_i, 0) + \frac{1-\alpha}{M(\alpha)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) + \frac{\alpha}{M(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{2} (\Delta t) \quad (4.110)$$

Now we do numerical approximation for the **Atangana-Baleanu integral**

$${}^{ABC}J_t^\alpha f(t) = f(0) + \frac{1-\alpha}{AB(\alpha)} f(t) + \frac{\alpha}{\Gamma(\alpha)AB(\alpha)} \int_0^t f(\tau) (t-\tau)^{\alpha-1} d\tau \quad (4.111)$$

At  $(x_i, t_{n+1})$  we present the numerical approximation as follows:

$$\begin{aligned} {}^{ABC}J_t^\alpha f(x, t) &= f(x_i, 0) + \frac{1-\alpha}{\Gamma(\alpha+1)} f(x_i, t_{n+1}) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^{t_{n+1}} f(x_i, \tau) (t_{n+1} - \tau)^{\alpha-1} d\tau \end{aligned} \quad (4.112)$$

$$\begin{aligned} {}^{ABC}J_t^\alpha f(x, t) &= f(x_i, 0) + \frac{1-\alpha}{\Gamma(\alpha+1)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{2} \int_0^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} d\tau \end{aligned} \quad (4.113)$$

$$\begin{aligned}
{}^{ABC}J_t^\alpha f(x, t) &= f(x_i, 0) + \frac{1 - \alpha}{\Gamma(\alpha + 1)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) \\
&+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{2\alpha} \left[ (t_{n+1} - t_i)^\alpha \Delta t^\alpha - (t_{n+1} - t_{j+1})^\alpha \Delta t^\alpha \right]
\end{aligned} \tag{4.114}$$

$$\begin{aligned}
{}^{ABC}J_t^\alpha f(x, t) &= f(x_i, 0) + \frac{1 - \alpha}{\Gamma(\alpha + 1)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) \\
&+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{2\alpha} \Delta t^\alpha [(n - j + 1)^\alpha - (n - j)^\alpha]
\end{aligned} \tag{4.115}$$

Then, finally we have:

$$\begin{aligned}
{}^{ABC}J_t^\alpha f(x, t) &= f(x_i, 0) + \frac{1 - \alpha}{\Gamma(\alpha + 1)} \left( \frac{f_i^{n+1} + f_i^n}{2} \right) \\
&+ \frac{1}{AB(\alpha)\Gamma(\alpha)} \sum_{j=0}^n \frac{f_i^{j+1} + f_i^j}{2} \Delta t^\alpha [(n - j + 1)^\alpha - (n - j)^\alpha]
\end{aligned} \tag{4.116}$$

#### 4.4.5.3 Lagrange Approximation

In this section we consider numerical approximation scheme that combines the fundamental theorem of fractional calculus and the two-step Lagrange polynomial, this has been observed from the works of Mekkaoui and Atangana, (2017). The Lagrange method in previous studies has proven to be beneficial in terms of being computationally less complex, yet comparable in accuracy (Yeh & Kwan, 1978).

Using Lagrange approximation method on the following equation expressed in Caputo sense.

$${}^C D_t^\alpha f(x, t) = F(f(x, t), t) \tag{4.117}$$

and using Riemann–Liouville we obtain:

$$f(x, t) = f(x, 0) + \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} F(f(x, \tau), \tau) d\tau \tag{4.118}$$

At  $(x_i, t_{n+1})$  we present the numerical approximation as follows:

$$f_i^{n+1} - f_i^0 = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \tau)^{\alpha-1} F(f(x_i, \tau), \tau) d\tau \tag{4.119}$$

$$f_i^{n+1} - f_i^0 = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} F(f(x_i, \tau), \tau) d\tau \tag{4.120}$$

Then  $[t_j, t_{j+1}]$

$$P_j(\tau) = \frac{\tau - t_j}{t_j - t_{j-1}} F(f_i^j, t_j) + \frac{\tau - t_{j-1}}{t_{j-1} - t_j} F(f_i^{j-1}, t_{j-1}) \quad (4.121)$$

$$f_i^{n+1} - f_i^0 = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} \left[ \frac{\tau - t_j}{t_j - t_{j-1}} F(f_i^j, t_j) + \frac{\tau - t_{j-1}}{t_{j-1} - t_j} F(f_i^{j-1}, t_{j-1}) \right] d\tau \quad (4.122)$$

$$= \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \left[ \frac{F(f_i^j, t_j)}{t_i - t_{j-1}} \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} (\tau - t_s) d\tau + F\left(\frac{f_i^{j-1}, \tau}{t_{j-1} - t_j}\right) \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} (\tau - t_{j-1}) d\tau \right] \quad (4.123)$$

Therefore we have:

$$f_i^{n+1} - f_i^0 = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{F(f_i^j, t_j)}{\Delta t} \frac{(\Delta t)^{\alpha+1}}{\alpha} \left[ -(n-j)^\alpha - \frac{(n-j)^{\alpha+1}}{\alpha+1} + \frac{(n-j+1)^{\alpha+1}}{\alpha+1} \right] + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \frac{F(f_i^{j-1}, t_{j-1})}{(-\Delta t)} \frac{(\Delta t)^{\alpha+1}}{\alpha} \left[ -(n-j-1)^\alpha - \frac{(n-j-1)^{\alpha+1}}{\alpha+1} \right] \quad (4.124)$$

$$f_i^{n+1} - f_i^0 = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \left[ F(f_i^j, t_j) (\Delta t)^\alpha \left( -(n-j)^\alpha - \frac{(n-j)^{\alpha+1}}{\alpha+1} + \frac{(n-j+1)^{\alpha+1}}{\alpha+1} \right) - F(f_i^{j-1}, t_{j-1}) (\Delta t)^\alpha \left( -(n-j-1)^\alpha - \frac{(n-j-1)^{\alpha+1}}{\alpha+1} + \frac{(n-j)^{\alpha+1}}{\alpha+1} \right) \right] \quad (4.125)$$

$$f_i^{n+1} = f_i^0 + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \left[ \frac{\Delta t^\alpha F(f_i^j, t_j)}{\Gamma(\alpha+2)} \left( (n-j+1)^\alpha (n-j+2+\alpha) - (n-j)^\alpha (n-j+2+2\alpha) - \frac{\Delta t^\alpha F(f_{i-1}^j, t_{j-1})}{\Gamma(\alpha+2)} \left( (n+1-j)^{\alpha+1} - (n-j)^\alpha (n-j+1+\alpha) \right) \right) \right] \quad (4.126)$$

#### 4.5 Model with power-law process

In this section we discretised the proposed diffusion equation considering the power-law function. Power-law process has been applied to different fractional advection-dispersion equations before, by different researchers (Benson et al., 2000; Tateishi et al., 2017). It is believed that processes such as Brownian motion are driven by power-law process, in diffusion process we consider power-law memory kernel.

Detailed analysis of the diffusion equation is considered where the process of power law is applied. The time derivative is converted to a fractional derivative whereby the derivative is the Caputo.

Below we recall and present the diffusion equation in the matrix.

$$(1 + \beta k_D) \frac{\partial C_m}{\partial t} = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (4.127)$$

We also present the Caputo derivative:

$${}_0^c D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) (t-\tau)^{-\alpha} d\tau \quad (4.128)$$

Then the numerical approximation of the above is presented below:

$$(1 + \beta k_D) \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) (t-\tau)^{-\alpha} d\tau = D_h(x) \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (4.129)$$

$$(1 + \beta k_D) \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) (t-\tau)^{-\alpha} d\tau = D_h(x) \frac{\partial^2 C_{m(x,t)}}{\partial x^2} - v_m \frac{\partial C_{m(x,t)}}{\partial x} \quad (4.130)$$

$$\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) (t-\tau)^{-\alpha} d\tau = \frac{1}{1 + \beta k_D} \left[ D_h(x) \frac{\partial^2 C_{m(x,t)}}{\partial x^2} - v_m \frac{\partial C_{m(x,t)}}{\partial x} \right] \quad (4.131)$$

For simplicity we let  $\frac{1}{1 + \beta k_D} \left[ D_h(x) \frac{\partial^2 C_{m(x,t)}}{\partial x^2} - v_m \frac{\partial C_{m(x,t)}}{\partial x} \right]$  to be equal to  $F(x, t, C_m(x, t))$

Then we have:

$$\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) (t-\tau)^{-\alpha} d\tau = F(x, t, C_m(x, t)) \quad (4.132)$$

Now applying the **Riemann–Liouville** integral we obtain the following:

$$C_m(x, t) - C_m(x, 0) = \frac{1}{\Gamma(\alpha)} \int_0^t F(x, \tau, C_m(x, \tau)) (t-\tau)^{\alpha-1} d\tau \quad (4.133)$$

Then at  $t = t_n$ , we have  $t_n = \Delta t n$ ,  $x_i = i\Delta x$ , thus at  $t_{n+1}$  we discretise.

$$C_m(x_i, t_{n+1}) - C_m(x_i, 0) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} F(x_i, \tau, C_m(x_i, \tau)) (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.134)$$

Now

$$C_{m,i}^{n+1} - C_{m,i}^0 = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} F(x_i, \tau, C_m(x_i, \tau)) (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.135)$$

We approximate  $F(x_i, \tau, C_m(x_i, \tau)) = P_j(\tau)$  at  $[t_{j-1}, t_{j+1}]$

$$P_j(\tau) = \frac{\tau - t_{j-1}}{t_j - t_{j-1}} F(x_i, t_j, C_{m,i}^j) + \frac{\tau - t_j}{t_{j-1} - t_j} F(x_i, t_{j-1}, C_{m,i}^{j-1}) \quad (4.136)$$

Thus :

$$C_{m,i}^{n+1} - C_{m,i}^0 = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} \left[ \frac{\tau - t_{j-1}}{\Delta t} F(x_i, t_j, C_{m,i}^j) - \frac{\tau - t_j}{\Delta t} F(x_i, t_{j-1}, C_{m,i}^{j-1}) \right] (t_{n+1} - \tau)^{\alpha-1} d\tau \quad (4.137)$$

Now using the integral routine presented above, we obtain the following:

$$\begin{aligned} C_{m,i}^{n+1} - C_{m,i}^0 = & \sum_{j=0}^n \left[ \frac{(\Delta t)^\alpha}{\Gamma(\alpha + 2)} F(x_i, t_j, C_{m,i}^j) \{ (n+1-j)^\alpha (n-j+2+\alpha) \right. \\ & - (n-j)^\alpha (n-j+2+2\alpha) \} \\ & - \frac{(\Delta t)^\alpha}{\Gamma(\alpha + 2)} F(x_i, t_{j-1}, C_{m,i}^{j-1}) \{ (n+2-j)^{\alpha+1} \\ & \left. - (n-j)^\alpha (n-j+1+\alpha) \} \right] \end{aligned} \quad (4.138)$$

However, we know that we have the following:

$$F(x_i, t_j, C_{m,i}^j) = \frac{1}{1 + \beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j}{\Delta x^2} - v_m \frac{C_{m,i+1}^j - C_{m,i-1}^j}{2\Delta x} \right] \quad (4.139)$$

$$F(x_i, t_j, C_{m,i}^{j-1}) = \frac{1}{1 + \beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1}}{\Delta x^2} - v_m \frac{C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1}}{2\Delta x} \right] \quad (4.140)$$

Then substituting the above two equations into equation (4.138) we get:

$$\begin{aligned}
C_{m,i}^{n+1} - C_{m,i}^0 &= \sum_{j=0}^n \frac{(\Delta t)^\alpha}{\Gamma(\alpha + 2)} \left\{ \frac{1}{1 + \beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j}{\Delta x^2} \right. \right. \\
&\quad \left. \left. - v_m \frac{C_{m,i+1}^j - C_{m,i-1}^j}{2\Delta x} \right] \right\} \{ (n-j+1)^\alpha (n-j+2+\alpha) \\
&\quad - (n-j+2+2\alpha)(n-j)^\alpha \} \\
&\quad - \frac{(\Delta t)^\alpha}{\Gamma(\alpha + 2)} \left\{ \frac{1}{1 + \beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1}}{\Delta x^2} \right. \right. \\
&\quad \left. \left. - v_m \frac{C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1}}{2\Delta x} \right] \right\} \{ (n-j+1)^{\alpha+1} - (n-j)^\alpha (n-j+1+\alpha) \}
\end{aligned} \tag{4.141}$$

Below we then present the stability analysis of the above numerical scheme, to achieve this, we consider  $C_{m,i}^j$  to be the exact solution of the equation and  $\overline{C_{m,i}^j}$  the approximate solution.

Thus :

$$\epsilon_{m,i}^j = C_{m,i}^j - \overline{C_{m,i}^j} \text{ the error} \tag{4.142}$$

Applying Fourier transform, we know that:

$$\epsilon_{m,i}^j = \delta_j e^{ik_e x}, \quad \epsilon_{m,i-1}^{j-1} = \delta_j e^{ik_e(x-\Delta x)} \tag{4.143}$$

$$\epsilon_{m,i+1}^{j+1} = \delta_{j+1} e^{ik_e(x+\Delta x)}, \quad \epsilon_{m,i+1}^{j+1} = \delta_{j+1} e^{ik_e(x-\Delta x)} \tag{4.144}$$

Then for simplicity we let:

$$\delta_{n,j}^\alpha = (n-j+1)^\alpha (n-j+2+\alpha) - (n-j+2+2\alpha)(n-j)^\alpha \tag{4.145}$$

and

$$\delta_{n,j-1}^\alpha = (n-j+1)^{\alpha+1} - (n-j)^\alpha (n-j+\alpha+1) \tag{4.146}$$

and

$$A_i = \frac{D_h(x_i)(\Delta t)^\alpha}{(1 + \beta k_D)\Delta x^2 \Gamma(\alpha + 2)} \tag{4.147}$$

$$B_i = \frac{-v_m \Delta t^\alpha}{2(1 + \beta k_D)\Delta x \Gamma(\alpha + 2)} \tag{4.148}$$

Then substituting the above we have:

$$\begin{aligned}
C_{m,i}^{j+1} - C_{m,i}^0 &= \sum_{j=0}^n \left[ A_i (C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j) + B_i \frac{(C_{m,i+1}^j - C_{m,i-1}^j)}{2\Delta x} \right] \delta_{n,j}^\alpha \\
&\quad - \sum_{j=0}^n \left[ A_i (C_{m,j+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1}) + B_i (C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1}) \right] \delta_{n,j-1}^\alpha
\end{aligned} \tag{4.149}$$

Now introducing an error, we have:

$$\begin{aligned}
& \delta_{n+1}e^{ik_e(x)} - \delta_0e^{ik_ex} \\
&= \sum_{j=0}^n [A_i(\delta_j e^{ik_e(x+\Delta x)} - 2\delta_j e^{ik_ex} + \delta_j e^{ik_e(x-\Delta x)}) \\
&+ B_i(\delta_j e^{ik_e(x+\Delta x)} - \delta_j e^{ik_e(x-\Delta x)})] \delta_{n,j}^\alpha \\
&- \sum_{j=0}^n [A_i(\delta_{j-1} e^{ik_e(x+\Delta x)} - 2\delta_{j-1} e^{ik_ex} + \delta_{j-1} e^{ik_e(x-\Delta x)}) \\
&+ B_i(\delta_{j-1} e^{ik_e(x+\Delta x)} - \delta_{j-1} e^{ik_e(x-\Delta x)})] \delta_{n,j-1}^\alpha
\end{aligned} \tag{4.150}$$

$$\begin{aligned}
\delta_{n+1} - \delta_0 &= \sum_{j=0}^n [A_i(\delta_j e^{ik_e\Delta x} - 2\delta_j + \delta_j e^{-ik_e\Delta x}) + B_i(\delta_j e^{ik_e\Delta x} - \delta_j e^{-ik_e\Delta x})] \delta_{n,j}^\alpha \\
&- \sum_{j=0}^n [A_i(\delta_{j-1} e^{ik_e\Delta x} - 2\delta_{j-1} + \delta_{j-1} e^{-ik_e\Delta x}) \\
&+ B_i(\delta_{j-1} e^{ik_e\Delta x} - \delta_{j-1} e^{-ik_e\Delta x})] \delta_{n,j-1}^\alpha
\end{aligned} \tag{4.151}$$

We know that:

$$e^{ik_e\Delta x} - 2 + e^{-ik_e\Delta x} = -4\text{Sin}^2\left[\frac{k_e\Delta x}{2}\right] \tag{4.152}$$

Thus, we have:

$$\begin{aligned}
\delta_{n+1} - \delta_0 &= \sum_{j=0}^n A_i \left[ -4\text{Sin}^2\left(\frac{k_e\Delta x}{2}\right) + B_i(2i\text{Sin}^2(k_e\Delta x)) \right] \delta_{n,j}^\alpha \delta_j \\
&- \sum_{j=0}^n \left[ -4\text{Sin}^2\left(\frac{k_e\Delta x}{s}\right) A_i + B_i\text{Sin}(k_e\Delta x) \right] \delta_{n,j}^\alpha \delta_{j-1}
\end{aligned} \tag{4.153}$$

The above can be reformulated as:

$$\begin{aligned}
\delta_{n+1} - \delta_0 &= \sum_{j=0}^{n-1} \left[ -4A_i\text{Sin}^2\left(\frac{k_e\Delta x}{2}\right) + 2iB_i\text{Sin}(k_e\Delta x) \right] \delta_{n,j}^\alpha \delta_j \\
&- \left[ -4A_i\text{Sin}^2\left(\frac{k_e\Delta x}{2}\right) + 2iB_i\text{Sin}(k_e\Delta x) \right] \delta_{n,j}^\alpha \delta_n \\
&+ \sum_{j=0}^{n-1} \left[ -4A_i\text{Sin}^2\left(\frac{k_e\Delta x}{2}\right) + 2iB_i\text{Sin}(k_e\Delta x) \right] \delta_{n,j-1}^\alpha \delta_j \\
&+ \left[ -4A_i\text{Sin}^2\left(\frac{k_e\Delta x}{2}\right) + 2i\text{Sin}(k_e\Delta x) \right] \delta_n^\alpha \delta_{n-1}
\end{aligned} \tag{4.154}$$

We prove the stability by introducing “n”, thus when h=0 we have:

$$\delta_1 - \delta_0 = \left[ -4A_i \sin^2 \left( \frac{k_e \Delta x}{2} \right) + 2iB_i \sin(k_e \Delta x) \right] \delta_{0,0}^\alpha \quad (4.155)$$

Therefore, we have:

$$\frac{\delta_1}{\delta_0} = \left[ 1 - 4A_i \sin^2 \left( \frac{k_e \Delta x}{2} \right) + 2iB_i \sin(k_e \Delta x) \right] \delta_{0,0}^\alpha \quad (4.156)$$

$$\left| \frac{\delta_1}{\delta_0} \right| = \delta_{0,0}^\alpha \sqrt{\left( 1 - 4A_i \sin^2 \left( \frac{k_e \Delta x}{2} \right) \right)^2 + 4B_i^2 \sin^2(k_e \Delta x)} \quad (4.157)$$

#### 4.6 Model with Caputo-Fabrizio

The Caputo-Fabrizio derivate has been applied to solve groundwater flow, free convection flow, fluid dynamics problem and advection diffusion problems (Atangana & Alkahtani, 2015; Ali et al., 2016).

Tateishi et al., (2017) in their study showed us that the Caputo-Fabrizio operator is characterised by the following: the waiting time distribution is deemed to be exponential and it recovers a diffusive process with stochastic resetting, the fractional order exponent is related to the resetting rate.

Again we bring forward the diffusion equation:

$$(1 + \beta k_D) \frac{\partial c_m}{\partial t} = D_h \frac{\partial^2 c_m}{\partial x^2} - v_m \frac{\partial c_m}{\partial x} \quad (4.158)$$

The Caputo-Fabrizio derivative is as follows:

$${}^{CF}D_t^\alpha f(t) = \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) \exp \left[ -\frac{\alpha}{1-\alpha} (t-\tau) \right] d\tau \quad (4.159)$$

Now introducing the derivative to the derived equation for matrix:

$$(1 + \beta k_D) \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) \exp \left[ -\frac{\alpha}{1-\alpha} (t-\tau) \right] d\tau = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \quad (4.160)$$

$$\begin{aligned}
(1 + \beta k_D) \frac{M(\alpha)}{(1 - \alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) \exp \left[ -\frac{\alpha}{1 - \alpha} (t - \tau) \right] d\tau \\
= D_h \frac{\partial^2 C_m(x, t)}{\partial x^2} - v_m \frac{\partial C_m(x, t)}{\partial x}
\end{aligned} \tag{4.161}$$

Now dividing with  $(1 + \beta k_D)$  we get:

$$\begin{aligned}
\frac{M(\alpha)}{(1 - \alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) \exp \left[ -\frac{\alpha}{1 - \alpha} (t - \tau) \right] d\tau \\
= \frac{1}{1 + \beta k_D} \left[ D_h \frac{\partial^2 C_m(x, t)}{\partial x^2} - v_m \frac{\partial C_m(x, t)}{\partial x} \right]
\end{aligned} \tag{4.162}$$

To simplify the equation we let  $\frac{1}{1 + \beta k_D} \left[ D_h \frac{\partial^2 C_m(x, t)}{\partial x^2} - v_m \frac{\partial C_m(x, t)}{\partial x} \right] = F(x, t, C_m(x, t))$

Therefore we can represent the above equation as the following:

$$\frac{M(\alpha)}{(1 - \alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) \exp \left[ -\frac{\alpha}{1 - \alpha} (t - \tau) \right] d\tau = F(x, t, C_m(x, t)) \tag{4.163}$$

$$\frac{M(\alpha)}{(1 - \alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) \exp \left[ -\frac{\alpha}{1 - \alpha} (t - \tau) \right] d\tau = F(x, t, C_m(x, t)) \tag{4.164}$$

We apply the associate integral to obtain the following:

$$C_m(x, t) - C_m(x, 0) = \frac{1 - \alpha}{M(\alpha)} F(x, t, C_m(x, t)) + \frac{\alpha}{M(\alpha)} \int_0^t F(x, \tau, C_m(x, \tau)) d\tau \tag{4.165}$$

Now at  $(x_i, t_{n+1})$  we have:

$$\begin{aligned}
C_m(x_i, t_{n+1}) - C_m(x_i, 0) \\
= \frac{1 - \alpha}{M(\alpha)} F(x_i, t_n, C_m(x_i, t_n)) + \frac{\alpha}{M(\alpha)} \int_0^{t_{n+1}} F(x_i, \tau, C_m(x_i, \tau)) d\tau
\end{aligned} \tag{4.166}$$

And at  $(x_i, t_n)$  we have:

$$\begin{aligned}
C_m(x_i, t_n) - C_m(x_i, 0) \\
= \frac{1 - \alpha}{M(\alpha)} F(x_i, t_{n-1}, C_m(x_i, t_{n-1})) + \frac{\alpha}{M(\alpha)} \int_0^{t_n} F(x_i, \tau, C_m(x_i, \tau)) d\tau
\end{aligned} \tag{4.167}$$

Then equation (4.166) minus equation (4.167) then we get:

$$\begin{aligned}
& C_m(x_i, t_{n+1}) - C_m(x_i, t_n) \\
&= \frac{1-\alpha}{M(\alpha)} \left[ F\left(x_i, t_n, C_m(x_i, t_n) - F(x_i, t_{n-1}, C_m(x_i, t_{n-1}))\right) \right. \\
&+ \frac{\alpha}{M(\alpha)} \int_0^{t_{n+1}} F(x_i, \alpha, \tau, C_m(x_i, \tau)) d\tau \\
&\left. - \frac{\alpha}{M(\alpha)} \int_0^{t_n} F(x_i, \tau, C_m(x_i, \tau)) d\tau \right] \tag{4.168}
\end{aligned}$$

Since we know that:

$$\int_a^b f(x)dx + \int_b^c f(x)dx = \int_a^c f(x)dx \tag{4.169}$$

Then we apply the above principle onto the following:

$$\begin{aligned}
& C_m(x_i, t_{n+1}) - C_m(x_i, t_n) \\
&= \frac{1-\alpha}{M(\alpha)} [F(x_i, t_n, C_m(x_i, t_n)) - F(x_i, t_{n-1}, C_m(x_i, t_{n-1}))] \\
&+ \frac{\alpha}{M(\alpha)} \int_{t_n}^{t_{n+1}} F(x_i, \tau, C_m(x_i, \tau)) d\tau \tag{4.170}
\end{aligned}$$

Therefore within  $[t_n, t_{n+1}]$  we approximate the function  $F(x_i, \tau, C_m(x_i, \tau))$  using Lagrange approximation.

$$F(x_i, \tau, C_m(x_i, \tau)) = P_i(\tau) \tag{4.171}$$

Then we obtain:

$$P_i(\tau) = \frac{\tau - t_{n-1}}{t_n - t_{n-1}} [F(x_i, t_n, C_m(x_i, t_n))] + \frac{\tau - t_n}{t_{n-1} - t_n} [F(x_i, t_{n-1}, C_m(x_i, t_{n-1}))] \tag{4.172}$$

Then we have:

$$\begin{aligned}
& C_m(x_i, t_{n+1}) - C_m(x_i, t_n) \\
&= \frac{1-\alpha}{M(\alpha)} [F(x_i, t_n, C_m(x_i, t_n)) - F(x_i, t_{n-1}, C_m(x_i, t_{n-1}))] \\
&+ \frac{\alpha}{M(\alpha)} \int_{t_n}^{t_{n+1}} P_i(\alpha) d\tau \tag{4.173}
\end{aligned}$$

Further we obtain:

$$\begin{aligned}
& C_m(x_i, t_{n+1}) - C_m(x_i, t_n) \\
&= \frac{1-\alpha}{M(\alpha)} [F(x_i, t_n, C_m(x_i, t_n)) - F(x_i, t_{n-1}, C_m(x_i, t_{n-1}))] \\
&+ \frac{\alpha}{M(\alpha)} \int_{t_n}^{t_{n+1}} \left[ \frac{\tau - t_{n-1}}{t_n - t_{n-1}} F(x_i, t_n, C_m(x_i, t_n)) d\tau \right]
\end{aligned} \tag{4.174}$$

Finally after integrating we obtain:

$$\begin{aligned}
& C_m(x_i, t_{n+1}) - C_m(x_i, t_n) \\
&= \frac{1-\alpha}{M(\alpha)} [F(x_i, t_n, C_m(x_i, t_n)) - F(x_i, t_{n-1}, C_m(x_i, t_{n-1}))] \\
&+ \frac{\alpha}{M(\alpha)} \left[ \frac{3}{2} \Delta t F(x_i, t_n, C_m(x_i, t_n)) - \frac{\Delta t}{2} F(x_i, t_{n-1}, C_m(x_i, t_{n-1})) \right]
\end{aligned} \tag{4.175}$$

#### 4.7 Model with Atangana-Baleanu

The Atangana-Baleanu fractional operator has been applied in different research areas as it is found to be suitable to model real world problems when compared to other existing fractional operators. By and large, this fractional operator has been applied in different fields include electronic circuits exhibiting chaotic behaviour, flow dynamics (convection and channel flow), the spread of diseases (Ebola virus and tuberculosis) (Abro et al., 2018; Alkahtani, 2016; Altaf Khan et al., 2018; Koca, 2018; Saqib et al., 2018).

The Atangana-Baleanu operator can be associated with a fractional diffusion equation with derivatives of distributed order. Furthermore, this operator has a crossover from stretched exponent to power-law when considering waiting time distribution and it captures the memory effects better (Tateishi et al., 2017).

The Atangana-Baleanu fractional operator is also considered on the equation below:

$$(1 + \beta k_D) \frac{\partial C_m}{\partial t} = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \tag{4.176}$$

The Atangana-Baleanu derivative is as follows:

$${}^{ABC}D_t^\alpha f(t) = \frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) E_\alpha \left( -\frac{\alpha}{1-\alpha} (t-\tau)^\alpha \right) d\tau \tag{4.177}$$

Now introducing the derivative to the derived equation for matrix:

$$(1 + \beta k_D) \frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau) E_\alpha \left( -\frac{\alpha}{1-\alpha} (t-\tau)^\alpha \right) d\tau = D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \tag{4.178}$$

Now dividing by the retardation factor  $(1 + \beta k_D)$  on both sides we get:

$$\frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) E_\alpha \left( -\frac{\alpha}{1-\alpha} (t-\tau)^\alpha \right) d\tau = \frac{1}{1+\beta k_D} \left[ D_h \frac{\partial^2 C_m}{\partial x^2} - v_m \frac{\partial C_m}{\partial x} \right] \quad (4.179)$$

To simplify the equation we let  $\frac{1}{1+\beta k_D} \left[ D_h \frac{\partial^2 C_m(x,t)}{\partial x^2} - v_m \frac{\partial C_m(x,t)}{\partial x} \right] = F(x, t, C_m(x, t))$

Therefore we can represent equation (4.179) as :

$$\frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{\partial}{\partial \tau} C_m(x, \tau) E_\alpha \left( -\frac{\alpha}{1-\alpha} (t-\tau)^\alpha \right) d\tau = F(x, t, C_m(x, t)) \quad (4.180)$$

We then apply an integral on both sides to obtain :

$$\begin{aligned} & C_m(x, t) - C_m(x_i, 0) \\ &= \frac{1-\alpha}{AB(\alpha)} F(x, t, C_m(x, t)) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} F(x, \tau, C_m(x, \tau)) d\tau \end{aligned} \quad (4.181)$$

At  $(x_i, t_{n+1})$  we have the following:

$$\begin{aligned} & C_m(x_i, t_{n+1}) - C_m(x_i, 0) \\ &= \frac{1-\alpha}{AB(\alpha)} F(x_i, t_n, C_m(x_i, t_n)) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} F(x_i, \tau, C_m(x_i, \tau)) d\tau \end{aligned} \quad (4.182)$$

Then we represent the equation as:

$$\begin{aligned} & C_m(x_i, t_{n+1}) - C_m(x_i, 0) \\ &= \frac{1-\alpha}{AB(\alpha)} F(x_i, t_n, C_m(x_i, t_n)) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} (t_{n+1}-\tau)^{\alpha-1} F(x_i, \tau, C_m(x_i, \tau)) d\tau \end{aligned} \quad (4.183)$$

Within the  $[t_j, t_{j+1}]$  interval, we approximate the function  $F(x_i, \tau, C_m(x_i, \tau))$  to a polynomial  $P_j(\tau)$ .

$$F(x_i, \tau, C_m(x_i, \tau)) = P_j(\tau) \quad (4.184)$$

Then we use the well-known Lagrange polynomial.

$$P_j(\tau) = \frac{\tau - t_{j-1}}{t_j - t_{j-1}} F(x_i, t_j, C_m(x_i, t_j)) + \frac{\tau - t_j}{t_{j-1} - t_j} F(x_i, t_{j-1}, C_m(x_i, t_{j-1})) \quad (4.185)$$

Replacing  $P_j(\tau)$  in the general equation we get:

$$\begin{aligned} & C_m(x_i, t_{n+1}) - C_m(x_i, 0) \\ &= \frac{1 - \alpha}{AB(\alpha)} F(x_i, t_n, C_m(x_i, t_n)) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=0}^n \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} \left[ \frac{\tau - t_{j-1}}{t_j - t_{j-1}} F(x_i, t_j, C_m(x_i, t_j)) \right. \\ &\left. + \frac{\tau - t_j}{t_{j-1} - t_j} F(x_i, t_{j-1}, C_m(x_i, t_{j-1})) \right] d\tau \end{aligned} \quad (4.186)$$

Now after integration, we obtain the following approximated solution.

$$\begin{aligned} & C_m(x_i, t_{n+1}) - C_m(x_i, 0) \\ &= \frac{1 - \alpha}{AB(\alpha)} F(x_i, t_n, C_m(x_i, t_n)) \\ &+ \frac{\alpha}{AB(\alpha)} \sum_{j=0}^n \left( \frac{(\Delta t)^2 F(x_i, t_j, C_m(x_i, t_j))}{\Gamma(\alpha + 2)} \right) \{ (n - j + 1)^\alpha (n - j + 2 \\ &- \alpha) - (n - j)^\alpha (n - j + 2 + 2\alpha) \} \\ &- \frac{(\Delta t)^\alpha}{\Gamma(\alpha + 2)} F(x_i, t_{j-1}, C_m(x_i, t_{j-1})) \{ (n - j + 1)^{\alpha+1} \\ &- (n - j)^\alpha (n - j + \alpha + 1) \} \end{aligned} \quad (4.187)$$

where :

$$\begin{aligned} & F(x_i, t_j, C_m(x_i, t_j)) \\ &= \frac{1}{1 + \beta k_d} \left[ D_h(x_i) \frac{C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j}{(\Delta x)^2} \right. \\ &- v_m(x_i) \frac{C_{m,i+1}^j - C_{m,i-1}^j}{2\Delta x} \left. \right] F(x_i, t_{j-1}, C_m(x_i, t_{j-1})) \\ &= \frac{1}{1 + \beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1}}{(\Delta x)^2} \right. \\ &- v_m(x_i) \frac{C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1}}{2\Delta x} \left. \right] \end{aligned} \quad (4.188)$$

Now replacing  $F(x_i, t_j, C_m(x_i, t_j))$  with equation (4.187) above we get:

$$\begin{aligned}
& C_{m,i}^{n+1} - C_{m,i}^0 \\
= & \frac{1-\alpha}{AB(\alpha)} \frac{1}{1+\beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^n - 2C_{m,i}^n + C_{m,i-1}^n}{(\Delta x)^2} - v_m(x_i) \frac{C_{m,i+1}^{n-1} - C_{m,i-1}^{n-1}}{2\Delta x} \right] \\
+ & \frac{\alpha}{AB(\alpha)} \sum_{j=0}^n \left( \frac{(\Delta t)^2 \frac{1}{1+\beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j}{(\Delta x)^2} - v_m(x_i) \frac{C_{m,i+1}^j - C_{m,i-1}^j}{2\Delta x} \right]}{\Gamma(\alpha+2)} \right) \{(n \\
- & j+1)^\alpha (n-j+2+\alpha) - (n-j)^\alpha (n-j+2+2\alpha)\} \\
- & \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \frac{1}{1+\beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1}}{(\Delta x)^2} \right. \\
- & \left. v_m(x_i) \frac{C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1}}{2\Delta x} \right] \{(n-j+1)^{\alpha+1} - (n-j)^\alpha (n-j+\alpha+1)\}
\end{aligned} \tag{4.189}$$

$$\begin{aligned}
& C_{m,i}^{n+1} - C_{m,i}^0 \\
= & \frac{1-\alpha}{AB(\alpha)} \frac{1}{1+\beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^n - 2C_{m,i}^n + C_{m,i-1}^n}{(\Delta x)^2} - v_m(x_i) \frac{C_{m,i+1}^{n-1} - C_{m,i-1}^{n-1}}{2\Delta x} \right] \\
+ & \frac{\alpha}{AB(\alpha)} \sum_{j=0}^n \left( \frac{(\Delta t)^2 \frac{1}{1+\beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j}{(\Delta x)^2} - v_m(x_i) \frac{C_{m,i+1}^j - C_{m,i-1}^j}{2\Delta x} \right]}{\Gamma(\alpha+2)} \right) \{(n \\
- & j+1)^\alpha (n-j+2+\alpha) - (n-j)^\alpha (n-j+2+2\alpha)\} \\
- & \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \frac{1}{1+\beta k_D} \left[ D_h(x_i) \frac{C_{m,i+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1}}{(\Delta x)^2} \right. \\
- & \left. v_m(x_i) \frac{C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1}}{2\Delta x} \right] \{(n-j+1)^{\alpha+1} - (n-j)^\alpha (n-j+\alpha+1)\}
\end{aligned} \tag{4.190}$$

Now we let :

$$\frac{1-\alpha}{AB(\alpha)} \frac{1}{(1+\beta k_D)} \frac{1}{(\Delta x)^2} = a_1 \tag{4.191}$$

and

$$\frac{1-\alpha}{AB(\alpha)} \frac{1}{(1+\beta k_D)} \frac{1}{2\Delta x} = a_2 \tag{4.192}$$

and

$$\frac{\alpha}{AB(\alpha)} \frac{(\Delta t)^2}{(1 + \beta k_D)} \frac{1}{\Gamma(\alpha + 2)} \frac{1}{(\Delta x)^2} \{(n - j + 1)^\alpha (n - j + 2 + \alpha) - (n - j)^\alpha (n - j + 2 + 2\alpha)\} = \delta_{n,\alpha}^j \quad (4.193)$$

and

$$\frac{\alpha}{AB(\alpha)} \frac{(\Delta t)^2}{(1 + \beta k_D)} \frac{1}{\Gamma(\alpha + 2)} \frac{1}{2\Delta x} \{(n - j + 1)^\alpha (n - j + 2 + \alpha) - (n - j)^\alpha (n - j + 2 + 2\alpha)\} = \delta_{n,\alpha}^{j,1} \quad (4.194)$$

and

$$\frac{(\Delta t)^\alpha}{\Gamma(\alpha + 2)} \frac{1}{(1 + \beta k_D)} \frac{1}{(\Delta x)^2} \{(n - j + 1)^{\alpha+1} - (n - j)^\alpha (n - j + \alpha + 1)\} = \delta_{n,\alpha}^{j,2} \quad (4.195)$$

and

$$\frac{(\Delta t)^\alpha}{\Gamma(\alpha + 2)} \frac{1}{(1 + \beta k_D)} \frac{1}{2\Delta x} \{(n - j + 1)^{\alpha+1} - (n - j)^\alpha (n - j + \alpha + 1)\} = \delta_{n,\alpha}^{j,3} \quad (4.196)$$

Now therefore, finally we get a simplified version of the equation:

$$\begin{aligned} C_{m,i}^{n+1} - C_{m,i}^0 &= D_h(x_i)(C_{m,i+1}^n - 2C_{m,i}^n + C_{m,i-1}^n)a_1 - v_m(x_i)(C_{m,i+1}^{n-1} - C_{m,i-1}^{n-1})a_2 \\ &+ \sum_{j=0}^n [D_h(x_i)(C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j)\delta_{n,\alpha}^j \\ &- v_m(x_i)(C_{m,i+1}^j - C_{m,i-1}^j)\delta_{n,\alpha}^{j,1}] \\ &- D_h(x_i)(C_{m,i+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1})\delta_{n,\alpha}^{j,2} \\ &- v_m(x_i)(C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1})\delta_{n,\alpha}^{j,3} \end{aligned} \quad (4.197)$$

Now doing stability for the above equation:

$$\begin{aligned} C_{m,i}^{n+1} - C_{m,i}^0 &= D_h(x_i)(C_{m,i+1}^n - 2C_{m,i}^n + C_{m,i-1}^n)a_1 - v_m(x_i)(C_{m,i+1}^{n-1} - C_{m,i-1}^{n-1})a_2 \\ &+ \sum_{j=0}^n [D_h(x_i)(C_{m,i+1}^j - 2C_{m,i}^j + C_{m,i-1}^j)\delta_{n,\alpha}^j \\ &- v_m(x_i)(C_{m,i+1}^j - C_{m,i-1}^j)\delta_{n,\alpha}^{j,1}] \\ &- D_h(x_i)(C_{m,i+1}^{j-1} - 2C_{m,i}^{j-1} + C_{m,i-1}^{j-1})\delta_{n,\alpha}^{j,2} \\ &- v_m(x_i)(C_{m,i+1}^{j-1} - C_{m,i-1}^{j-1})\delta_{n,\alpha}^{j,3} \end{aligned} \quad (4.198)$$

Now  $C_{m,i}^{n+1} - C_{m,i}^0$  replacing with and we get  $\delta_{n+1}e^{ik_m(x)} - \delta_0e^{ik_m(x)}$

then:

$$\begin{aligned}
& \delta_{n+1}e^{ik_m(x)} - \delta_0e^{ik_m(x)} \\
&= D_h(x_i)(\delta_n e^{ik_m(x+\Delta x)} - 2\delta_n e^{ik_m(x)} + \delta_n e^{ik_m(x-\Delta x)})a_1 \\
&- v_m(x_i)(\delta_{n-1} e^{ik_m(x+\Delta x)} - \delta_{n-1} e^{ik_m(x-\Delta x)})a_2 \\
&+ \sum_{j=0}^n [D_h(x_i)(\delta_j e^{ik_m(x+\Delta x)} - 2\delta_j e^{ik_m(x)} + \delta_j e^{ik_m(x-\Delta x)})\delta_{n,\alpha}^j \\
&- v_m(x_i)(\delta_j e^{ik_m(x+\Delta x)} - \delta_j e^{ik_m(x-\Delta x)})\delta_{n,\alpha}^{j,1}] \\
&- D_h(x_i)(\delta_{j-1} e^{ik_m(x+\Delta x)} - 2\delta_{j-1} e^{ik_m(x)} + \delta_{j-1} e^{ik_m(x-\Delta x)})\delta_{n,\alpha}^{j,2} \\
&- v_m(x_i)(\delta_{j-1} e^{ik_m(x+\Delta x)} - \delta_{j-1} e^{ik_m(x-\Delta x)})\delta_{n,\alpha}^{j,3}
\end{aligned} \tag{4.199}$$

Then we have :

$$\begin{aligned}
& e^{ik_m(x)}(\delta_{n+1} - \delta_0) \\
&= D_h(x_i)(\delta_n(e^{ik_m(x)}e^{ik_m(\Delta x)}) - 2\delta_n e^{ik_m(x)} \\
&+ (\delta_n(e^{ik_m(x)}e^{ik_m(-\Delta x)})))a_1 \\
&- v_m(x_i)(\delta_{n-1}(e^{ik_m(x)}e^{ik_m(\Delta x)}) - (\delta_{n-1}(e^{ik_m(x)}e^{ik_m(-\Delta x)})))a_2 \\
&+ \sum_{j=0}^n [D_h(x_i)(\delta_j(e^{ik_m(x)}e^{ik_m(\Delta x)}) - 2\delta_j e^{ik_m(x)} \\
&+ (\delta_j(e^{ik_m(x)}e^{ik_m(-\Delta x)})))\delta_{n,\alpha}^j \\
&- v_m(x_i)(\delta_j(e^{ik_m(x)}e^{ik_m(\Delta x)}) - \delta_j(e^{ik_m(x)}e^{ik_m(-\Delta x)}))\delta_{n,\alpha}^{j,1}] \\
&- D_h(x_i)(\delta_{j-1}(e^{ik_m(x)}e^{ik_m(\Delta x)}) - 2\delta_{j-1}e^{ik_m(x)} \\
&+ \delta_{j-1}(e^{ik_m(x)}e^{ik_m(-\Delta x)}))\delta_{n,\alpha}^{j,2} - v_m(x_i)(\delta_{j-1}(e^{ik_m(x)}e^{ik_m(\Delta x)}) \\
&- \delta_{j-1}(e^{ik_m(x)}e^{ik_m(-\Delta x)}))\delta_{n,\alpha}^{j,3}
\end{aligned} \tag{4.200}$$

Then we have :

$$\begin{aligned}
(\delta_{n+1} - \delta_0) &= D_h(x_i)(\delta_n e^{ik_m(\Delta x)} - 2\delta_n + \delta_n e^{ik_m(-\Delta x)})a_1 \\
&- v_m(x_i) \left( \delta_{n-1} e^{ik_m(\Delta x)} - \delta_{n-1} (e^{ik_m(-\Delta x)}) \right) a_2 \\
&+ \sum_{j=0}^n \left[ D_h(x_i) (\delta_j e^{ik_m(\Delta x)} - 2\delta_j + \delta_j (e^{ik_m(-\Delta x)})) \delta_{n,\alpha}^j \right. \\
&- v_m(x_i) (\delta_j e^{ik_m(\Delta x)} - \delta_j e^{ik_m(-\Delta x)}) \delta_{n,\alpha}^{j,1} \\
&- D_h(x_i) (\delta_{j-1} e^{ik_m(\Delta x)} - 2\delta_{j-1} + \delta_{j-1} e^{ik_m(-\Delta x)}) \delta_{n,\alpha}^{j,2} \\
&\left. - v_m(x_i) (\delta_{j-1} (e^{ik_m(\Delta x)}) - \delta_{j-1} (e^{ik_m(-\Delta x)})) \delta_{n,\alpha}^{j,3} \right]
\end{aligned} \tag{4.201}$$

Now simplifying the equation further, we get :

$$\begin{aligned}
(\delta_{n+1} - \delta_0) &= D_h(x_i)(\delta_n (e^{ik_m(\Delta x)} - 2 + e^{ik_m(-\Delta x)}))a_1 \\
&- v_m(x_i) \left( \delta_{n-1} (e^{ik_m(\Delta x)} - e^{ik_m(-\Delta x)}) \right) a_2 \\
&+ \sum_{j=0}^n \left[ D_h(x_i) \left( \delta_j (e^{ik_m(\Delta x)} - 2 + e^{ik_m(-\Delta x)}) \right) \delta_{n,\alpha}^j \right. \\
&- v_m(x_i) \left( \delta_j (e^{ik_m(\Delta x)} - e^{ik_m(-\Delta x)}) \right) \delta_{n,\alpha}^{j,1} \\
&- D_h(x_i) \left( \delta_{j-1} (e^{ik_m(\Delta x)} - 2 + e^{ik_m(-\Delta x)}) \right) \delta_{n,\alpha}^{j,2} \\
&\left. - v_m(x_i) \left( \delta_{j-1} (e^{ik_m(\Delta x)} - e^{ik_m(-\Delta x)}) \right) \delta_{n,\alpha}^{j,3} \right]
\end{aligned} \tag{4.202}$$

Now we let :

$$k_m(\Delta x) = \theta \tag{4.203}$$

And we let :

$$-k_m(\Delta x) = -\theta \tag{4.204}$$

Therefore when replacing with  $\theta$  and  $-\theta$  we get the following equation :

$$\begin{aligned}
(\delta_{n+1} - \delta_0) &= D_h(x_i)(\delta_n (e^{i\theta} - 2 + e^{-i\theta}))a_1 - v_m(x_i) \left( \delta_{n-1} (e^{i\theta} - e^{-i\theta}) \right) a_2 \\
&+ \sum_{j=0}^n \left[ D_h(x_i) \left( \delta_j (e^{i\theta} - 2 + e^{-i\theta}) \right) \delta_{n,\alpha}^j \right. \\
&- v_m(x_i) \left( \delta_j (e^{i\theta} - e^{-i\theta}) \right) \delta_{n,\alpha}^{j,1} \\
&- D_h(x_i) \left( \delta_{j-1} (e^{i\theta} - 2 + e^{-i\theta}) \right) \delta_{n,\alpha}^{j,2} \\
&\left. - v_m(x_i) \left( \delta_{j-1} (e^{i\theta} - e^{-i\theta}) \right) \delta_{n,\alpha}^{j,3} \right]
\end{aligned} \tag{4.205}$$

Then we know that :

$$e^{i\theta} + e^{-i\theta} = 2\cos\theta \quad (4.206)$$

and, that :

$$e^{i\theta} - e^{-i\theta} = 2i\sin\theta \quad (4.207)$$

Then equation (4.205) becomes :

$$\begin{aligned} (\delta_{n+1} - \delta_0) &= D_h(x_i)(\delta_n(2\cos\theta - 2))a_1 - v_m(x_i)(\delta_{n-1}(2i\sin\theta))a_2 \\ &+ \sum_{j=0}^n \left[ D_h(x_i) \left( \delta_j(2\cos\theta - 2) \right) \delta_{n,\alpha}^j - v_m(x_i) \left( \delta_j(2i\sin\theta) \right) \delta_{n,\alpha}^{j,1} \right. \\ &\left. - D_h(x_i) \left( \delta_{j-1}(2\cos\theta - 2) \right) \delta_{n,\alpha}^{j,2} - v_m(x_i) \left( \delta_{j-1}(2i\sin\theta) \right) \delta_{n,\alpha}^{j,3} \right] \end{aligned} \quad (4.208)$$

$$\begin{aligned} \delta_{n+1} &= \delta_0 + 4D_h(x_i)\sin^2\left(\frac{\theta}{2}\right) * a_1\delta_n - 2i\sin\theta \int_{n-1} v_m(x_i)a_2 \\ &+ \sum_{j=0}^n \left[ -D_h(x_i) * 4\sin^2\left(\frac{\theta}{2}\right) * \delta_{n,\alpha}^j + 4D_h(x_i) * \delta_{j-1}\sin^2\left(\frac{\theta}{2}\right) * \delta_{n,\alpha}^{j,2} \right. \\ &\left. - v_m(x_i)\delta_{j-1}2i\sin\theta * \delta_{n,\alpha}^{j,3} \right] \end{aligned} \quad (4.209)$$

When  $h=0$ , we have :

$$\delta_1 = \delta_0 - 4D_h(x_i)\sin^2\left(\frac{\theta}{2}\right) * a_1\delta_0 \quad (4.210)$$

We want to show that :

$$\left| \frac{\delta_1}{\delta_0} \right| < 1 \quad (4.211)$$

Then :

$$|\delta_1| = |\delta_0| \left| 1 - 4D_h(x_i)\sin^2\left(\frac{\theta}{2}\right) * a_1 \right| \quad (4.212)$$

$$\left| \frac{\delta_1}{\delta_0} \right| < 1 \text{ imply that } \left| 1 - 4D_h(x_i)\sin^2\left(\frac{\theta}{2}\right) * a_1 \right| < 1 \quad (4.213)$$

$$\left| 1 - 4D_h(x_i)\sin^2\left(\frac{\theta}{2}\right) * a_1 \right| < 1 \text{ for all values of } m \text{ are equal to } k_m\Delta x \quad (4.214)$$

$$|1 - 4D_h(x_i)a_i| < 1 \quad (4.215)$$

$$|1 - 4D_h(x_i)a_i| = \begin{cases} -1 + 4D_h(x_i)a_1 - 2 < 1 - 4D_h(x) * a_1 < 1 \\ -1 + 4D_h(x_i)a_1 - 2 < -4D_h(x_i) * a_1 < 0 \end{cases} \quad (4.216)$$

That means that:

$$4D_h(x_i)a_i < 2 \quad (4.217)$$

$$D_h(x_i)a_i < \frac{1}{2} \quad (4.218)$$

$$D_h(x_i) < \frac{1}{2a_1} \quad (4.219)$$

This we consider to satisfy the 1<sup>st</sup> condition.

Therefore we have:

$$\left| \frac{\delta_1}{\delta_0} \right| < 1 \Rightarrow D_h(x_i) < \frac{1}{2}a_1 \quad (4.220)$$

We assume that for all values of  $h > 1$  and therefore:

$$\left| \frac{\delta_h}{\delta_0} \right| < 1 \text{ we want to show that } \left| \frac{\delta_{n+1}}{\delta_0} \right| < 1 \quad (4.221)$$

However,

$$\begin{aligned} |\delta_{n+1}| = & \left| \delta_0 - 4D_h(x_i)\text{Sin}^2\left(\frac{\theta}{2}\right)a_1\delta_n - 2i\text{Sin}\theta * \delta_{n-1} * v_m(x_1)a_2 \right. \\ & + \sum_{j=0}^n \left[ -D_h(x_i) * 4\text{Sin}^2\left(\frac{\theta}{2}\right)\delta_{n,\alpha}^j + 4D_h(x_i) * \delta_{j-1}\text{Sin}^2\left(\frac{\theta}{2}\right)\delta_{n,\alpha}^{j,2} \right. \\ & \left. \left. - 4v_m(x_i)\delta_{j-1} * \text{Sin}\theta * \delta_{n,\alpha}^{j,3} \right] \right| \quad (4.222) \end{aligned}$$

$$\begin{aligned} |\delta_{n+1}| = & \left\| \left[ \delta_0 - 4D_h(x_i)\text{Sin}^2\left(\frac{\theta}{2}\right) * a_1 * \delta_n + \sum_{j=0}^n \left( -4\text{Sin}^2\left(\frac{\theta}{2}\right)\delta_{n,\alpha}^j D_h(x_i)\delta_n \right) \right. \right. \\ & \left. \left. + i \left( -2\text{Sin}\theta\delta_{n-1}v_m(x_i)a_2 + \sum_{j=0}^n -2v_m(x_i)\delta_{j-1}\text{Sin}\theta * \delta_{n,\alpha}^{j,3} \right) \right] \right\| \quad (4.223) \end{aligned}$$

$$\begin{aligned}
|\delta_{n+1}| < \left| |\delta_0| - 4D_h(x_i) \text{Sin}^2\left(\frac{\theta}{2}\right) * a_1 |\delta_n| + \sum_{j=0}^n \left( -4 \text{Sin}^2\left(\frac{\theta}{2}\right) \delta_{n,\alpha}^j D_h(x_i) \right) |\delta_j| \right. \\
\left. + i \left( 2 \text{Sin}\theta * v_m(x_i) a_2 |\delta_{n-1}| + \sum_{j=0}^n -2v_m(x_i) * \text{Sin}\theta * \delta_{n,2}^{j,3} |\delta_{j-1}| \right) \right| \quad (4.224)
\end{aligned}$$

By introduction of hypothesis:

$$|\delta_{n+1}| < |\delta_0| \left\| \left[ 1 - 4D_h(x_i) + i \left( 2 \text{Sin}\theta * v_m(x_i) * a_2 + \sum_{j=0}^n (-2v_m(x_i) \text{Sin}\theta * \delta_{n,2}^{j,3}) \right) \right] \right\| \quad (4.225)$$

see the final equations

Then we have:

$$\left| \frac{\delta_{n+1}}{\delta_0} \right| < 1 \Rightarrow \sqrt{\left( \left( 1 - 4D_h(x_i) \sin^2 \left( \frac{\theta}{2} \right) a_2 + \sum_{j=0}^n \left( -4 \sin^2 \left( \frac{\theta}{2} \right) \delta_{n,j}^i D_h(x_i) \right) \right)^2 + \left( 2 \sin \theta v_n(x_i) a_2 + \sum_{j=0}^n (-2v_m(x_i) \sin \theta * \delta_{n,2}^{j,3}) \right)^2 \right)} < 1 \quad (4.226)$$

The numerical scheme will be stable if :

$$\text{Min} \left\{ D_h(x_i) < \frac{1}{2a_2}, \sqrt{\left( \left( 1 - 4D_h(x_i) \sin^2 \left( \frac{\theta}{2} \right) a_2 + \sum_{j=0}^n \left( -4 \sin^2 \left( \frac{\theta}{2} \right) \delta_{n,j}^i D_h(x_i) \right) \right)^2 + \left( 2 \sin \theta v_n(x_i) a_2 + \sum_{j=0}^n (-2v_m(x_i) \sin \theta * \delta_{n,2}^{j,3}) \right)^2 \right)} < 1 \right\} \quad (4.227)$$

## 5 Simulations with the Classical Differentiation

In this section we present the results of simulations obtained when using the classical differentiation to explain diffusion-advection processes as the solute is transported over time and space.

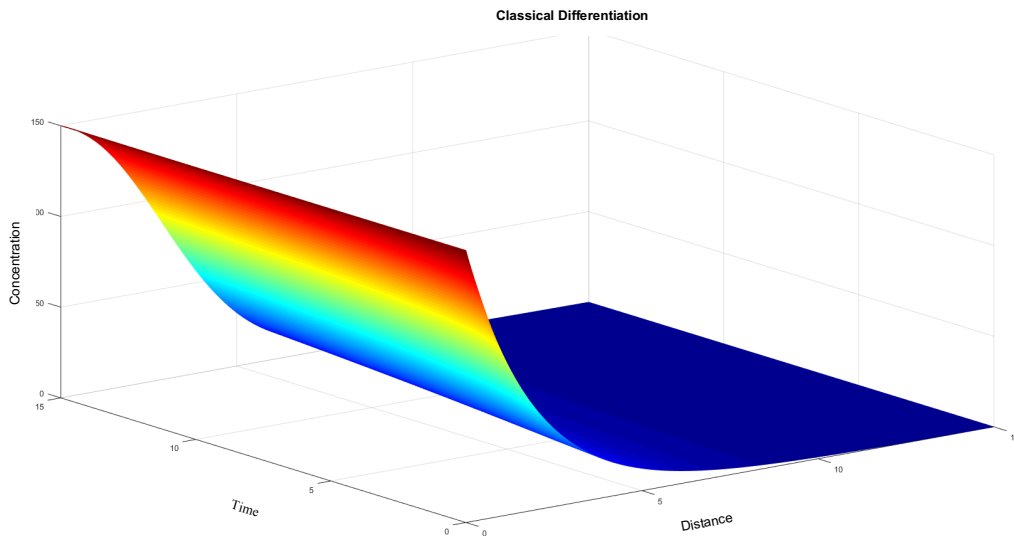
The community of academics and practitioners in science, engineering and other disciplines have assumed that the advection velocity ( $v_m$ ) is constant so as the advection flux of the solute, in this section we demonstrate that the advection velocity is not constant and show that its impact on concentration gradient over space.

Furthermore, in this section we discuss that the fractional operators introduced to the diffusion-advection equation offer great level of efficiency in describing diffusion and advection in complex systems and that the advection velocity ( $v_m$ ) varies over space, therefore we conclude to say that the advection velocity is space depended.

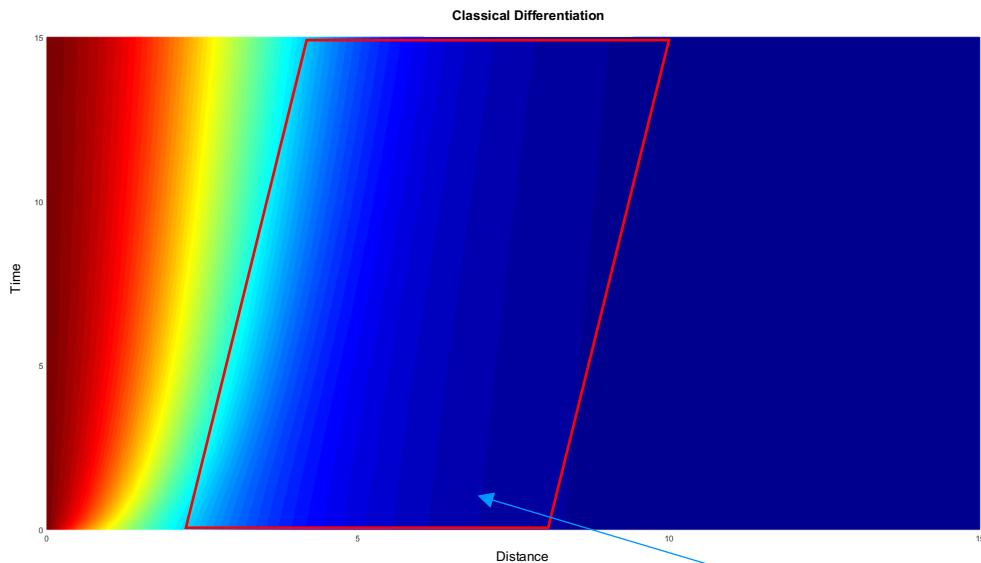
### 5.1 Simulation with the Classical Diffusion Equation

#### 5.1.1 First Scenario for the Classical Differentiation Model

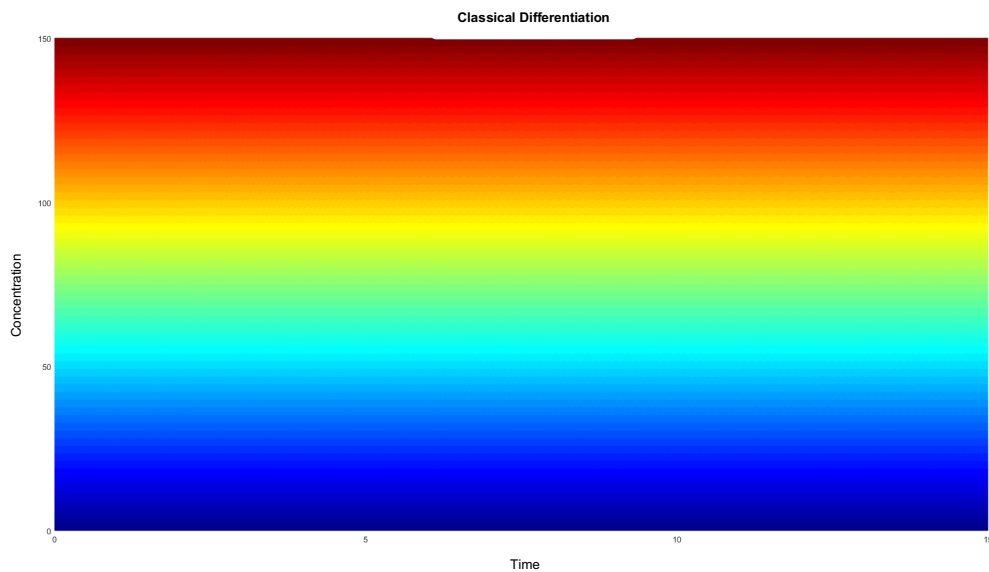
The presentation of the first classical differential model for diffusion-advection is shown in figures below. Shown on the figure 5-1 below it can be observed that the concentration-time distribution over space is distinctively characterised by exponential and power-law behaviour.



**Figure 5-1:** Concentration versus time over a distance where the initial concentration ( $C_0 = 150$ ) and time is ( $T_{max} = 15$ ), a time step of ( $\Delta t = 0,01$ ) and distance assumed at ( $X_{max} = 15$ ). Other variables assumed include the following  $K_D = 0,15$ ;  $\lambda = 0,5$  and where  $v_m(x) = e^{-x}$ ; and  $D_h(x) = \frac{1}{1+x}$



**Figure 5-2:** Showing concentration decay over time and space-domain, the cross-over behaviour between the initial concentration is observed on the above figure. We can easily see the impact of advection velocity and the corresponding concentration depletion in the domain. The salient parameters for this simulation are the initial concentration ( $C_0 = 150$ ) and time is ( $T_{max} = 15$ ), a time step of ( $\Delta t = 0,01$ ) and distance assumed at ( $X_{max} = 15$ ).



**Figure 5-3:** Showing concentration decay over time in the space domain.

In figure 5-3, we observe that the concentration depletion is also a function of time in the domain space, however the driver of the processes, in the main, is the advection velocity.

In the above model we have been able to show that the advection velocity ( $v_m$ ) is not constant and so is as the advection flux (solute) as it has been shown above that it is space depended.

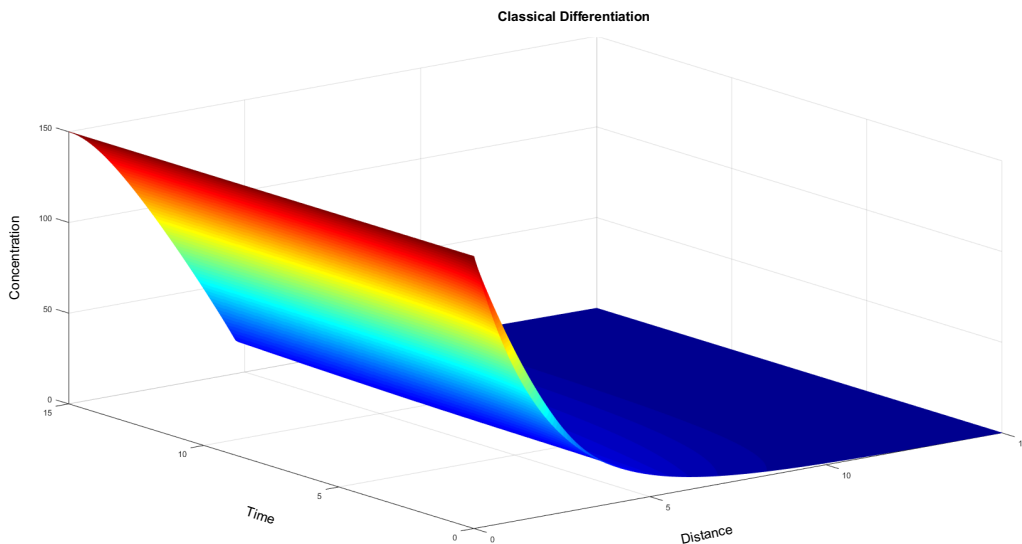
### 5.1.2 Second Scenario for the Classical Differentiation Model

The presentation of the second classical differential model for diffusion-advection is shown in figures below. The assumptions made for the second classical differentiation model are presented in Table 5-1.

**Table 5-1:** Assumptions made for the second model

Variables assumed for the second scenario		
$\Delta x = 0,01$	$\Delta t = 0,01$	$T_{max} = 15$
$X_{max} = 15$	$C_0 = 150$	$K_D = 0,15$
$D_{h(x)} = \sin(x + 1)$	$\lambda = 0,5$	$v_{m(x)} = 2e^{(-x)}$

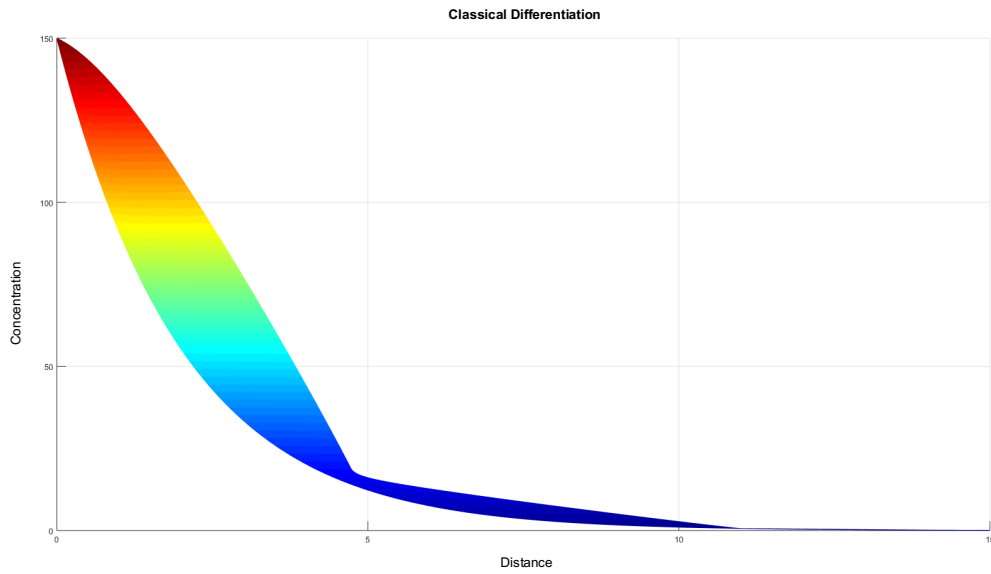
In this section we provide the sine-series representation of the diffusion-advection model with an increase of the advection-velocity by a factor of 2. The impact of the changed variables on the concentration flux is also demonstrated.



**Figure 5-4:** Concentration versus time over a distance where the initial concentration ( $C_0 = 150$ ) and time is ( $T_{max} = 15$ ), a time step of ( $\Delta t = 0,01$ ) and distance assumed at ( $X_{max} = 15$ ). Other variables assumed include the following  $K_D = 0,15$ ;  $\lambda = 0,5$ ;  $D_{h(x)} = \sin(x)$  and where  $v_{m(x)} = e^{(-x)}$ .

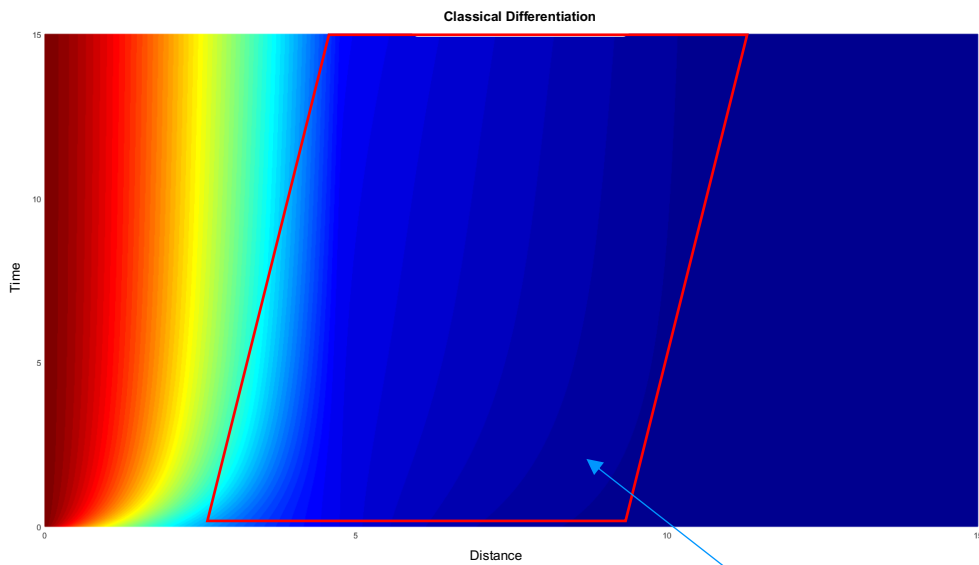
In figure 5-4 again we observed that the concentration-time distribution over space is distinctively characterised by exponential and power-law behaviour.

However in Figure 5-5 we further clearly observe the change in concentration and the impact of the variable advection velocity in space, furthermore, that advection velocity is a function of space.

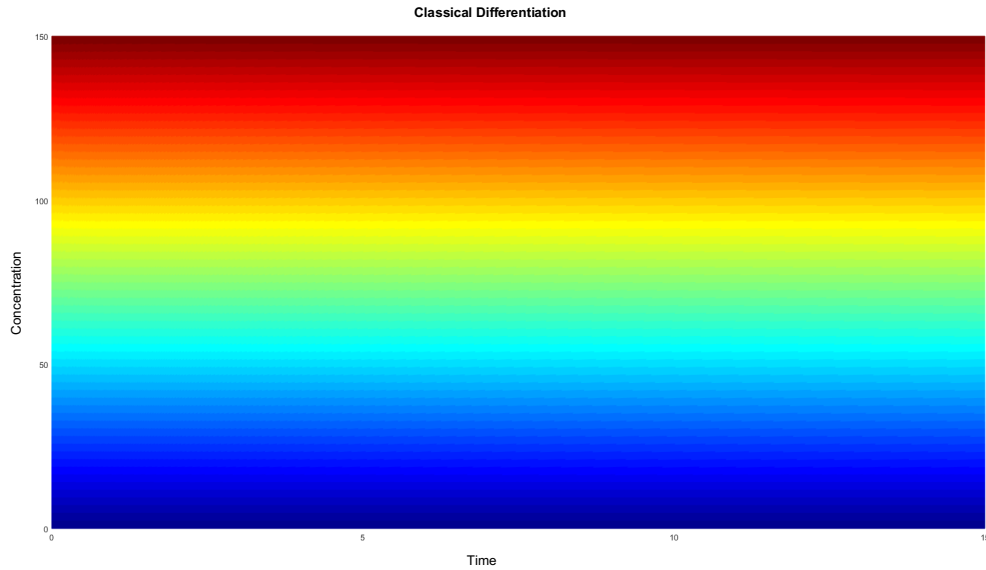


**Figure 5-5:** Concentration gradient variation over space at an initial concentration ( $C_0 = 150$ ) and the distance assumed is at ( $X_{max} = 15$ ).

We can observe that the concentration gradient is characterised by exponential and power-law behaviour.



**Figure 5-6:** Showing concentration decay over time and space-domain, the cross-over behaviour between the initial concentration is observed on the above figure. The cross-over behaviour is represented better by comparison to the other presented in figure 5-2.



**Figure 5-7:** Showing concentration decay over time in the space domain.

In figure 5-7, we also observe that the contamination concentration distribution as it is depleted over time in the space domain, however the process is driven in the main by the advection velocity.

In the above model we have been able to show that the advection velocity ( $v_m$ ) is not constant and so is as the advection flux (solute) as it has been shown above that it is space depended.

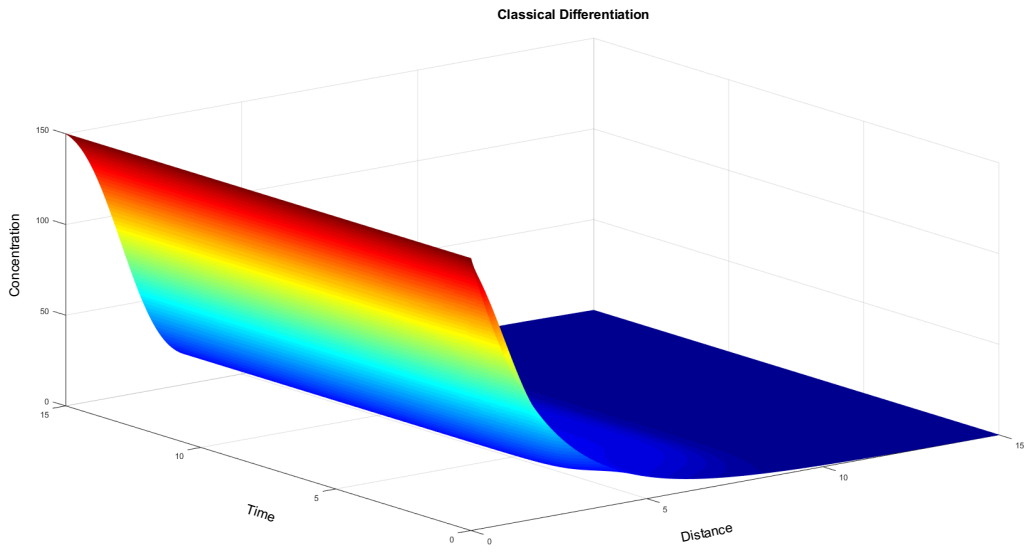
### 5.1.3 The Third Scenario for Classical Differentiation Model

The presentation of the third classical differential model for diffusion-advection is shown in figures below. The assumptions made for the second classical differentiation model are presented in Table 5-2.

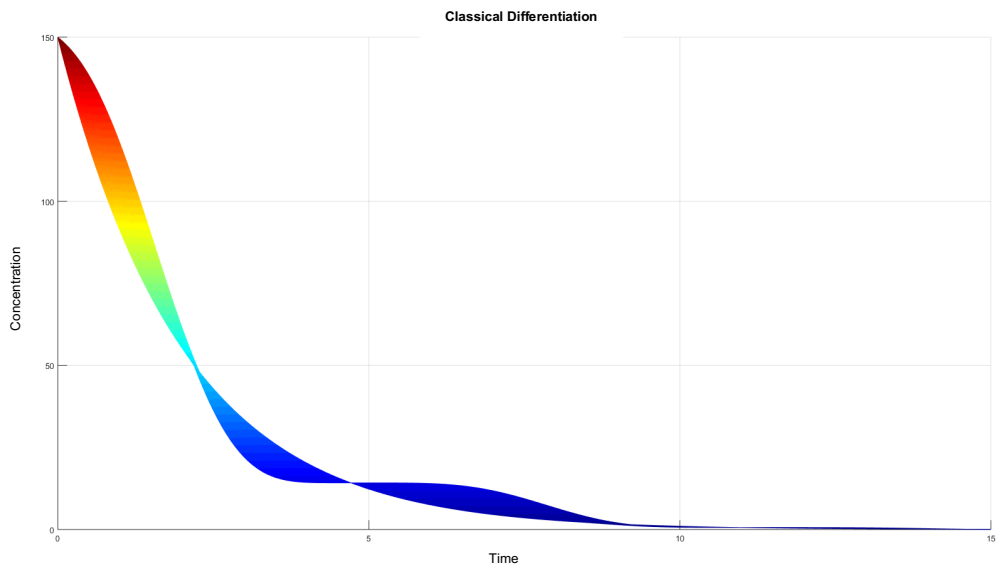
**Table 5-2:** Assumptions made for the second model

Variables assumed for the third scenario		
$\Delta x = 0,01$	$\Delta t = 0,01$	$T_{max} = 15$
$X_{max} = 15$	$C_0 = 150$	$K_D = 0,15$
$D_{h(x)} = \sin(x + 1)$	$\lambda = 0,5$	$v_{m(x)} = \cos(x + 1)$

In figure 5-8, we observed that the concentration-time distribution over the space domain and that the concentration decay is characterised by power-law behaviour.



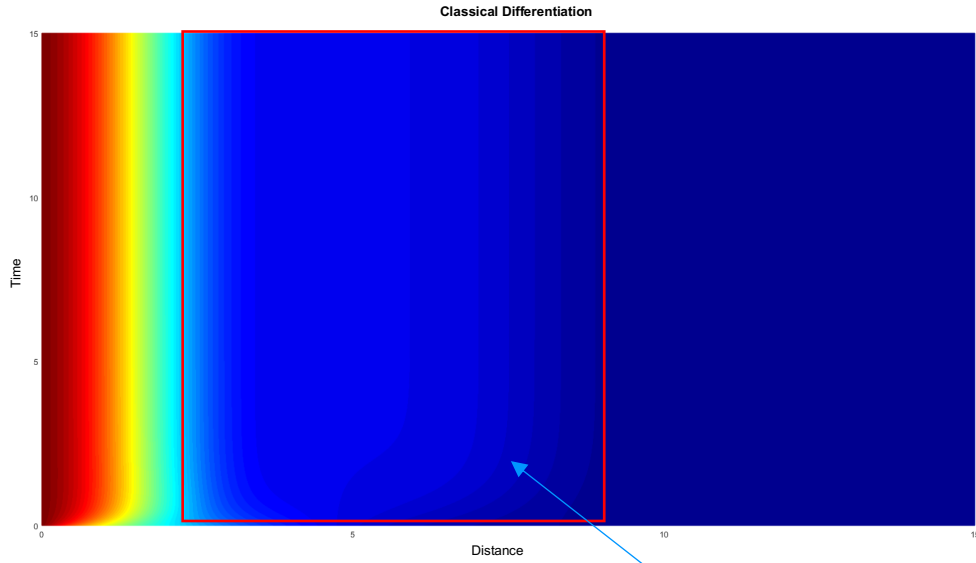
**Figure 5-8:** The concentration of solute versus time over a distance is presented, where the initial concentration ( $C_0 = 150$ ) and time is ( $T_{max} = 15$ ), a time step of ( $\Delta t = 0,01$ ) and distance assumed at ( $X_{max} = 15$ ). Other variables assumed include the following  $K_D = 0,15$ ;  $\lambda = 0,5$ ;  $D_h(x) = \sin(x)$  and where  $v_m(x) = \cos(x)$ .



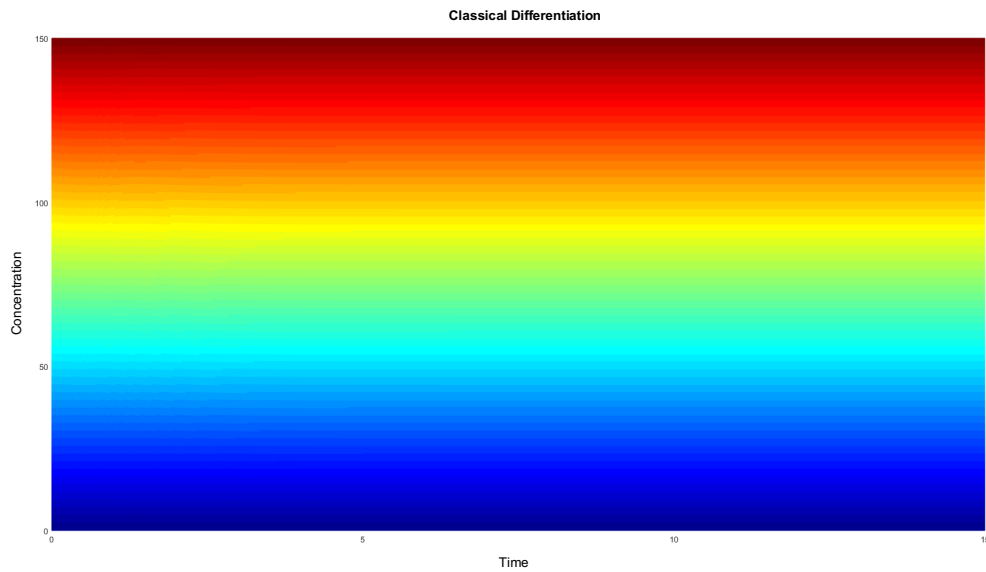
**Figure 5-9:** Concentration declivity over time where the initial concentration is at ( $C_0 = 150$ ) and the distance assumed is at ( $X_{max} = 15$ ).

We can observe that the concentration gradient is characterised, by and large, by the exponential and power-law behaviour. Furthermore we observe changes in concentration over time and effects of the advection velocity ( $v_m(x)$ ).

In figure 5-10, we show cross-over behaviour of the solute concentration in time and space.



**Figure 5-10:** concentration decay over time and space-domain, the cross-over behaviour between the initial concentration is observed on the above figure. the cross-over behaviour is represented better by comparison to the other presented in figure 5-2 and 5-6.



**Figure 5-11:** Showing concentration decay over time in the space domain

The pattern of contamination concentration distribution as it is depleted over time in the space domain is presented in figure 5-11, the process is driven by the advection velocity.

In the above model we have been able to show that the advection velocity ( $v_m$ ) is not constant and so is as the advection flux (solute) as it has been shown above that it is space depended.

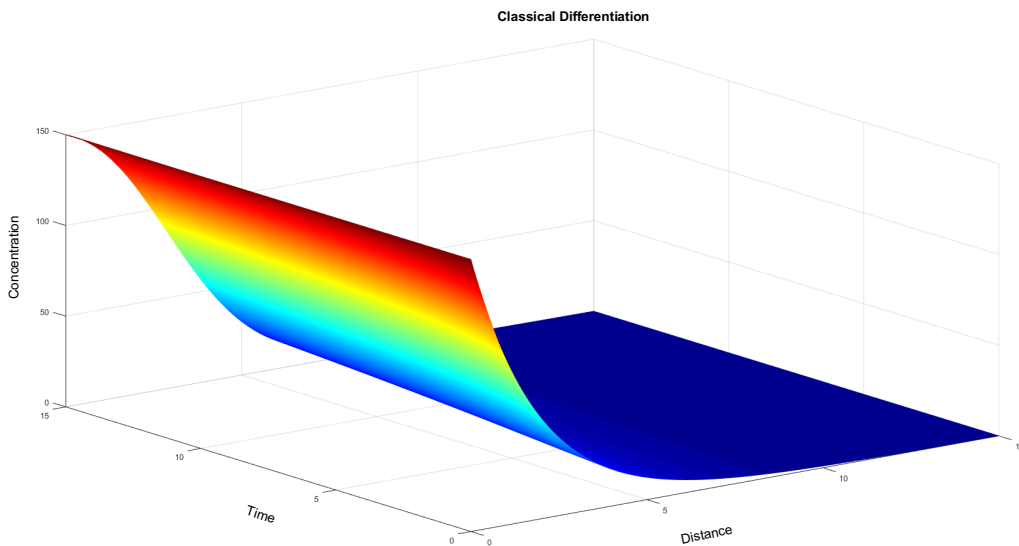
### 5.1.4 The Fourth Scenario for the for Classical Differentiation Model

The presentation of the third classical differential model for diffusion-advection is shown in figures below. The assumptions made for the second classical differentiation model are presented in Table 5-3.

**Table 5-3:** Assumptions made for the second model

Variables assumed for the 4 <sup>rd</sup> scenario		
$\Delta x = 0,01$	$\Delta t = 0,01$	$T_{max} = 15$
$X_{max} = 15$	$C_0 = 150$	$K_D = 0,15$
$D_{h(x)} = \cos(x)$	$\lambda = 0,5$	$v_{m(x)} = \cos(x)$

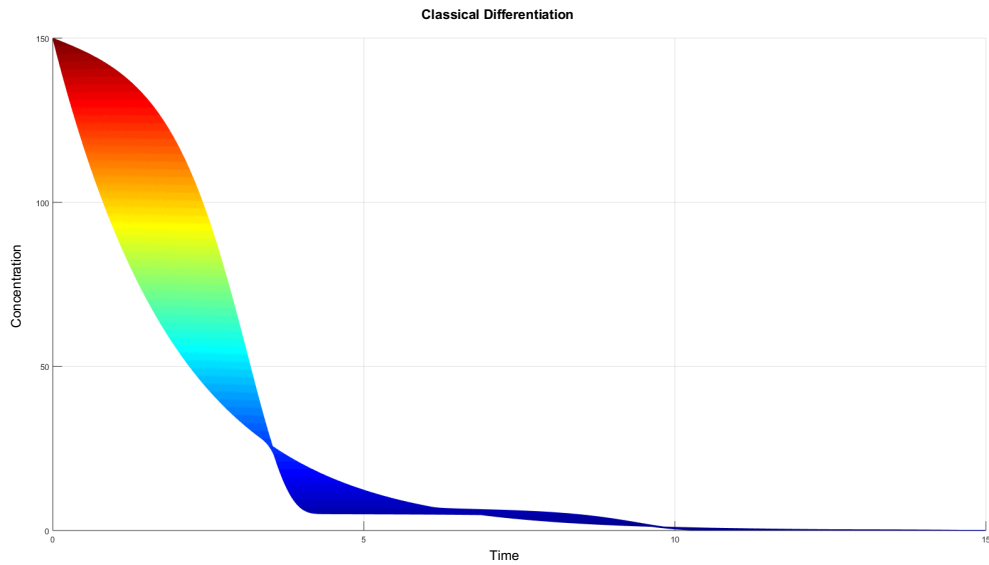
In figure 5-12, we also observed that the concentration-time distribution over the space domain and that the concentration decay behaviour is characterised by power-law.



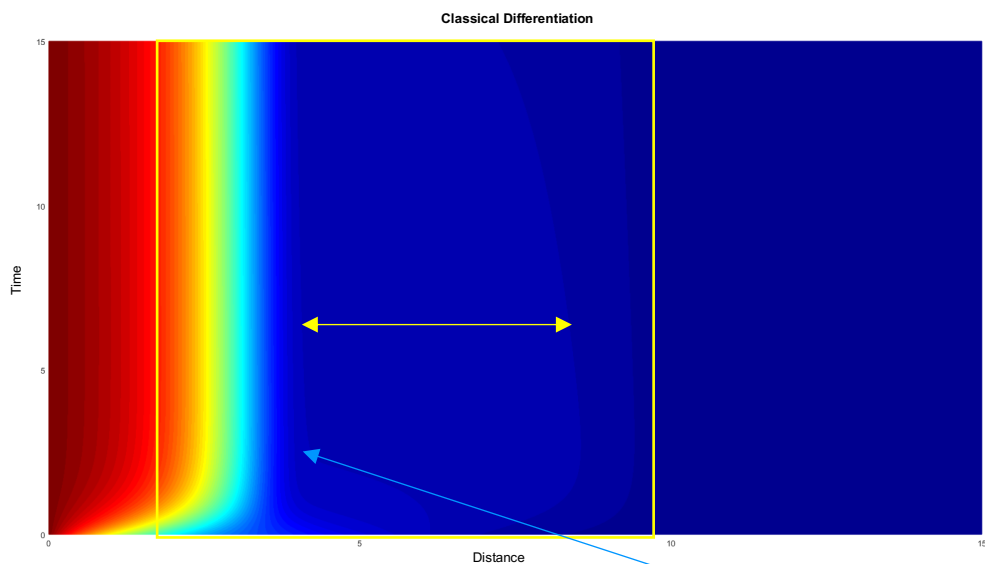
**Figure 5-12:** The concentration of solute versus time over a distance is presented, where the initial concentration ( $C_0 = 150$ ) and time is ( $T_{max} = 15$ ), a time step of ( $\Delta t = 0,01$ ) and distance assumed at ( $X_{max} = 15$ ). Other variables assumed include the following  $K_D = 0,15$ ;  $\lambda = 0,5$ ;  $D_{h(x)} = \cos(x)$  and where  $v_{m(x)} = \cos(x)$ .

In figure 5-12, again we observe that the concentration-time distribution over the space domain and that the concentration decay behaviour is characterised by power-law.

In figure 5-13, we observe that the concentration gradient is characterised by exponential and power-law behaviour. Furthermore, we observe changes in concentration over time and effects of the advection velocity ( $v_{m(x)}$ ).

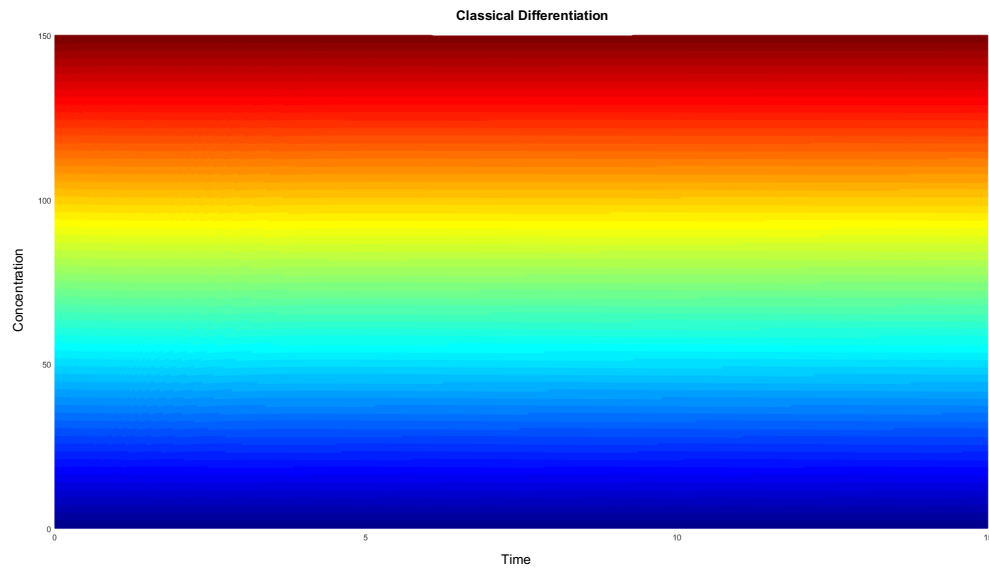


**Figure 5-13:** Concentration declivity over time where the initial concentration is at ( $C_0 = 150$ ) and the distance assumed is at ( $X_{max} = 15$ ).



**Figure 5-14:** Showing concentration decay over time and space-domain, the cross-over behaviour between the initial concentration is observed on the above figure. the cross-over behaviour is represented better by comparison to the other presented in figure 5-2, 5-6 and 5-10.

In figure 5-14, the concentration cross-over behaviour is prominent and it can be clearly seen that concentration distribution is driven by the advection velocity and that it is space dependent the is not a space variation.



**Figure 5-15:** Concentration decay over time in the space domain is shown.

The pattern of contamination concentration distribution as it is depleted over time in the space domain is presented in figure 5-15, the process is driven by the advection velocity.

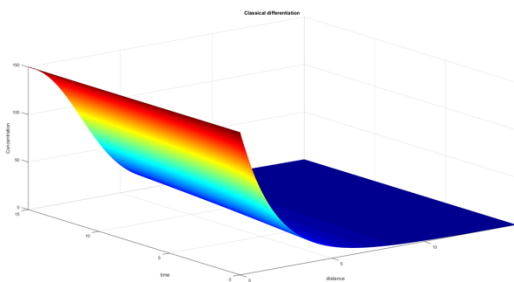
In the above model we have been able to show that the advection velocity ( $v_m$ ) is not constant and so is as the advection flux (solute) as it has been shown above that it is space depended.

## 6 Summary Discussion

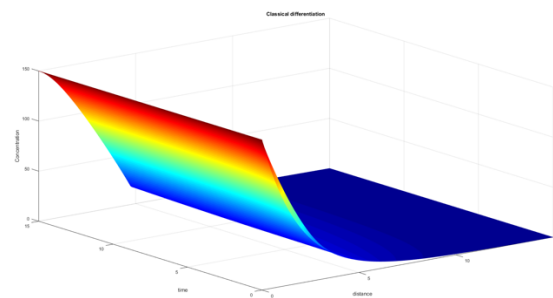
Summary discussion of the results obtain and presented in section 5 of this thesis are presented. Four scenarios were considered to model with classical differentiation, they included changing salient variables.

### 6.1 Diffusion-Advection Equation with Classical Differentiation

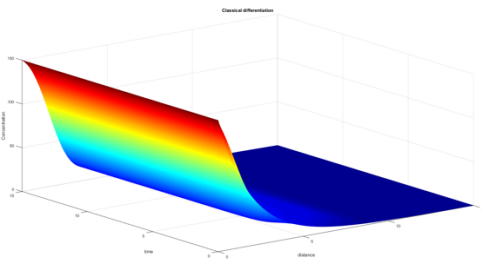
First, we present summary findings of the contamination concentration transport over time in space.



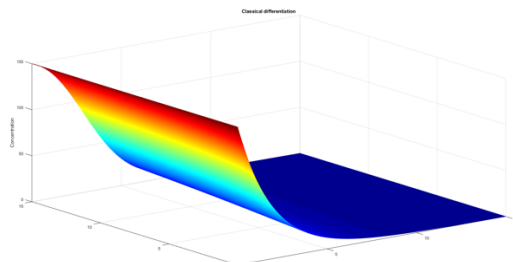
**Figure 6-1:** for  $C_0 = 150$ ; ( $T_{max} = 15$ ), ( $\Delta t = 0,01$ ) distance ( $X_{max} = 15$ );  $K_D = 0,15$ ;  $\lambda = 0,5$  and where  $v_m(x) = e^{(-x)}$ ; and  $D_h(x) = \frac{1}{1+x}$



**Figure 6-2:** for ( $C_0 = 150$ ); ( $T_{max} = 15$ ); ( $\Delta t = 0,01$ ) distance ( $X_{max} = 15$ )  $K_D = 0,15$ ;  $\lambda = 0,5$ ;  $D_h(x) = \sin(x)$  and where  $v_m(x) = e^{(-x)}$



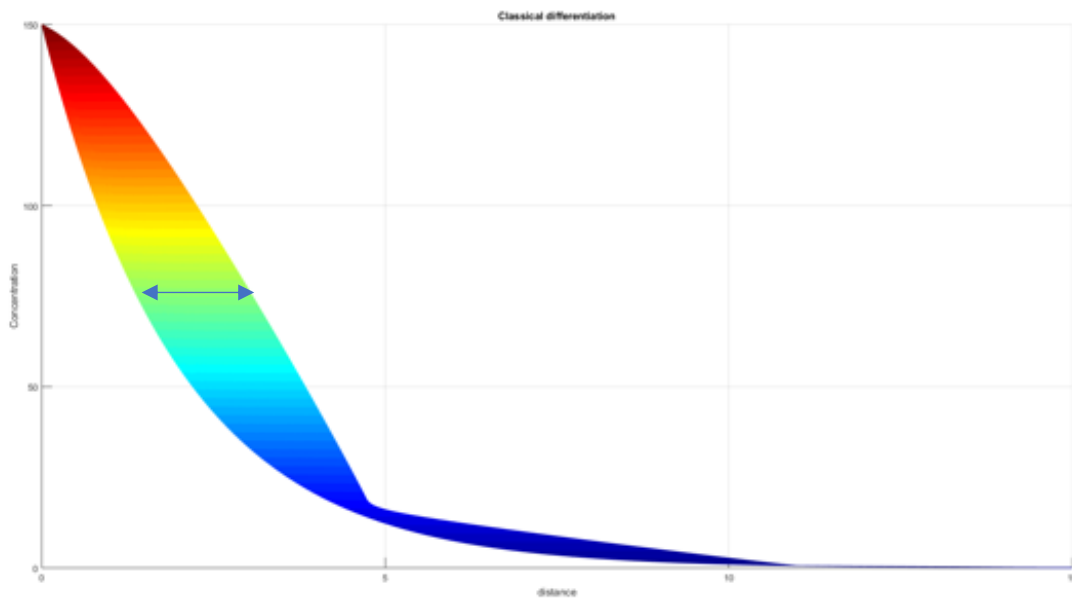
**Figure 6-3:** for ( $C_0 = 150$ ); ( $T_{max} = 15$ ), ( $\Delta t = 0,01$ ); distance ( $X_{max} = 15$ );  $K_D = 0,15$ ;  $\lambda = 0,5$ ;  $D_h(x) = \sin(x)$  and where  $v_m(x) = \cos(x)$ .



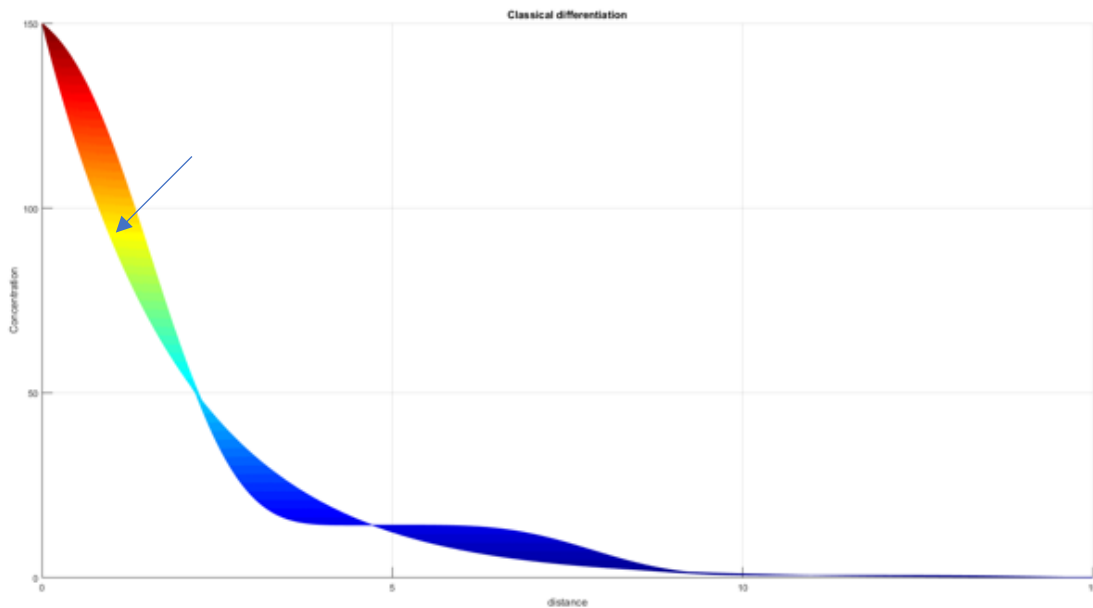
**Figure 6-4:** for ( $C_0 = 150$ ); ( $T_{max} = 15$ ), ( $\Delta t = 0,01$ ) distance ( $X_{max} = 15$ );  $K_D = 0,15$ ;  $\lambda = 0,5$ ;  $D_h(x) = \cos(x)$  and where  $v_m(x) = \cos(x)$ .

In all the above figures we observe that similarities of concentration decay over time and in space (*in the matrix*) follows the exponential decay and power-law process. Furthermore, the concentration evanescing is space depended and is induced by the advection velocity as we see that over the distance or travel time the concentration is fading.

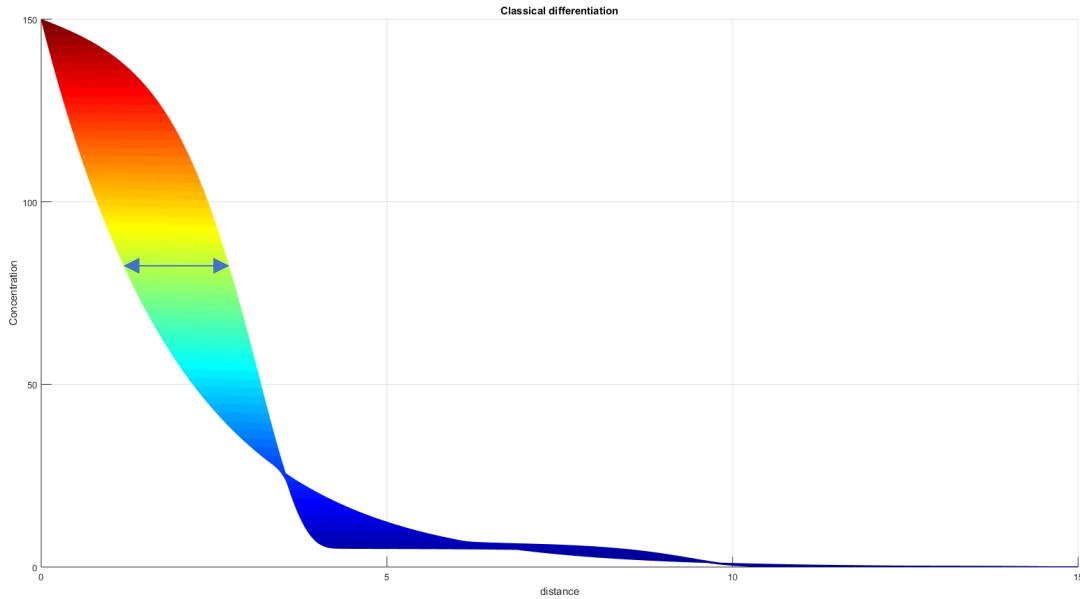
The concentration of solute over the distance in the space-domain is expressed in figures 6-5 to 6-7 in the next page.



**Figure 6-5:** Concentration gradient variation over space at an initial concentration ( $C_0 = 150$ ) and the distance assumed is at ( $X_{\max} = 15$ ) when  $D_{h(x)} = \sin(x)$  and  $v_{m(x)} = e^{-x}$



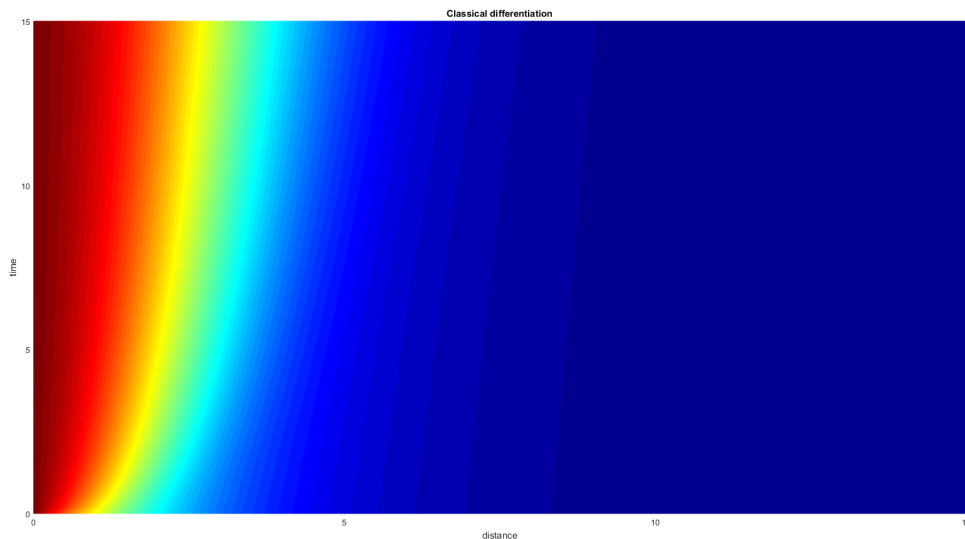
**Figure 6-6:** Concentration declivity over time where the initial concentration is at ( $C_0 = 150$ ) and the distance assumed is at ( $X_{\max} = 15$ ) when  $D_{h(x)} = \sin(x)$  and  $v_{m(x)} = \cos(x)$ .



**Figure 6-7:** Concentration declivity over time where the initial concentration is at ( $C_0 = 150$ ) and the distance assumed is at ( $X_{\max} = 15$ ) when  $D_{h(x)} = \cos(x)$  and  $v_{m(x)} = \cos(x)$ .

The highlighted areas (in arrows) in figure 6-5 to 6-7, show concentration attenuation, the attrition is driven by the advection velocity. This shows that contamination movement follow preferential paths as dictated by the advection velocity, therefore it is not right to assume constant advection velocity across the space-domain.

The concentration attenuation over time in the space-domain is discussed below.



**Figure 6-8:** Concentration attenuation in the space-domain over time.

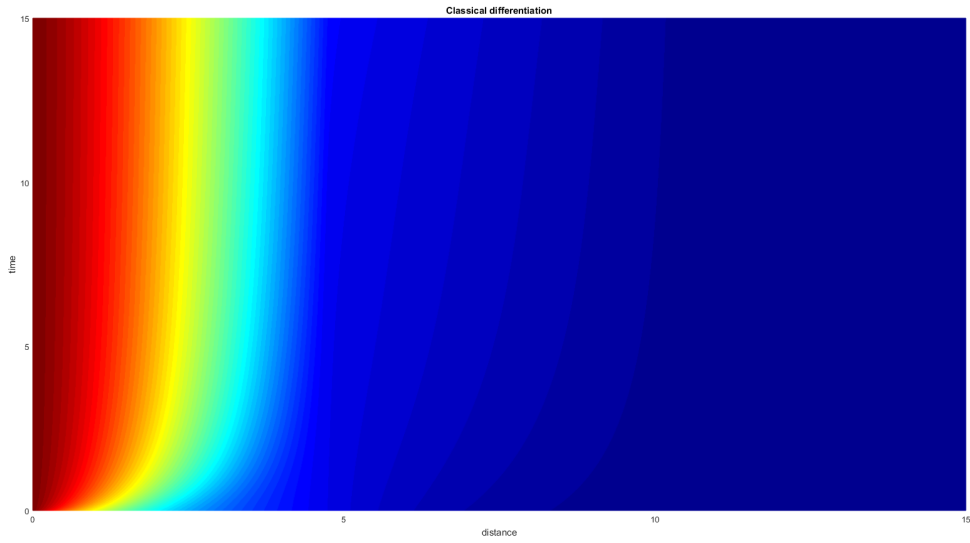


Figure 6-9: Concentration attenuation in the space-domain over time.

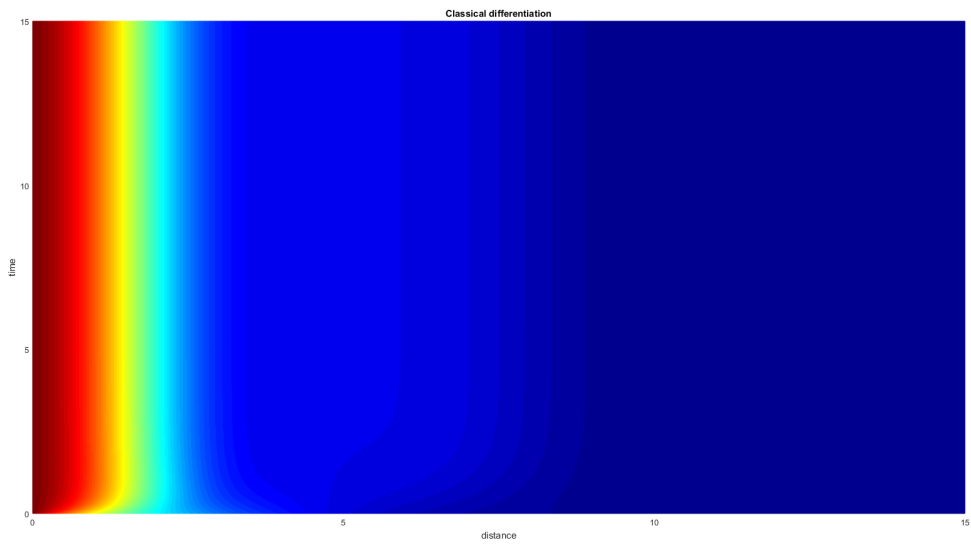


Figure 6-10: Concentration attenuation in the space-domain over time.

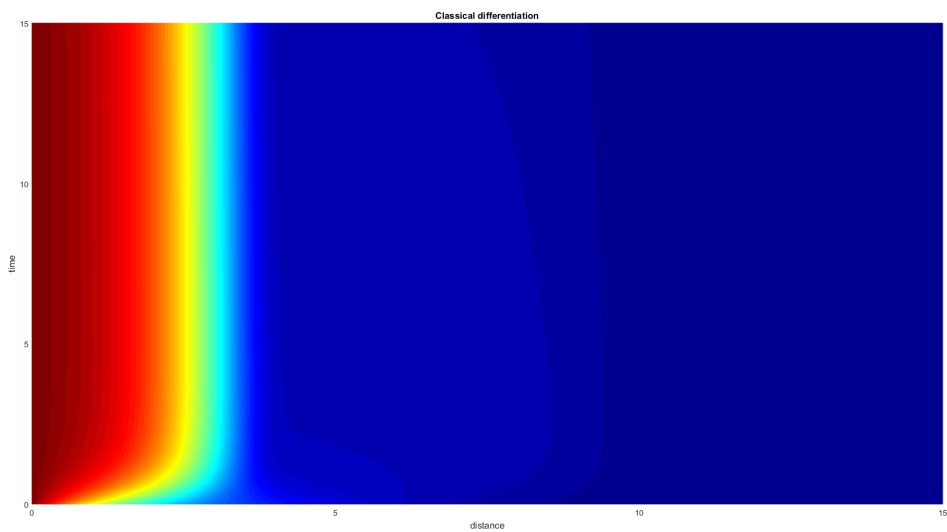


Figure 6-11: Concentration attenuation in the space-domain over time.

The above figures demonstrate a cross-over behaviour from the initial concentration over space. This goes to show that at different conditions in space i.e. fracture or matrix, the concentration will vary across the space-domain.

## 7 Conclusion

Modeling real world problems have been a serious worry for researchers in all the fields of science, technology and engineering. Whereas prediction of future behaviours of a given real world problem depends upon the output of the mathematical model and the data collected.

In general, if the collected data are not in good agreement with the mathematical model, one must ask the following questions: does the mathematical model really replicate the observed facts? or does the collected data really represent the real world problem? if the answer to the first question is yes then, it is clear that the collected data are not free of uncertainties, therefore, such data should undergo thorough uncertainty investigation, an easier way to solve such problem is perhaps to solve the equation  $f(x + mT) = f(x)$  where the parameters  $m$  represent the number of time the data was collected and  $T$  the period within which such data was collected, thus after removal of uncertainties, the corrected data can then be matched with mathematical model to give proper prediction. If the answer of the first question is no and that of the second is yes, then, the suggested model should be revised.

Within the field of groundwater, movement of contamination or impurities within the geological formation has attracted the attention of many researchers. The initial suggested mathematical model considers the concept of differentiation based on the rate of change and the associate coefficient representing aquifer parameters are assumed to be constant across the aquifer. Although, this model has been used with some success within the field of groundwater, one has to note that such model did not take into consideration the transport from the matrix into a fracture, also the model does include into the mathematical formulation the transfer terms from the matrix rock to fracture, more importantly, the model does not account for the aperture size.

Finally the model does consider processes like power law, fading memory and crossover, while these processes are associated to properties of the geological formation. In this thesis we suggested a new model that follows the principle of mass conservation theory, however, the model is taking into account the movement from matrix soil to fracture, addition a transfer term was included although some part were neglected. The first model was constructed using the classical differentiation, however, it was found out that the new dispersion coefficient is space dependent also the velocity was obtained as function of space. This new model was solved numerically using some new suggested numerical schemes. The conditions under which the used numerical scheme is stable and converge were also presented in this thesis in detail.

To include into mathematical formulation the effect of long-range dependency that corresponds to movement within a finite fracture, the concept of fractional differential and integral operators with power law kernel was used to modify the classical model. The obtained model was also analysed accordingly. To include into mathematical formulation the fading memory effect that correspond to the movement within a geological formation with elastic properties the classical model was modified using the well-known Caputo-Fabrizio fractional differential operator, a new numerical scheme was used to solve this model and stability analysis was presented in detail.

Finally, to include into mathematical formulation the crossover effect, the Atangana-Baleanu fractional differential operator was used to extend the classical model also the conditions under which the stability and the convergence are reached were presented in details. One of the great finding in this thesis is the fact that the variable dispersion and velocity even with classical case are able to replicate the effect of change in fracture aperture.

## 8 Conclusion

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