A NEW METHOD FOR MODELING GROUNDWATER FLOW PROBLEMS: FRACTIONAL-STOCHASTIC MODELING

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DECLARATION

I, Mohau L. Mahantane, declare that the dissertation hereby submitted by me for the Magister Scientiae degree at the University of the Free State (Institute for Groundwater Studies) in the Faculty of Natural and Agricultural Sciences, is my own independent work and that I have not previously submitted it at any other institution of higher education.

More importantly, I declare that all sources cited have been acknowledged by means of a list of references.

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ABSTRACT

To date, groundwater flow problems are still increasingly becoming a great environmental concern worldwide. This is among some of the reasons that many researchers from various fields of science have focused much of their attention in formulating new mathematical equations and models that could be used to capture and understand the behavior of groundwater flow with respect to space and time. The main aim of this study was to develop a new concept for modeling groundwater flow problems. The approach involved coupling of differential operators with stochastic approach. Literature proves that each of these two concepts has shown a great success in modeling complex real-world problems. But we argued that differential equations with constant coefficient are not fit to capture complexities with statistical setting. Therefore, to solve such a problem in this study, we considered a classical one-dimensional advection-dispersion equation for describing transport in porous medium and then applied stochastic approach to convert groundwater velocity (v), retardation (R) and the dispersion (D) constant coefficients into probability distribution. The next step was to employ the concept of fractional differentiation where we substituted the time derivative with the time fractional differential operator. Thereafter, we applied the Caputo, Caputo-Fabrizio and the Atangana-Baleanu fractional operators and derived conditions under which the exact solution for each derivative can be obtained. We then suggested the numerical solutions using the newly established numerical scheme of the Adams-Bashforth in the case of the aforementioned three (3) different types of differential operators. By combining the two concepts, we developed a new method to capture groundwater flow problems that could not be possible to capture using differential operators or stochastic approach alone. This new approach is believed to be a future technique for modeling complex groundwater flow problems. After solving the new model numerically, the condition for stability was also tested using the Von Neumann stability analysis method. Lastly, we presented numerical simulations using a software package called MATLAB.

Keywords: Advection-dispersion equation, Stochastic approach, Fractional differentiation, Adams-Bashforth, Numerical analysis, Stability analysis

LIST OF GREEK NOTATIONS

α	Alpha
λ	Lambda
τ	Tau
δ	Zeta
∂	Partial differential
Γ	Gamma
ρ	rho
μ	Mu
Σ	Sigma
Δ	Delta
γ	Gamma
ψ	Psi
Φ	Phi
ε	Epsilon
σ	Sigma

ABBREVIATIONS AND NOTATIONS

eq.	Equation
ADE	Advection-dispersion equation
D	Dispersion Coefficient
v	Seepage velocity
R	Retardation factor
t	Time
exp	Exponent
1-D	One-dimensional
f	Function
ϵ	Element of
C	Concentration
cos	Cosine
sin	Sine

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CHAPTER 1: INTRODUCTION

1.1 BACKGROUND AND RATIONALE

One of the real-world's most complicated and challenging issue to be represented by means of simple mathematical models and/or equations is the issue facing groundwater investigations, as it requires the modeler's detailed understanding about the geologic structure and the response of the aquifer through which groundwater moves. Thus, modeling such a problem remains a challenging task because the response and geological structure of the aquifer through which groundwater travels is invisible and changes with space and time (Atangana and Bildik, 2013). For example, assessment of groundwater contamination and its remediation remains among the most complex hydrogeological issues to quantify due to the heterogeneity of geological medium and also demands knowing and understanding the physical, chemical and biological properties of a contaminant to be dealt with. In an aquifer system, in saturated zones for instance, solutes are transported together with flowing water, thus, groundwater serves as the main causative substance for the movement of those pollutants from one area to another (Dong, 2006). Hence, the volume of a pollutant that is likely to be present in groundwater is determined by the aforementioned properties (i.e. physical, chemical and biological properties). Thus, two main transport processes, namely, advection and hydrodynamic dispersion (DellaSala and Goldstein, 2017) govern solute migration in the subsurface.

In groundwater investigations, researchers employ the transport equation (see eq. 1.1) known as advection-dispersion equation (ADE) to quantify the movement of a contaminant within an aquifer system. This equation (eq. 1.1) accounts for the mass balance of pollutants over the entire volume of an aquifer system (DellaSala and Goldstein, 2017). Thus, advection and hydrodynamic dispersion are the two main physical processes influencing the migration of solutes through the entire volume of a porous medium (Freeze and Cherry, 1979).

The ADE shown below is from a published paper "A generalized advection-dispersion equation" by Atangana (2014).

$$D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - \lambda RC = R\frac{\partial C}{\partial t} + f(x,t) \tag{1.1}$$

Initial and boundary conditions may be presented as:

$$C(x,0) = 0, \qquad C(0,t) = c_0 \exp(-\alpha t) \tag{1.2}$$

and,

$$C_{\mathrm{x}}(\infty,t) = 0 \tag{1.3}$$

where, D is the coefficient of dispersion, v and R are the average linear groundwater velocity and the retardation factor, respectively. λ is the constant for radioactive decay, c_0 denotes the initial concentration, α is the positive constant and $f(x,t)$ may be any source or sink term in the system. But the assumption can be made that there is no sink or source in groundwater pollution and $f(x,t)$ is then ignored in such circumstances.

The movement of solutes in an aquifer system as stated in the previous paragraphs is due to the processes of *advection* and *hydrodynamic dispersion.* Thus, the movement occurring under process of advection is mainly influenced by the fluid flow within the pore spaces, while the hydrodynamic dispersion process that may comprise both molecular diffusion with respect to concentration gradients, and mechanical dispersion as a result of pore fluids moving along the tortuous flow paths of porous media. When a pollutant is introduced in the groundwater system, advection becomes the main transport process influencing the movement of that particular pollutant through a geologic medium at some early stages (DellaSalla and Goldstein, 2017). This is because during advection process, the dissolved solutes are transported together with groundwater moving in bulk flows. For this reason, contaminant migration occurring under this process is said to travel at an equal speed as the average linear groundwater velocity. Therefore, a conclusion may be drawn that the advection process influences the arrival of pollutants at a certain location

(Vandenbohede, 2003). In other words, the main determining factor in advection process is average linear groundwater flow velocity/seepage velocity.

Furthermore, during advection transport process, the seepage velocity is reliant on geologic medium properties such as average permeability, the hydraulic gradient as well the effective porosity of the medium (DellaSala and Goldstein, 2017). Moreover, since the process of advection is the movement of dissolved mass due to flowing groundwater, it can therefore be calculated by applying Darcy's law (Patil and Chore, 2014). In geologic media characterized by high permeability material, advection process results in an increased solute migration in the more porous medium (Gillham *et al*., 1984). This proves that in reality, heterogeneity does exist in the subsurface and the solute transport due to advection through different types of formations is a non-uniform process hence seepage velocity will vary with space. To add, in subsurface locations where the porous medium exhibits fractures, the rate at which pollutants are transported will differ depending on the geological setting of those fractures (Silveira and Usunoff, 2009). For instance, higher seepage flow velocities will be measured in locations where the solute moves through the highly fractured medium as compared to the non-fractured areas within an aquifer system.

In addition, during advection process, as solutes are transported from one location to another by the bulk movement of flowing groundwater, they are also subjected to different stages of mixing and spreading known as the dispersion. This is due to the presence of heterogeneities in porous medium which results in groundwater flow velocity variations as a with respect to space and time (Fitts, 2002). Thus, the interaction of solutes with pores of different sizes causes a migrating plume to disperse along the flow paths as a result of groundwater flow velocity variations. For example, as the plume migrates, some of the solutes move at increased rates through pore openings while other solutes move slowly due to interactions at grain boundaries and with large pores. Furthermore, in situations where groundwater flow is laminar and constant, the process of advection contributes to longitudinal dispersion of solutes, but no transversal dispersion. However, in reality subsurface groundwater flows are not uniform, and there exist variant groundwater flow velocities and molecular diffusion, which both cause transversal dispersion of solutes along groundwater flow directions (Fitts, 2002). Subsequently, as these solutes are spread in longitudinal and transversal manner along the flow paths, they tend to be subjected to mechanical mixing and dilution effects due to the process known as mechanical dispersion (DellaSala and Goldstein, 2017).

To add, based on the information from the previous paragraph it is clear that groundwater flow velocity variations resulting from tortuosity of porous medium flow paths also contribute to mechanical dispersion. Thus, mechanical dispersion can therefore be viewed as a microscopic and macroscopic process due to these fluctuations in groundwater flow velocity (Anderson, 1984). On microscopic scale, for non-homogeneous medium, longitudinal mechanical mixing will be experienced if the mixing happens along groundwater flow paths, and transversal if the mixing occurs at right-angles to groundwater flow paths (DellaSala and Goldstein, 2017; Schulze-Makuch, 2009). During solute transportation, the dispersion of solutes due to variations in groundwater flow velocity is also dependant on the structure of geologic medium through which the dissolved mass travels and how it interacts with the aquifer material either physically or chemically along the way (Dietrich, *et al*., 2005; Sahimi, 1995). For example, in heterogeneous geological medium, these solutes travel along paths differing in lengths and through pores with differing sizes. That is, some paths lengths are longer while others are short (converging and diverging flow paths) and therefore it becomes a complex issue for a modeler to predict when a contaminant will reach a certain place. Possibly, this converging and diverging effect of flow paths is likely to cause a contaminant to accumulate greater volumes within the subsurface as some fluid particles collide and some disperse with distance along flow paths.

Similarly, with differing pores sizes, when a contaminant moves through larger pore spaces, the rate of movement increases because the flow path is widened and physical interaction of the flowing solutes with solid surface of the medium is reduced hence less friction is involved. On the other hand, when solute movement is happening closer to grain boundaries, the physical contact will cause solutes to travel slowly as a result of exposure to increased pore roughness. Thus, solute particles not in contact with the medium phase will flow faster than those in contact with the solid phase. Furthermore, as the plume migrates, the spreading and dilution that occur in the process cause the concentration of a contaminant to decrease with distance from its source. On macroscopic scale (Kinzelbach, 1992), the factor determining mechanical dispersion is the medium hydraulic conductivity which varies in space due to aquifer heterogeneity. These variations in geologic hydraulic conductivity either vertically or horizontally possibly cause flow paths irregularity, which also lead to a change in the direction of groundwater flow hence contaminant dispersion. Even if one might be familiar with how the process of dispersion occurs but capturing these variations in hydraulic conductivity (non-homogeneities) still remains challenging (Knox *et al*., 1993). Therefore, one can conclude that in actual facts, the quantification of groundwater flow and solute transport requires a thorough understanding of the aquifer geometry. Hence the need for the formulation of a model that will account for these heterogeneities.

It is therefore among some of the reasons, that many models have been developed by numerous researchers in the field of hydrogeology with the attempt to suggest a model that will best describe subsurface groundwater flow, although no fully realistic findings as yet (Atangana and Bildik, 2013). Thus, modeling groundwater flow systems remains a challenging aspect because the subsurface through which this flow occurs is not visible and can change with time and space. Moreover, due to the invisibility of the nature of groundwater flow processes, mathematical equations are defined for groundwater movement to facilitate in the investigation of transport and fate of pollutants for risk management purposes. In this study, modeling of groundwater flow problems will be based on the modification of the aforementioned one-dimensional (1-D) advection-dispersion equation (ADE) by coupling of fractional differential and integral operators with stochastic approach. Hence, the need to account for random movement of groundwater and solute transport with respect to heterogeneity of aquifer systems.

1.1.1 Stochastic Approach

How a contaminant will travel in groundwater is dependent on aquifer geohydraulic and geochemical properties, and these properties are said to vary with space within aquifer systems (Skaggs and Barry, 1996). As a result, it becomes a very challenging issue to characterise and provide a detailedillustration of aquifer heterogeneity. Thus, groundwater flow and transport parameters are in nature associated with uncertainty.In most groundwater problems, the aquifer spatial heterogeneity with respect to variable hydraulic conductivity is one of the main aspects in hydrogeology that impedes the means to feasibly characterize contaminated groundwater areas (Gómez-Hernández *et al*., 2016). In fact, not only aquifer heterogeneity results in uncertainty of hydrogeological models, but field data as well (Baalousha, 2011).

In addition, a lot of assumptions or approximations are involved during formulation of mathematical equations, and are believed to pose higher possibilities of uncertainties in modeling results (Baalousha, 2011; Baalousha and Köngeter, 2006). These uncertainties in groundwater modeling can therefore be accounted by application of stochastic techniques. With such an approach, when modeling groundwater movement and solute migration the values of aquifer properties and parameters that impact on the flow and transport are treated as random, so that their uncertainties can be accounted for (Dagan, 2002). Thus, the stochastic approach provides a way to address these uncertainties using probability functions or related quantities such as statistical moments.

Advantages of Stochastic Methods

Numerous stochastic techniques have been developed for investigating solute movement in randomly heterogeneous aquifers. However, according to Dagan (2002), the Monte Carlo Simulations (MCS) and First-order approximation in log-conductivity variance (weak variance) are the two stochastic methods that were mostly used for solution over the past decades. In addition, Baalousha (2003) also mentioned that the most widely used methods in stochastic modeling are the Monte Carlo Simulations, First-Order Second Moment Method (FOSM) and First-Order Reliability Method (FORM). However, stochastic approach using the Monte Carlo method is still the most famously applied method for analyzing uncertainty in hydrogeological models (Baalousha, 2011; Kunstmanna and Kastensb, 2006; Liou and Der Yeh, 1997). With the Monte Carlo Simulations (Dagan, 2002), the solution of flow and transport problems is achieved by performing repeated runs or executions through computation, and a sample output for each execution is produced. This computerized technique employs random sampling statistical methods based on probability distribution functions (Kwak and Ingall, 2007). With first-order approximation in log-conductivity variance, the equations of flow and transport are utilized in a power series to find first-order approximation (Dagan, 2002). There are other several numerical perturbation methods that have been proposed, although are not as efficient as the Monte Carlo approach when it comes to application in complex real-world situations (Li *et al*., 2004; Li *et al*., 2003). It is therefore very important to point out that stochastic methods have both advantages and limitations. The advantages and limitations addressed in sections below are based on the aforementioned stochastic methods.

The advantages of MCS as outlined by Dagan (2002) are based on its conceptual simplicity, generality, and comprehensive representation of results. Due to its conceptual simplicity, it provides a clear description of heterogeneity even when there is little available spatial or temporal data about the aquifer system in place. Hence, gives a modeler the capability to resolve the risk and address any uncertainty arising from any made estimations (Daniel *et al*., 2011). Thus, MCS is a very straightforward method to employ even in situations where there is limited field data. Accordingly, it is very simple to apply when dealing with both linear and non-linear stochastic flow and transport problems (Neuman, 2004). Apart from being a fit technique to apply in groundwater modeling, numerical MCS also produces results of better precision or accuracy (Baalousha, 2003). In fact, MCS has found its way in solution of many real-world systems given that it can handle uncertainty as well as variability associated with model parameters (Kwak and Ingall, 2007).

Furthermore, some modifications of MCS such as Latin hypercube have been developed afterwards and is considered to significantly decrease the time needed for computation (Baalousha, 2011; Zhang and Phinder, 2003). In addition, another stochastic method requiring a low computational time and effort for use as an alternative to Monte Carlo method (Baalousha, 2003) is the First-Order Reliability method (FORM). In most of its applications, FORM involves a less number of runs or simulations and this makes it to be more computationally efficient than MCS. It also yields good results in terms of accuracy (Manoj, 2016). However, this advantage only holds in situations dealing with solutions of less complicated real life problems. Next, another suggested method is the First-Order-Second Moment (FOSM) method (Manoj, 2016), which also does not require a large number of computations compared to MCS but a disadvantage is that it yields poor results in terms of accurateness. With first-order approximation in log-conductivity variance, clear linearization approach is applied to the equations to achieve simplified results (Dagan, 2002). Thus, this technique enables the results to be handled analytically or semi-analytically with simplified data application.

Additionally, in situations where there is inadequate data or a high level in data uncertainty, stochastic methods enable an uncertainty factor to be included in the modeling process. This in turn produces more meaningful model outcomes and enable better interpretations, which will help with easy model application when solving real-world situations (Ohio-EPA, 2007). Since modeling process involves making a lot of assumptions and estimations about the randomness of model properties, thus, stochastic modeling enables the validity of those assumptions to be tested statistically. Furthermore, because stochastic techniques have the ability to account for flow and transport parameter uncertainty (Skaggs and Barry, 1996), they are also very useful in providing the modeler with an understanding of any possible impacts associated with heterogeneity on hydrogeological processes and models (Renard, 2007).

Limitations of Stochastic Methods

Despite the aforementioned advantages of stochastic techniques, some limitations for MCS method are that, the application of this method in three-dimensional (3-D) simulations becomes computationally too demanding and may require the extension of the grid size (Dagan, 2002). That is, quite a number of repeated computations are required to achieve a proper precision with MCS (Baalousha, 2003). In addition, in situations where a contaminant transport has a large number of variables MCS becomes inefficient. Although the Latin hypercube method is considered to reduce the time requirements, it still also comes with huge computational costs (Yidana *et al*., 2016). With first-order log-conductivity variance, the results generated are said to be valid only for small variances (Dagan, 2002). To add, its analytical solutions do not become realistic in situations with variable mean flow and transient conditions as well as where complex boundaries exist.

Furthermore, with FORM method aforementioned as another alternative method to MCS, the disadvantage is that it requires optimization approach in order to achieve the most feasible results at a particular point (Baalousha, 2003). Consequently, this procedure is very complex hence more time and is very cost intensive, hence the likely increase in uncertainty of produced results. In addition, it also requires a substantial amount of variables when dealing with contaminant transport problems. Another challenge when employing a stochastic approach to simulate transport processes is that, it is not easy to compute the ensemble moments of solute concentration in a way that will account for the effects of some significant non-linearities (Li *et al.,* 2004). According to Li *et al.* (2003), the numerical performance is what they suppose must be the main issue when it comes to the use of stochastic techniques in groundwater investigations.

1.1.2 Definitions of some well-known Fractional Derivatives

The notion of fractional differentiation as indicated in published research works is vastly becoming a useful approach in the field of groundwater science when addressing the concept of heterogeneity, viscoelasticity, fading memory etc. There are quite a number of fractional differential operators that exist, although very few of them have been applied in the fields of scientific research to solve problems of real world. The Riemann-Liouville and the Caputo derivatives are regarded as the most commonly used fractional derivatives (Atangana and Bildik, 2013). Recently, some new fractional operators such as the Atangana-Baleanu and the Caputo-Fabrizio derivative have been proposed. Accordingly, these fractional operators have also shown their usefulness in the field of scientific research. The definition for each of these fractional derivatives is presented below.

Definition for Riemann-Liouville fractional derivative:

$$D^{\alpha} f(t) = \frac{1}{\Gamma(n-\ \alpha)} \frac{d^n}{dt^n} \int_a^t \frac{f(x)}{(t-x)^{\alpha+1-n}}\, dx, \qquad n - 1 < \alpha < n. \tag{1.4}$$

Definition for Caputo fractional derivative of function f is presented as:

$${}_0^C D_t^{\alpha} f(t) = \frac{1}{\Gamma(n\ -\ \alpha)} \int_0^t (t-x)^{n-\ \alpha-1} \frac{d^n}{dx^n} (f'(x))\, d,. \quad n - 1\ < \alpha \leq n. \tag{1.5}$$

Definition for Caputo-Fabrizio fractional derivative is given as follows:

Let $f \in H^1\ (a, b), b >\ a, \alpha \in [0, 1]$

Then,

$${}_0^{CF} D_t^{\alpha} f(t) = \frac{M(\alpha)}{1\ -\ \alpha)} \int_a^t f'(x)\, exp \left[-\alpha\ \frac{t-x}{1-\ \alpha}\right] dx, \tag{1.6}$$

However, if the function does not belong to $H^1(a, b)$ then, the derivative is redefined as follows:

$${}_0^{CF} D_t^{\alpha} f(t) = \frac{\alpha M(\alpha)}{1\ -\ \alpha)} \int_a^t (f(t) -\ f(x))\, exp \left[-\alpha\ \frac{t-x}{1-\ \alpha}\right] dx. \tag{1.7}$$

Definition for Atangana-Baleanu fractional derivative in the sense of Caputo is given as:

Let $f \in H^1(a, b), a < b, \alpha \in [0,1]$

Then,

$${}_a^{ABC} D_t^{\alpha} \big(f(t)\big) = \frac{AB(\alpha)}{1-\ \alpha} \int_a^t f'(x) E_{\alpha} \left[-\alpha \frac{(t-x)^{\alpha}}{1-\ \alpha}\right] dx, \qquad 0\ < \alpha <\ 1. \tag{1.8}$$

Atangana-Baleanu fractional derivative definition in the Riemann-Liouville sense is given as:

Let $f \in H^1(a,b), a < b, \alpha \in [0,1]$

Then,

$$ {}^{ABR}_{\ a}D_t^{\alpha}\big(f(t)\big) = \frac{AB(\alpha)}{1-\ \alpha}\frac{d}{dt}\int_{a}^{t} f(x)E_{\alpha}\left[-\alpha\frac{(t-x)^{\alpha}}{1-\ \alpha}\right]dx, \qquad 0\ < \alpha <\ 1. \tag{1.9}$$

The fractional integral for Atangana-Baleanu derivative of order α of a function f (t), is given as:

$$ {}^{AB}_{\ a}I_t^{\alpha}\big(f(t)\big) = \frac{1-\alpha}{B(\alpha)}\ f(t) + \frac{\alpha}{B(\alpha)\Gamma(\alpha)}\int_a^t f(\tau)(t-\tau)^{\alpha-1}d\tau. \tag{1.10}$$

The definition of Mittag-Leffler function $E_{\alpha,\beta}$ is given as:

$$E_{\alpha,\beta}(t) = \ \sum_{m\,=\,0}^{\infty}\frac{t^m}{\Gamma(\alpha m+\beta)'}(\alpha >\ 0), \beta >\ 0). \tag{1.11}$$

It is therefore very essential to have a better understanding of some of the advantages and limitations associated with these fractional order derivatives before employing them to solve problems addressed in this research.

Advantages of Fractional Differentiation

As stated earlier that the most widely used fractional derivatives in the field of scientific research are the Riemann-Liouville, Caputo, Caputo-Fabrizio and Atangana-Baleanu fractional derivatives. Thus, this section highlights some of the advantages associated with these fractional operators. For instance, the Caputo fractional derivative has shown its significant advantage when solving real-world problems. The Caputo differential operator which utilizes the power law, is more suitable for modeling elastic, homogeneous subsurface. Accordingly, this derivative enables the use of both standard initial and boundary conditions during modeling process (Atangana and Secer, 2013), and has the ability to present the initial conditions with a clear definition (Sontakke and Shaikh, 2015). In addition, the Caputo derivative is said to be mathematically bounded, which implies that the derivative of a constant in Caputo sense is zero (0). Furthermore, the Riemann-Liouville fractional derivative is also suitable for solution of real world problems such as in the field of viscoelasticity (Heymans and Podlubny, 2005). This fractional derivative also has the ability to depict issues related to anomalous diffusion process (Li *et al*., 2011). To add, both the Riemann-Liouville and Caputo fractional derivatives can be used in various areas of science including application to model heat flow in the field of engineering (Yang *et al.*, 2016; Hristov and El Ganaoui, 2013; Hussein, 2015).

In addition, the fractional integrals of both the Caputo and Riemann-Liouville are very useful when deriving solution of linear fractional differential equations (Gladkina *et al*., 2018). Also, these fractional derivatives are considered as non-local operators but have singular kernels. Nonetheless, the non-locality of their kernels has the ability to account for the memory effect (Zhang *et al*., 2017). Alternatively, Caputo and Fabrizio (2015) proposed a new modified version of Caputo fractional derivative with the aim to overcome some of the drawbacks that were encountered with the Caputo and Riemann-Liouville fractional derivatives. This new fractional derivative is known as the Caputo-Fabrizio (CF) fractional derivative and is based on the exponential law. It is a very suitable derivative to model subsurface heterogeneities and structures at different scales (Al-Salti *et al*., 2016; Caputo and Fabrizio, 2016). Furthermore, the CF operator employs an exponential kernel with no singularities (Ali *et al*., 2016). Therefore, due to the non-singularity of its kernel, the memory effect can be well addressed (Atangana and Alkahtani, 2015; Atangana and Alqahtani, 2016). To add, this derivative is appropriate for use with both the Laplace and Fourier transforms (Caputo and Fabrizio, 2015).

Another fractional operator, which is found to be very accurate in solving more complex real-world systems, is the Atangana-Baleanu fractional derivative. This differential operator is based on the Mittag-Leffler law (Atangana and Alqahtani, 2016) and is more suitable to model all types of geologic formations including the homogeneous, heterogeneous and viscoelastic subsurfaces. The Mittag-Leffler function is also very appropriate to solutions involving linear and non-linear fractional differential equations. This differential operator (AB derivative) comes along with some additional advantages over other fractional operators because it employs both non-local and non-singular kernels (Atangana and Koca, 2016). Due to the non-singularity and non-locality of its kernel, it allows an easy expression with regard to the behavior of groundwater flow in viscoelastic materials (Alkahtani and Atangana, 2016; Ali *et al*., 2016) and the effect of memory within the structure at different scales. To add, this derivative is fit for use with the Laplace transform (Ali *et al*., 2016). In actual facts, the Atangana-Baleanu fractional derivative incorporates all the properties of other fractional derivatives and this makes it a very useful tool to address issues of real-world situations (Zhang *et al.,* 2017).

Limitations of Fractional Differentiation

Although these fractional derivatives are becoming more advantageous in the field of science, they have some limitations for application in other scenarios. For example, the Riemann-Liouville has some drawbacks especially when coupled with fractional differential equations to solve real-world problems. Unlike the Caputo, the derivative of a function for a constant term in Riemann-Liouville sense does not equal to zero (Atangana and Secer, 2013). In addition, with the Riemann-Liouville derivative, the description of initial conditions of non-integer order is a requirement and if not provided with a clear definition, then its application remains a complex issue (Sontakke and Shaikh, 2015). Even though the Caputo derivative is the most popular, but it is quite intensive to apply as it requires the fractional derivative of a function to be calculated before performing the computations of such a function in Caputo sense (Atangana and Secer, 2013). In addition, the Caputo derivative is only suited for differentiable functions.

Furthermore, both the Caputo and Riemann-Liouville are non-local fractional derivatives with singular kernels. As a result, the singularity of the kernel restricts their application when solving problems in real-world scenarios (Zhang *et al*., 2017). Thus, the description of the heterogeneity at different scales cannot be fully accounted with fractional derivatives utilizing a singular kernel. Again, with the Caputo-Fabrizio fractional derivative, although it was pointed out that its kernel is non-singular, but the operator is still not considered non-local (Atangana and Koca, 2016).

1.2 PROBLEM STATEMENT

Modeling of contaminated groundwater systems is a very challenging issue due to the invisibility of the nature of groundwater flow processes, as well as spatial variability of the subsurface environments. In actual facts, what really happens in the field is different from what models performed under laboratory experiments portray, hence uncertainties inherent in porous medium will have an effect on the transport and fate of a contaminant in the subsurface (Qin *et al*., 2008). These uncertainties as mentioned in previous paragraphs emerge from different sources and may have an undesirable impact on model predictions. Thus, the processes describing the flow and transport of contaminants in the geologic medium are considered stochastic (Lin and Tartakovsky, 2010). Some literature however, assumes that the aquifer parameters are constant at every point within the geological formation. Nevertheless, such assumptions become practically invalid because the subsurface is characterized by heterogeneity and aquifer parameters are not known with certainty. It is therefore very preferable to capture such uncertainties and heterogeneities using the concept of stochastic modeling. Nonetheless, some models fail to provide reliable groundwater flow estimates due to their inability to account for the heterogeneity, viscoelasticity and memory effect. The concept of differentiation is therefore very suitable to model groundwater flow behavior in different types of geological formations. It is therefore among some of the reasons that different mathematical models are nowadays being suggested with the aim to come up with a model that will enhance the solution of groundwater flow related problems with great success.

In this study, modeling of groundwater flow problems will be based on the aforementioned 1-D advection-dispersion equation (ADE) by coupling the concept of fractional differential and integral operators with stochastic approach in order to account for the uncertainty of parameters within the advection-dispersion equation, that impact on the groundwater flow and transport of contaminants in the subsurface. Despite the great advantages of both fractional differentiation and stochastic approach previously mentioned, the main challenge is that in the past decades these two approaches were each applied separately for solution of real-world problems. Therefore, this study is going to utilize the advantages of both fractional derivatives and stochastic methods to formulate a new method for modeling groundwater flow problems. This new approach is developed with the idea of capturing randomness with respect to flow and contaminant transport within the aquifer systems and account for the heterogeneity and memory effects by incorporating the concept of fractional differentiation.

1.3 AIMS AND OBJECTIVES

The study aims to develop a new method for modeling groundwater flow problems by incorporating the concept of fractional differentiation and stochastic approach into transport equation. This is done with the purpose of accounting for the heterogeneity and memory effects at field scale.

Objectives

The aim will be achieved through the following objectives:

1.3.1 Reviewing of a simple one-dimensional advection-dispersion equation.

1.3.2 Application of stochastic approach to perform the uncertainty analysis on the parameters that are associated with flow and contaminant transport.

1.3.3 Quantification of the mean and variances of dispersion coefficient (D), seepage velocity (v) and retardation factor (R).

1.3.4 Solution of advection-dispersion equation using numerical method based on the probability distributions of input parameters.

1.3.5 Modification of a one-dimensional (1-D) advection-dispersion equation by making use of fractional differentiation.

1.3.6 Obtaining the approximate solutions using the concept of fractional derivatives and stochastic approach.

1.3.7 Obtaining a modified transport equation using the concept of uncertainties function.

1.4 RESEARCH FRAMEWORK

The framework used to achieve the aim and objectives of this study is presented as follows:

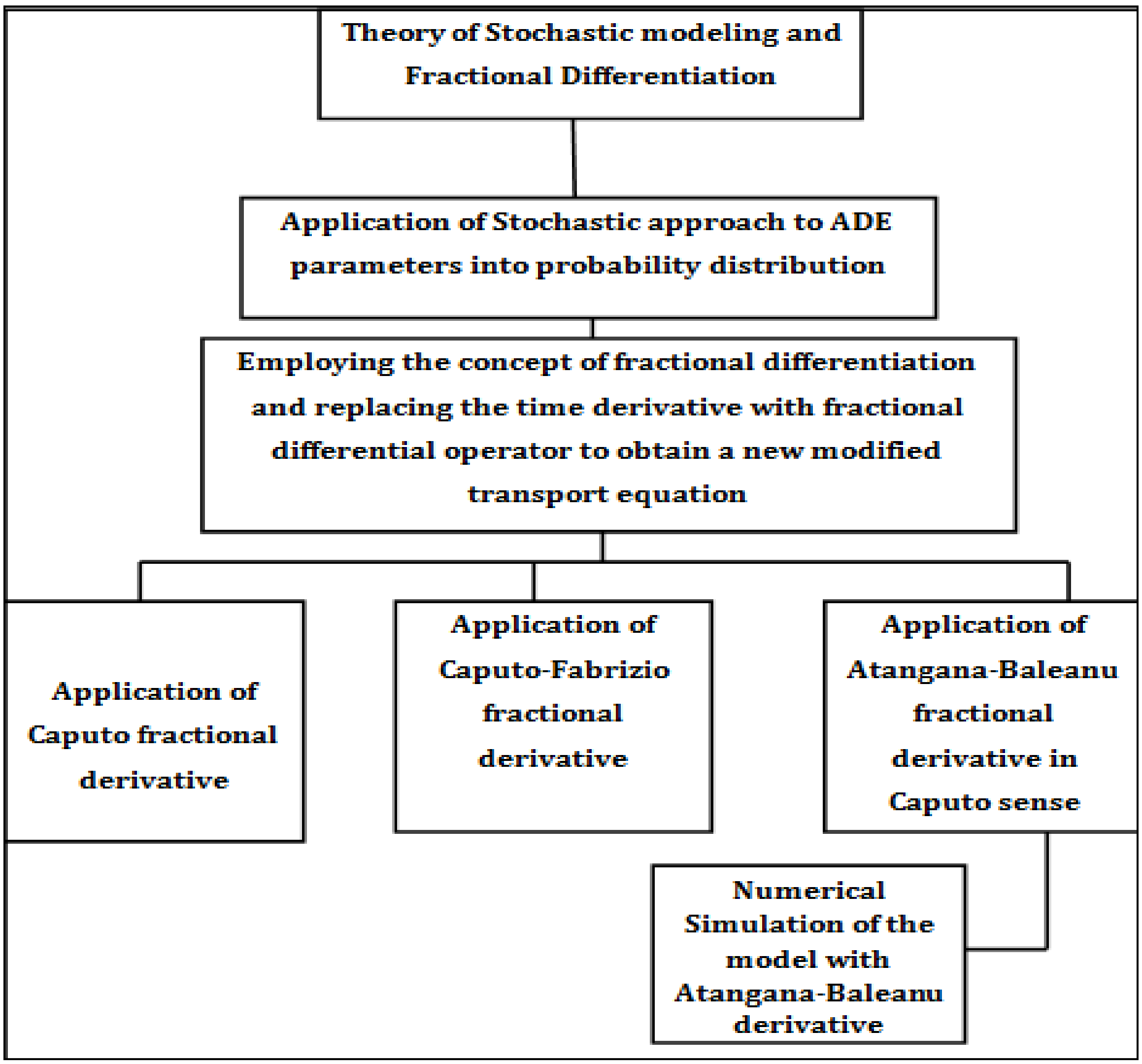

Figure 1: Study Research framework

1.5 DISSERTATION OUTLINE

This dissertation is outlined as follows: Chapter 1 provides a background to the behavior of a migrating contaminant under the advection and dispersion transport processes within a porous groundwater system. This chapter also provides us with the advantages and limitations associated with stochastic approach and fractional differentiation as these concepts will be used to model groundwater flow problems in this study. In addition, the definitions and properties of most widely used fractional derivatives in fields of science are also presented. Chapter 2 presents the application of these two concepts to the modification of advection-dispersion transport equation. Furthermore, Chapter 3 provides the numerical solution of groundwater flow and transport within a porous medium in the case of Caputo, Caputo-Fabrizio and Atangana-Baleanu fractional derivatives. Finally, Chapter 4 and 5 entail the analysis of stability and presentation of numerical simulations in the case of Atangana-Baleanu derivative, respectively. Thereafter, the conclusion follows.

CHAPTER 2: FRACTIONAL-STOCHASTIC MODELING

2.1 INTRODUCTION

Within an aquifer system, the contaminants usually travel with moving groundwater, and thus, any geologic material properties and aquifer parameters influencing the behavior of groundwater flow are very likely to affect the movement of contaminants within aquifers (Jaiswal and Kumar, 2011). However, the major challenge is that, the natural environments through which these contaminants move are invisible and stochastic processes influencing flow and solute movement are not or cannot be known with certainty. It is therefore very essential to account for the parameter uncertainty into models in order to boost confidence in model predictions (Illangasekare and Saenton, 2004). Hence, the need for a mathematical model that will better simulate the uncertainties associated with flow and contaminants transport within any given geologic medium under various conditions. Because flow and solute transport is a non-uniform process, a number of stochastic techniques and fractional operators have been suggested in the literature with the focus of developing a better model that will account for the heterogeneity effects of the porous media.

This chapter therefore gives an overview of some important parameters within advection-dispersion equation that impact on groundwater flow and contaminant transport, their definitions as well as their associated probability distributions. Next, the brief discussion of the processes governing solute movement and the definitions of some important fractional derivatives in the field of science. Actually, this section gives an insight of how fractional derivatives and stochastic techniques are going to be employed for successful capturing of randomness with respect to flow and solute transport in porous media.

2.2 STOCHASTIC MODELING

As mentioned in the previous sections that the processes describing flow and transport of contaminants in the subsurface are considered stochastic, therefore, stochastic methods are very preferable when describing the behavior of solute movement in media characterized by random heterogeneity. Thus, a stochastic model represents a situation where uncertainty exists. In other words, it is a process that has some kind of randomness. A stochastic model of subsurface solute migration therefore describes the random movement of fluids in a porous media due to velocity variations influenced by the interactions between the fluid and the solid phase of the media (Verwoerd, 2004). Thus, to describe this subsurface stochastic flow and solute movement, the application of advection-dispersion equation (ADE) equation is considered (Lin and Tartakovsky, 2010). This means that, as indicated in Chapter 1, all the flow and solute transport parameters of interest must be treated as random so that their uncertainties can be accounted for.

Some literature however, approach the solution using ADE along with a set of initial and boundary conditions by assuming dispersion and velocity as constants (Jaiswal and Kumar, 2011). For example, Chegenizadeh *et al*., (2014) presented a 2-D Convection-Dispersion Equation to analyze contaminant movement through the soil, where the water content, dispersion coefficient and velocity were all assumed to be uniform. Another study was presented by Runkel (1996), in which they derived an analytical solution to advection-dispersion equation based on the constant-parameter for a continuous load of a finite duration, where a fixed, constant flow rate was maintained and the resultant dispersion assumed to be constant with space. However, these approaches become practically invalid at field scale (van Kooten, 1996) because in nature, heterogeneity does exist in subsurface environments (Wu *et al.*, 2004). And so, it must not be neglected during groundwater flow investigations so that any errors in model results can be avoided, hence incorrect model predictions.

In reality, parameters influencing flow and solute transport are not constants. However, depend on the temporal and spatial scales of the aquifer heterogeneities through which flow and transport takes place (Kumar *et al*., 2012). Consequently, to well describe solute migration in heterogeneous medium, the coefficients of ADE used must not be treated as constants (Sanskrityayn and Kumar, 2016; Simpson, 1978; Matheron and de Marsily, 1980; Pickens and Grisak, 1981a), but rather described as random. Therefore, to account for the concept of heterogeneity, this study will employ the theory of stochastic modeling, where constant parameters within the advection-dispersion transport equation are converted into distribution.

In this section, some important parameters within the ADE as well as transport processes that influence solute movement in the subsurface are briefly discussed. As stated in Chapter 1 that there are two main transport mechanisms through which a contaminant can migrate in groundwater systems including the advection and dispersion. Therefore, when a pollutant is first introduced in groundwater, advection process plays a key role in the transportation of such a pollutant at some early stages. Thus, the advection process refers to the transport of solutes from one location to another due to the bulk movement of flowing groundwater in the subsurface. In addition, the rate at which these solutes are transported depends on the velocity of flowing groundwater. The influencing velocity is therefore referred to as seepage velocity (v) or average water velocity (Dietrich *et* al., 2005).

The one-dimensional (1-D) transport equation, which describes the movement of a solute influenced by advection alone, is given as:

$$\frac{\partial C\ (x,t)}{\partial t} = -\ v_x \frac{\partial C\ (x,t)}{\partial x}. \tag{2.1}$$

The advection mass-flux ($J_{a,i}$) representing the movement of a contaminant with flowing groundwateris expressed as:

$$J_x = \ nCv_i, \tag{2.2}$$

where, C is the concentration of the transported solute and n is the total porosity.

Furthermore, as the process of solute movement progresses, the pollutants tend to be subjected to different stages of mixing with distance from the source, through a process known as hydrodynamic dispersion. The hydrodynamic dispersion results from variations in flow velocities and can comprise of molecular diffusion (at low flow velocities) and mechanical dispersion at increased velocities. The mechanical dispersion process resulting from increased flow velocities fluctuations then causes the spreading of a contaminant either longitudinal or transverse to the direction of groundwater flow, depending on the heterogeneity in hydraulic conductivity (Liu *et al*., 2004). Thus, mechanical dispersion is triggered by the mechanisms illustrated in Figure 2.

That is,

a) Due to some soil pores being large in size than others, this therefore allows water particles to move through them in a faster motion than those moving through tiny pores (slowed motion).
b) Another factor is that, some of the water particles move along more tortuous flow paths, which results in longer times travelled but for the same linear distance.
c) In addition, movement of water particles occurring close to the soil pores is very slow due pore-water friction resulting from interactions between water particles and the edges of the pores, but faster at the center because of less or no friction involved.

The one-dimensional (1-D) dispersive transport equation, which describes the movement of a solute as influenced by dispersion alone, is given as:

$$\frac{\partial C\ (x,t)}{\partial t} = D\,\frac{\partial^2 C\ (x,t)}{\partial x^2}. \tag{2.3}$$

The dispersive mass flux is given by:

$$J_{d,i} = -D_{d,ij}\,\frac{\partial C}{\partial x_i}, \tag{2.4}$$

where, D is the dispersive tensor.

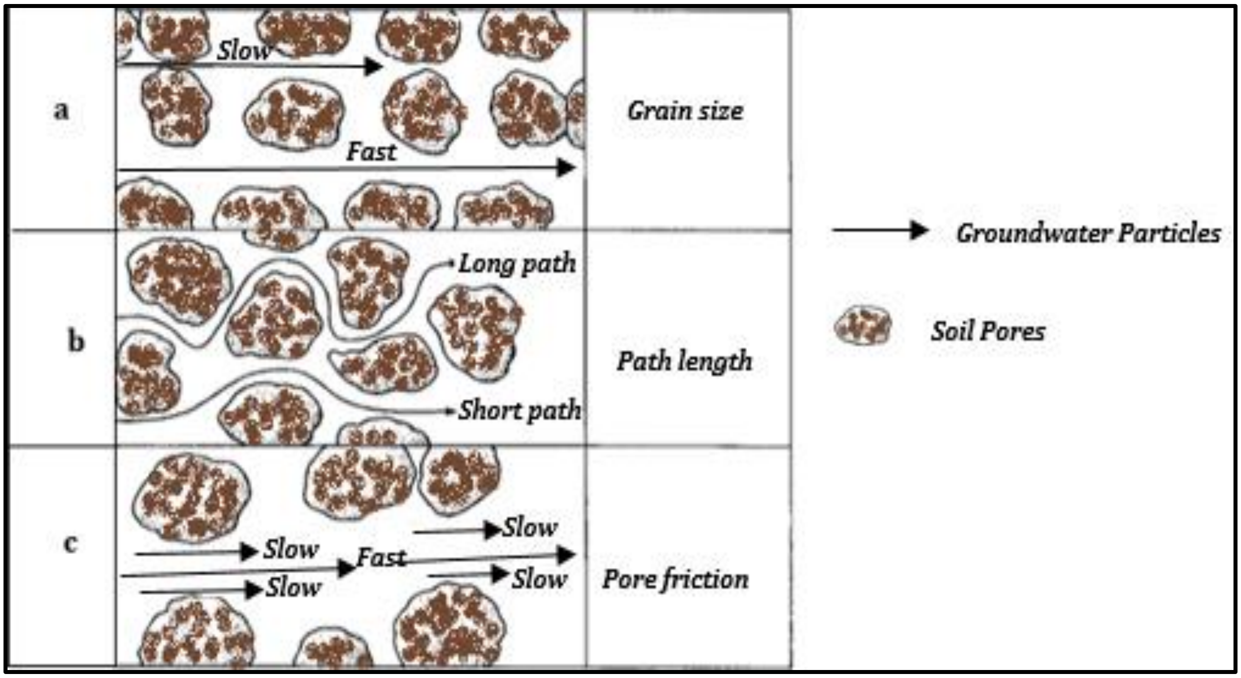

Figure 2: Factors causing mechanical dispersion (Freeze and Cherry, 1979)

However, during solute transport, the sorption reaction (interactions between the fluid and solid phase) sometimes becomes the determining factor for the movement and fate of contaminants in the subsurface, and thus, sorption must not be neglected during contamination risk assessment and management (Miller and Weber, 1986).

2.2.1 Parameters within Advection-Dispersion Transport Equation

Having being said previously, that the movement of solutes in the subsurface is well described in terms of the ADE. Therefore, some important groundwater flow and transport parameters considered in this research are discussed below. These include the seepage velocity (v), dispersion coefficient (D) and the retardation factor (R).

2.2.1.1 Seepage Velocity/Average Linear Velocity (v)

The seepage velocity of the flowing groundwater is undoubtedly a parameter that influences the movement and mixing of solutes in groundwater. This is the velocity of groundwater calculated from Darcy's law and is simply described as the bulk movement of water per unit time per unit cross-sectional area of available voids. It can simply be expressed as (Dietrich *et al*., 2005):

$$v_i = \frac{q_i}{n_e}, \tag{2.5}$$

where, v_i is the seepage, n_e and q_i are the effective porosity and the specific discharge, respectively.

The seepage velocity as previously mentioned, influences the transport of dissolved mass through a process known as advection. Thus, the pore velocity is considered as one of the main parameters governing the transport of pollutants in the subsurface (Zhang and Winter, 2000). The distribution of this flow velocity is considered not uniform, hence varies with both space and time due to the presence of inhomogeneity and anisotropy in porous media (Fitts, 2002). In nature, different aquifer systems differ in terms of their geologic settings with regard to distance, and thus, the existence of variable field flow velocities is a reality. For instance, velocity of a fluid flowing through fractures will differ from flow velocities at locations where the aquifer exhibits no fractures because of differing geological properties.

It is therefore very important not to assume constant coefficients when describing solute migration with ADE (Sanskrityayn and Kumar, 2016; Simpson, 1978; Matheron and de Marsily, 1980; Pickens and Grisak, 1981a). In addition, groundwater flow velocities are said to be spatially and temporally dependent (Sanskrityayn and Kumar, 2016). Accordingly, the temporal dependency in flow velocities is due to time variable hydraulic gradient while the spatial dependency is a cause of hydraulic conductivity, which varies with location (Yadav and Kumar, 2018).

2.2.1.2 Dispersion Coefficient (D)

The dispersion coefficient is simply defined as a measure of the spreading of a flowing fluid as influenced by the geological setting of the porous media, resulting from both the coefficients of mechanical dispersion and molecular diffusion within a porous geological system. The influencing factor for the solute dispersion at microscopic scale is the spatial variability of flow velocities due to porous media characteristics such as porosity, tortuosity and dead-end pores (Hunt *et al*., 2010). This means that the degree of a spreading solute is reliant on distributions groundwater flow velocity within the porous media. Alternatively, dispersion at a macroscopic scale is caused by velocity fluctuations arising from variable hydraulic conductivities (Fleurant and Van Der Lee, 2001). Thus, the dispersion processes are considerably scale dependent (Raoof and Hassanizadeh, 2013), that is, differ from one scale to another. For instance, field scale studies have indicated that the dispersion coefficient increases with distance as the contaminant travels away from the point of source (Serrano, 1988; Sudiky and Cherry, 1979; Dieulin *et al*., 1980). Moreover, dispersivity can be determined based on two components. That is, the longitudinal dispersivity occuring along the local groundwater flow velocity and the transverse dispersivity taking place perpendicular to groundwater velocity.

Since dispersion is dependent on flow velocities, then molecular diffusion will dominate only at low flow velocities whereas mechanical dispersion occurs at high flow velocities. However, according to Moezed *et al*., (2009); Gillham and Cherry (1982), molecular diffusion is only considered at flow velocities not greater than 10 cm s^{-1}. To add, the macro-dispersion coefficient, which is quantified based on the average linear velocity of groundwater may be expressed as follows (Lee *et al*., 2018; Zheng and Bennett, 2002).

$$D_e(x) = [\alpha_L(x) - \alpha_T(x)]\frac{v_i v_j}{\bar{v}} + D_0(x), \quad i,j = 1,2, \tag{2.6}$$

where, $D_e(x)$ is macro-dispersion coefficient, $\alpha_L(x)$ and $\alpha_T(x)$ are the longitudinal and transverse dispersivities, respectively. v_i and v_j are the groundwater velocities occurring indifferent points within the porous fractures, and $\bar{v}$ is the measure of seepage velocity. Whereas, $D_0(x)$ is the coefficient of effective molecular diffusion.

2.2.1.3 Retardation Factor (R)

The retardation factor (R) may be referred to as the measure of the amount of contaminant as slowed through sorption by the geologic materials relative to groundwater flow velocity.

Accordingly, when a contaminant is transported in groundwater, the movement and fate along the flow directions may be affected by its interactions with the medium phase especially in low flow velocities, thus, resulting in retardation of solute movement (van Kooten, 1996). This is because different types of pollutants react differently with different aquifer materials depending on the nature of flow paths along which they travel as well as variable rates at which groundwater flow occurs. Once retardation occurs, the rate of movement of a contaminant tend to be slower than that of groundwater, hence contaminant fate at that stage will differ depending on the geologic settings of the medium. According to Schäfer and Kinzelbach, (1995), the retardation factor is a random variable in space.

Thus, the spatial variability in both field flow velocity and retardation factor is considered as the factor influencing the migration of reactive solutes through porous media characterised by heterogeneity (Mojida and Vereecken, 2004). In cases where sorption does not occur at all, the rate at which solute movement happens can therefore be determined based on groundwater flow velocities (Fitts, 2002). This means that all the solute particles found in the free-phase (non-adsorbing) are susceptible to advection and dispersion mechanisms.

The retardation factor (R) is expressed as:

$$R = 1 + \left(\frac{\rho_b K_d}{N}\right), \qquad (2.7)$$

where, R is the retardation coefficient (unitless parameter), ρ_b is the aquifer bulk density (M/L^3), K_d is the distribution coefficient (L^3/M) and N is the porosity (L^3/L^3).

2.2.2 Illustration of Probability Distributions Associated with Groundwater Flow and Solute Transport Parameters

In nature, groundwater flow models are associated with uncertainties, and thus, these uncertainties can also be addressed by employing stochastic (statistical) approach. However, the main challenge to application of these approach is that, the statistical characteristics of random variables of interest (e.g. the mean, variance, covariance etc.) must first be estimated before stochastic techniques can be employed (Dong *et al*., 2017). Nevertheless, such statistical characteristics are very difficult to calculate when limited or insufficient data is available. Therefore, when doing stochastic analysis, researchers address any uncertainty that may be present in hydrogeological parameters by means of a probability density function (PDF) (Baalousha, 2003). Thus, a model is considered stochastic if any of its parameters conforms to a probability distribution.

Additionally, the most famously used geostatistical approach in stochastic analysis when describing the heterogeneity of the aquifer in terms of first and second moments of a probability distribution function (*pdf*), are mainly known as the mean and the variance/covariance, respectively (Illangasekare and Saenton, 2004). Note that, this probability distribution can vary between the variables and/or change with location (Dey, 2010).

When performing statistical analysis, if a certain parameter distribution is not known, but a set of data points $\{x_1, x_2 \dots x_n\}$ is available (Loucks *et al*., 2005), then the statistical moments of unknown distribution of x can be determined based on the sample values using the given eqs. (2.8 and 2.9).

That is, if n points in the aquifer are sampled, then the sample estimate for the mean is given by:

$$\bar{x} = \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right) = \frac{x_1 + x_2 + \dots x_n}{n}. \tag{2.8}$$

By taking note that $\bar{x}$ is the mean, with the $(x_1 + x_2 + \dots x_n)$ denoting the sum of all samples or observations, and n representing the sample number. Then, the sample estimate for the variance is obtained as:

$$\sigma_x^2 = S_x^2 = \frac{1}{n}\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right),$$

$$\sigma_x^2 = \frac{(x_1 - \bar{x}) + (x_2 - \bar{x}) + \cdots (x_n - \bar{x})}{n}, \tag{2.9}$$

$$\sigma_x^2 = \frac{(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + \ldots (x_n - \bar{x})^2}{n}.$$

Thus, the focus of this section is to express parameters within groundwater transport equation $(D, v \; and \; R)$ in terms of their statistical moments (*mean and variance*) and probability distributions. Normally, the type of statistical distribution employed depends on the situation to be dealt with. The illustrations are presented as follows:

For the Dispersion Coefficient (D):

Let us suppose the range of D, such that $D \in [a_1, a_2, \ldots a_n]$

Therefore, the arithmetic mean and variance denoting to dispersion coefficient (D) can simply be estimated from the following equations.

Mean:

$$\bar{\mathrm{D}} = \frac{1}{n}\left(\sum_{i=1}^{n} a_i\right) = \frac{a_1 + a_2 + \ldots + a_n}{n}. \tag{2.10}$$

Variance:

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(a_i - \bar{D})^2. \tag{2.11}$$

The variance and the mean dispersion coefficient can be approximated by both the normal (Gaussian) and log-normal (log-Gaussian) distributions. However, according to Hiscock and

Bense (2014), both laboratory and field observations show that the spreading of solute mass due to dispersion in a porous media follows a normal (Gaussian) distribution.

We convert the constant dispersion (D) input parameter into distribution and use the normal distribution as follows:

$$\widehat{D} = \overline{D} + \gamma N(\overline{D}, \sigma^2), \tag{2.12}$$

where, γ is the stochastic constant and $N(\cdot)$ represents the normal distribution given as:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\overline{D})^2}{2\sigma^2}\right], \tag{2.13}$$

where, $\overline{D}$ is the mean for the dispersion coefficient.

On the other hand, the variance and the mean for the dispersion coefficient in terms of the log-normal distribution may be approximated as follows.

$$\widehat{D} = \overline{D} + \gamma \log N\,(\overline{D}, \sigma^2), \tag{2.14}$$

where, γ is the stochastic constant and $\log N(\cdot)$ represents the log-normal distribution given as:

$$f(x) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{(\ln x-\overline{D})^2}{2\sigma^2}\right]. \tag{2.15}$$

For the Seepage Velocity (v):

We suppose the range of v, such that $v \in [b_1, b_2, \dots b_n]$

Then, the mean denoting to seepage velocity (v) is given as:

$$\bar{v} = \frac{1}{n}\left(\sum_{i=1}^{n} b_i\right) = \frac{b_1 + \ b_2 + \ldots + b_n}{n}. \tag{2.16}$$

Variance:

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(b_i - \bar{v})^2. \tag{2.17}$$

The probability distribution of groundwater velocity is said to be direction dependent. Thus, the probability distribution can change with location, meaning that longitudinal and transverse velocities will have different probability distributions (Dey, 2010). Cooke *et al*. (1995) and Biggar & Nielsen (1976) applied several probability distributions including the log-Gaussian, beta, gamma, Weibull, Pearson Type V and the Gumbel distributions in their work to approximate the variance and the mean seepage velocity distribution. Nevertheless, the velocity is well described by log-normal (non-Gaussian) than normal (Gaussian) distribution (Englert, 2003). However, with variances less than 0.1, the probability distribution of velocities conforms to a Gaussian shape (Fleurant and Van Der Lee, 2001).

We follow the same procedure as in dispersion coefficient estimation in the previous section to convert the constant velocity (v) input parameter into distribution and apply the normal distribution as follows:

$$\hat{v} = \ \bar{v} + \gamma N(\bar{v}, \sigma^2), \tag{2.18}$$

where, γ is the stochastic constant and $N(\cdot)$ represents the normal distribution given as:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{(x-\bar{v})^2}{2\sigma^2}\right]. \tag{2.19}$$

where, $\bar{v}$ is the mean estimate for the groundwater velocity.

Moreover, the variance and the mean for the seepage velocity can also be approximated using the log-normal distribution as follows.

$$\hat{v} = \bar{v} + \gamma \log N\,(\bar{v}, \sigma^2), \tag{2.20}$$

where, γ is the stochastic constant and $\log N\,(\cdot)$ represents the log-normal distribution given as:

$$f(x) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{(\ln x - \bar{v})^2}{2\sigma^2}\right]. \tag{2.21}$$

For Retardation Factor (R):

We assume the range of R, such that $R \in [c_{1,} c_2, \dots c_n]$

Similarly, the mean denoting to retardation factor (R) is given as:

$$\bar{R} = \frac{1}{n}\left(\sum_{i=1}^{n} c_i\right) = \frac{c_1 + c_2 + \ldots + c_n}{n}. \tag{2.22}$$

Variance:

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(c_i - \bar{R})^2. \tag{2.23}$$

The variance and mean distribution of the retardation factor can be approximated by log-normal distribution (Lemaire and Bjerg, 2017). Consequently, the distribution of K_d values is commonly assumed to be log-normally distributed (Kaplan *et al*., 1995; Van Genuchten and Wierenga, 1986; Hillel, 1980).

Likewise, we follow the same procedure to transform the constant retardation factor into probability distribution as follows:

$$\hat{R} = \bar{R} + \gamma N(\bar{R}, \sigma^2), \tag{2.24}$$

where, γ is the stochastic constant and $N(\cdot)$ represents the normal distribution given as:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\bar{R})^2}{2\sigma^2}\right], \tag{2.25}$$

where, $\bar{R}$ is the mean estimate denoting to retardation factor.

To add, the variance and the mean for the retardation factor may be approximated using the log-normal distribution as follows.

$$\hat{R} = \bar{R} + \gamma \log N\,(\bar{R}, \sigma^2), \tag{2.26}$$

where, γ is the stochastic constant and $\log N\,(\cdot)$ represents the log-normal distribution given as:

$$f(x) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{(\ln x-\bar{R})^2}{2\sigma^2}\right]. \tag{2.27}$$

Besides the importance of stochastic modeling being able to capture some statistical setting of nature with great success, it is however, not fit capture some behavior of nature such as fading memory. For instance, fading memory for groundwater velocity fluctuations. It is therefore preferable to employ the concept of fractional differentiation to account for those scenarios that stochastic methods is unable to capture such as the effect of memory and viscoelasticity in porous media.

Substituting the ADE input parameters *v, D and R* with their transformed statistical distributions as $\hat{v}$, $\hat{D}$ and $\hat{R}$ respectively, such that eq. (1.1) becomes a new modified advection-dispersion equation.

First, let us recall the distributions presented earlier for each sample where,

$$\widehat{D} = \overline{D} + \gamma N(\overline{D}, \sigma^2), \qquad \hat{v} = \bar{v} + \gamma N(\bar{v}, \sigma^2), \qquad \hat{R} = \bar{R} + \gamma N(\bar{R}, \sigma^2).$$

Therefore, eq. (1.1) is transformed into the following equation:

$$\frac{\partial C(x,t)}{\partial t} = \left(\overline{D} + \gamma N(\overline{D}, \sigma^2)\right)\frac{\partial^2 C(x,t)}{\partial x^2} - \left(\bar{v} + \gamma N(\bar{v}, \sigma^2)\right)\frac{\partial C(x,t)}{\partial x} - \left(\bar{R} + \gamma N(\bar{R}, \sigma^2)\right)\lambda C(x,t), \tag{2.28}$$

or,

$$\widehat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t) = \frac{\partial C(x,t)}{\partial t}. \tag{2.29}$$

We then present an illustration of the above equation (2.29) based on the theory of fractional differentiation to generate equation (2.30) below. We substitute the time derivative $\left(\frac{\partial C}{\partial t}\right)$ with a time fractional operator $\left({}_0^F D_t^{\alpha}\right)$ and obtain the following form of equation:

$${}_0^F D_t^{\alpha} C(x,t) = \widehat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t). \tag{2.30}$$

2.3 FRACTIONAL DIFFERENTIATION

As indicated in Chapter 1, this study is as well going to employ the concept of fractional differentiation with the focus of developing of a new method that will help in the solution of problems related to groundwater flow and solute transport in real world situations. The concept of differential and integral operators has the benefits to account for some of the phenomena that cannot be captured with stochastic approach and these may include the memory effect and viscoelasticity of the porous media at different scales. In addition, the development or advancement made with regard to fractional calculus has also shown some great success in the investigation of transport within the groundwater systems (Mirza and Vieru, 2016). Literature suggests that the most commonly used fractional derivatives in the fields of science are the Riemann-Liouville, Caputo, Caputo-Fabrizio and the Atangana-

Baleanu derivatives (refer to Chapter 1). In this section, we recall some of the advantages and the definitions of these fractional operators. Some examples from literature in which these derivatives have been applied are also given. Next, we employ these fractional operators to our transport equation to derive a modified equation that will be used to solve problems of real world.

Riemann-Liouville Fractional Derivative (RLFD)

The RLFD, which is based on power law kernel has shown some success in the fields of science including application in physics for simulations of anomalous diffusion (Li *et al*., 2011; Zhuang *et al*., 2008; Ervein *et al*., 2007), viscoelasticity flows (Baleanu and Fernandez, 2017; Liu and Li, 2015; Mainardi, 2010). To add, it can also be applied to address the non-Markovian anomalous subdiffusive processes (Zhuang *et al.*, 2008). Furthermore, it is an appropriate derivative for use in solution of linear fractional differential equations (FDEs) (Gladkina *et al*., 2018; Antoly *et al*., 2006). For example, Owolabi (2018) applied the RL derivative to model chaotic differential equations in which the focus of his work was on the stability analysis and numerical solution of chaotic time fractional equations. It is also a suitable derivative for use with the Laplace transform with respect to time and space components (Atangana and Kilicman, 2013), but it is argued that its Laplace transform presents insignificant physical terms (Mirza and Vieru, 2016).

Definition for Riemann-Liouville derivative of fractional orderα of function $f(t)$is given as:

$$ {}_{0}^{RL}D_{t}^{\alpha} f(t) = \frac{d^n}{dt^n} D^{-(n-\alpha)}\, f(t) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_0^t (t-\tau)^{n-\alpha-1}\, f(\tau) d\tau. \qquad (2.31) $$

The Riemann-Liouville fractional integral of order α for a function $f(t) \in C^1([0,b],\mathbb{R}^n)$; $b > 0$ is given as:

$$ {}_{0}^{RL}I_{t}^{\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1}\, f(\tau) d\tau, 0 < \alpha < \infty. \qquad (2.32) $$

where, $\Gamma(\cdot)$ is the Euler's gamma function.

Caputo Fractional Derivative (CFD)

The CFD, which is also based on power function, is a fractional operator very appropriate for use to solution of linear fractional differential equations (FDEs) (Gladkina *et al*., 2018; Anatoly *et al*., 2006; Stefan *et al*., 1993). This derivative is very appropriate than the RL derivative when addressing real world problems as it can enhance the description of standard initial and boundary conditions (Kavvas *et al*., 2017; Podlubny, 1998). The CFD also enhances the description of the effect of memory effect, but lacks accuracy due to the singularity of its kernel (Gómez-Aguilar, *et al.*, 2016; Caputo and Fabrizio, 2015). In addition, this derivative has shown its great success for use with the Laplace transform with respect to time and space components of fractional operators. For example, Atangana and Kiliçman (2013) managed to derive an analytical solution of the space-time Caputo fractional derivative of classical hydrodynamic advection-dispersion equation. Another study was done by Wanga *et* al. (2007), where they used the definition of Caputo derivative to determine solutions of time-fractional diffusion equation and its applications in fractional quantum mechanics.

Definition for Caputo fractional derivative:

Let $b > 0, f \in H^1(0,b)$ and $0 < \alpha > 1$, *then the Caputo fractional derivative of function of* $f(t)$ *of order* α*is given as*:

$$ {}_0^cD_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} f'(\tau)d\tau. \tag{2.33}$$

Now, let us recall our eq. (2.29). Then, by replacing the time-derivative with Caputo time-fractional derivative we obtain the following:

$$ {}_0^CD_t^\alpha C(x,t) = \widehat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda\hat{R}C(x,t), \tag{2.34}$$

or,

$$\frac{1}{\Gamma(1-\alpha)}\int_0^t (t-\tau)^{-\alpha} f'(\tau)d\tau = \widehat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda\hat{R}C(x,t).$$

Caputo-Fabrizio Fractional Derivative (CFFD)

A new version of fractional derivative (Caputo-Fabrizio derivative) was recently proposed by Caputo and Fabrizio in order to overcome the limitations observed with the aforementioned Caputo and Riemann-Liouville derivatives. This new derivative with fractional order with non-singular kernel is considered among some of the very useful fractional derivatives based on its abilities to account for medium heterogeneities and structures at different scales (Al-Salti *et al*., 2016; Caputo and Fabrizio, 2016). The definition of Caputo-Fabrizio derivative is based on the convolution of a first order derivative with exponential function and it is also very useful in the expression of diffusion substances at various scales (Atangana and Alkahtani, 2015).

Furthermore, the Caputo-Fabrizio temporal-fractional derivative is fit for use with the Laplace transform, whereas the Fourier transform can be incorporated for spatial representations of the Caputo-Fabrizio derivative (Shan and Khan, 2016). For instance, Mirza and Vieru (2016) were able to obtain a solution to their study involving the use of Laplace transform with respect to the temporal variable t, as well as the sine-Fourier and the exponential-Fourier transforms with respect to y and x variables, respectively. To validate the capabilities of this new derivative, Alkahtani and Atangana (2016) successfully applied the new CFFD with fractional order to determine the behavior of the movement of waves on the surface of shallow water by making use of the properties of this new derivative as it can depict the migration of substances at different scales.

The definition of fractional Caputo-Fabrizio derivative:

Let $f \in H^1(a,b), b > a, \alpha \in [0,1]$, *then the definition of the Caputo-Fabrizio fractional derivative is given as follows:*

$$
{}_{0}^{CF}D_t^{\alpha} f(t) = \frac{M(\alpha)}{1-\alpha} \int_a^t f'(\tau) \exp\left[-\alpha \frac{t-\tau}{1-\alpha}\right] d\tau, \tag{2.35}
$$

$$
{}_{0}^{CF}D_t^{\alpha} f(t) = \frac{\alpha M(\alpha)}{1-\alpha} \int_a^t (f(t) - f(\tau)) \exp\left[-\alpha \frac{t-\tau}{1-\alpha}\right] d\tau, \tag{2.36}
$$

Nevertheless, if the function is not within $H^1(a,b)$ then, the derivative is redefined as follows:

$$
{}_{0}^{CF}D_t^{\alpha} f(t) = \frac{\alpha M(\alpha)}{1-\alpha)} \int_a^t (f(t) - f(\tau)) \exp\left[-\alpha \frac{t-\tau}{1-\alpha}\right] d\tau. \tag{2.37}
$$

Similarly, we recall our eq. (2.29) and then replace the time-derivative with Caputo-Fabrizio time-fractional operator to generate the following:

$$
{}_{0}^{CF}D_t^{\alpha} C(x,t) = \widehat{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v} \frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t),
$$

or, (2.38)

$$
\frac{M(\alpha)}{1-\alpha} \int_a^t exp\left[-\frac{\alpha}{1-\alpha}(t-\tau)\right] f'(\tau) d\tau = \widehat{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v} \frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t).
$$

Atangana-Baleanu Fractional Derivative (ABFD)

The ABFD, based on the generalized Mittag-Leffler law is a fractional operator suggested by Atangana and Baleanu, and comprises both the non-local and non-singular kernels (Atangana and Baleanu, 2016). This means that the AB derivative is very fit for use when modeling the complexity of real-world problems within different kinds of geologic materials to address the concept of heterogeneity, viscoelasticity and the memory effect (Atangana and Baleanu, 2016; Atangana and Alqahtani, 2016). In addition, it is a very suitable derivative for use with the Laplace transform to describe some physical problems with initial conditions. To highlights among some of its applications with great success, Atangana and Alqahtani (2016) applied this derivative to the model of groundwater movement through an unconfined aquifer. In their study, the solution to the model incorporated the application of Mittag-Leffler function, which allows better description of the complexity of natural phenomena. To achieve their aim, they obtained the analytical and numerical solutions by making use of the Laplace transform operator and Crank-Nicolson technique, respectively. Furthermore, another study by Djida *et al*. (2016) entailed an application of Atangana-Baleanu fractional integral to model groundwater flow within a leaky aquifer. The approach to the solution of their problem was also based on Mittag-Leffler functions, then the analytical and numerical analysis were employed to derive their new model. In addition, Gómez-Aguilar *et al*. (2016)were able to employ Atangana-Baleanu fractional derivative in Liouville-Caputo and Riemann-Liouville sense to study electromagnetic waves in dielectric media.

Definition of Atangana-Baleanu fractional derivative in Riemann-Liouville sense is given as:

Let $f \in H^1(a,b), b > a, \alpha \in [0,1]$

Then,

$$ {}^{ABR}_{\ a}D_t^{\alpha}\big(f(t)\big) = \frac{B(\alpha)}{1-\alpha}\frac{d}{dt}\int_a^t f(\tau)E_\alpha\left[-\alpha\frac{(t-\tau)^\alpha}{1-\alpha}\right]d\tau;\ \ 0 < \alpha < 1. \tag{2.39}$$

Definition of Atangana-Baleanu fractional derivative in Caputo sense is given as:

Let $f \in H^1(a,b), b > a, \alpha \in [0,1]$

Then,

$$ {}^{ABC}_{\ a}D_t^{\alpha}\big(f(t)\big) = \frac{B(\alpha)}{1-\alpha}\int_a^t f'(\tau)E_\alpha\left[-\alpha\frac{(t-\tau)^\alpha}{1-\alpha}\right]d\tau; \qquad 0 < \alpha < 1. \tag{2.40}$$

Likewise, we recall eq. (2.29) and substitute the time-derivative with Atangana-Baleanu non-local fractional operator in Caputo sense to obtain the following:

$$ {}^{ABC}_{\ 0}D^{\alpha}_{t} C(x,t) \ = \ \widehat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda\hat{R}C(x,t), $$

or, (2.41)

$$ \frac{B(\alpha)}{1-\ \alpha}\int_{a}^{t} E_{\alpha}\left[-\frac{\alpha}{1-\ \alpha}(t-\tau)^{\alpha}\right] f'(\tau)d\tau = \widehat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda\hat{R}C(x,t). $$

The Atangana-Baleanu fractional integral of order αofa function f (t) is given as:

$$ {}^{AB}_{\ a}I^{\alpha}_{t}\big(f(t)\big) = \frac{1-\alpha}{B(\alpha)}\, f(t) + \frac{\alpha}{B(\alpha)\Gamma(\alpha)}\int_{a}^{t} f(\tau)(t-\tau)^{\alpha-1}d\tau. \tag{2.42} $$

The definition of Mittag-Leffler function $E_{\alpha,\beta}$is given as:

$$ E_{\alpha,\beta}(t) = \sum\nolimits_{m\,=\,0}^{\infty}\frac{t^m}{\Gamma(\alpha m+\beta)'}(\alpha >\ 0), \quad (\beta >\ 0). \tag{2.43} $$

Since literature provides quite a number of studies confirming the success of stochastic techniques and fractional differentiation application in various scientific research areas, including application in hydrogeology. However, these two approaches were both in the past years, applied separately in modeling concepts. Therefore, the theory behind this research is that, coupling of both stochastic techniques and the concepts of fractional differentiation can be used to enhance the development of a new approach towards estimation of groundwater flow and solute transport with the focus of accounting for any random motion, heterogeneity effects, viscoelasticity and the memory effect within the porous media. More importantly, the study will combine the two approaches in order to develop a modified groundwater transport equation that will better capture the behavior of advection and dispersion processes in complex groundwater systems.

CHAPTER 3: NUMERICAL SOLUTIONS

3.1 INTRODUCTION

Due to the changing behavior of the transport phenomenon in terms of time and space, the numerical solution of ADE becomes a challenging task. Therefore, there is a need for the formulation of a more acceptable numerical method in terms of stability, accuracy, algorithmic simplicity and computational efficiency (Andújar *et* al., 2011). There are various numerical solution techniques reported in the literature for solving advection-dispersion equation. Thus, the aim of this study as indicated earlier focuses on the development of a new approach for modeling groundwater related flow problems, by incorporating both the concept of fractional differentiation and stochastic techniques to develop a new groundwater transport equation.

Subsequently, this chapter presents some fractional derivatives and their applications in modeling groundwater problems. Next, the numerical solutions and stability analysis for each exact solution will also be provided.

3.2 NUMERICAL APPROXIMATIONS OF FRACTIONAL OPERATORS

In this section, the numerical approximations of the most widely used fractional derivatives are presented, notably the Caputo, Caputo-Fabrizio and Atangana-Baleanu fractional derivatives.

3.2.1 Numerical Approximation of the Caputo Derivative

As mentioned earlier in this study, the Caputo derivative which is based on the power function is very appropriate for modeling homogeneous, elastic geologic materials (refer to Chapter 2). It is also a suitable derivative for use with the Laplace transform with respect to time and space components of fractional operators. For the purpose of numerical analysis, Caputo fractional derivative is numerically approximated based on its definition as follows.

Let n be a positive integer greater than 1, then:

$$ {}_0^C D_t^{\alpha}\big(f(t_n)\big) = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_n} (t_n-\tau)^{-\alpha} \frac{d}{dt} f(\tau)\, d\tau. \tag{3.1} $$

Employing Crank-Nicolson Scheme yields:

$$ {}_0^C D_t^{\alpha}\big(f(t_n)\big) = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_n} (t_n-\tau)^{-\alpha} \frac{f(\Delta\tau+\tau)-f(\tau)}{\Delta\tau} d\tau, \tag{3.2} $$

$$ {}_0^C D_t^{\alpha}\big(f(t_k)\big) = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} \frac{f(t_{k+1})-f(t_k)}{\Delta t} (t_n-\tau)^{-\alpha} d\tau, \tag{3.3} $$

$$ = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \frac{f(t_{k+1})-f(t_k)}{\Delta t} \int_0^{t_n} (t_n-\tau)^{-\alpha} d\tau, \tag{3.4} $$

If $y = (t_n - \tau), y = t_n - t_{k+1}, y = t_n - t_k$ and, $dy = -d\tau \Rightarrow d\tau = -dy$

Then,

$$ {}_0^C D_t^{\alpha}\big(f(t_k)\big) = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \frac{f(t_{k+1})-f(t_k)}{\Delta t} \int_{t_n-t_k}^{t_n-t_{k+1}} y^{-\alpha}\,(-dy), \tag{3.5} $$

For any variable, $-\int_a^b f(x)dx = \int_b^a f(x)dx$

Therefore,

$$ {}_0^C D_t^{\alpha}\big(f(t_k)\big) = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \frac{f(t_{k+1})-f(t_k)}{\Delta t} \int_{t_n-t_{k+1}}^{t_n-t_k} y^{-\alpha}\, dy, \tag{3.6} $$

$$ = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \frac{f(t_{k+1})-f(t_k)}{\Delta t} \left(\int_{t_n-t_{k+1}}^{t_n-t_k} \frac{y^{-\alpha+1}}{-\alpha+1} \right), \tag{3.7} $$

$$ = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \frac{f(t_{k+1})-f(t_k)}{\Delta t} \left(\frac{y^{-\alpha+1}}{-\alpha+1} \right) \Bigg|_{t_n-t_{k+1}}^{t_n-t_k}, \tag{3.8} $$

Let $t = \Delta t,\ t_k = k\Delta t,\ t_n = n\Delta t,\ t_n - t_k = n\Delta t - k\Delta t,\ t_n - t_{k+1} = n\Delta t - (k+1)\Delta t$

$$ {}_0^C D_t^\alpha\big(f(t_n)\big) = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n} \frac{f(t_{k+1}) - f(t_k)}{\Delta t} \{(n\Delta t - k\Delta t)^{1-\alpha} \tag{3.9} $$
$$ - (n\Delta t - (k+1)\Delta t)^{1-\alpha}\}, $$

$$ = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n} \frac{f(t_{k+1}) - f(t_k)}{\Delta t} (\Delta t)^{1-\alpha}\{(n-k)^{1-\alpha} - (n-k-1)^{1-\alpha}\}. \tag{3.10} $$

3.2.2 Numerical Approximation to Caputo-Fabrizio (CF) Derivative

The Caputo-Fabrizio derivative is a new derivative with non-singular kernel recently introduced by Caputo and Fabrizio based on exponential law. It has shown a great success in the describing the heterogeneity of subsurface at different scales (refer to Chapter 2). Since the medium heterogeneity is among the factors that influence the behavior of groundwater flow and transport, this study will therefore employ the CF derivative in the solution of advection and dispersion problems.

The well-known Caputo-Fabrizio operator is given as:

$$ {}_0^{CF} D_t^\alpha f(t_n) = \frac{M(\alpha)}{1-\alpha} \int_0^{t_n} \frac{\partial}{\partial t} f(t) \exp\left[-\frac{\alpha}{1-\alpha}(t_n - \tau)\right] d\tau. \tag{3.11} $$

For simplicity of the numerical analysis, numerical approximation of the Caputo-Fabrizio derivative is presented as:

Let $n \geq 0$, then:

$$ {}_0^{CF} D_t^\alpha f(t_n) = \frac{M(\alpha)}{1-\alpha} \sum_{k=0}^{n} \int_{t_k}^{t_{k+1}} \frac{f(t_{k+1}) - f(t_k)}{\Delta t} exp\left[-\frac{\alpha}{1-\alpha}(t_n - \tau)\right] d\tau, \tag{3.12} $$

$$ = \frac{M(\alpha)}{1-\alpha} \sum_{k=0}^{n} \frac{f(t_{k+1}) - f(t_k)}{\Delta t} \int_{t_k}^{t_{k+1}} exp\left[-\frac{\alpha}{1-\alpha}(t_n - \tau)\right] d\tau, \tag{3.13} $$

Let, $y = (t_n - \tau), y = t_n - t_{k+1}, y = t_n - t_k$ and, $dy = -d\tau \Rightarrow d\tau = -dy$

Then,

$$ {}_{0}^{CF}D_t^{\alpha} f(t_n) = \frac{M(\alpha)}{1-\ \alpha} \sum_{k=0}^{n} \frac{f(t_{k+1}) -\ f(t_k)}{\Delta t} \int_{t_{n-}\ t_k}^{t_n - t_{k+1}} exp\ \left[-\frac{\alpha}{1-\ \alpha}\ y \right] dy, \tag{3.14} $$

$$ = \frac{M(\alpha)}{1-\ \alpha} \sum_{k=0}^{n} \frac{f(t_{k+1}) -\ f(t_k)}{\Delta t} \left\{ \frac{1-\alpha}{\alpha} \exp \Big|_{t_{n-}\ t_k}^{t_{n-}\ t_{k+1}} \right\}, \tag{3.15} $$

$$ = \frac{M(\alpha)}{1-\ \alpha} \sum_{k=0}^{n} \frac{f(t_{k+1}) -\ f(t_k)}{\Delta t} \left\{ \exp\left[\frac{1-\alpha}{\alpha} (t_n - t_{k+1}) \right] - \exp\left[\frac{1-\alpha}{\alpha} (t_n -\ t_k) \right] \right\}, \tag{3.16} $$

$$ = \frac{M(\alpha)}{1-\ \alpha} \sum_{k=0}^{n} \frac{f(t_{k+1}) -\ f(t_k)}{\Delta t} \psi_{n,k}^{\alpha}, \tag{3.17} $$

Where,

$$ \psi_{n,k}^{\alpha} = \exp\left[\frac{1-\alpha}{\alpha} (t_n - t_{k+1}) \right] - \exp\left[\frac{1-\alpha}{\alpha} (t_n -\ t_k) \right]. $$

The Caputo-Fabrizio fractional integral of order α of a function $\mu(x,t)$is given as:

$$ {}_{0}^{CF}I_t^{\alpha} \mu(x,t) = \frac{1-\alpha}{M(\alpha)} \mu(x,t) + \frac{\alpha}{M(\alpha)} \int_0^t \mu(x,\tau) d\tau. \tag{3.18} $$

At (x_i, t_n) we have,

$$ {}_{0}^{CF}I_t^{\alpha} \mu(x_i,t_n) = \frac{1-\alpha}{M(\alpha)} \mu(x_i,t_n) + \frac{\alpha}{M(\alpha)} \int_0^{t_n} \mu(x_i,\tau) d\tau, \tag{3.19} $$

$$ = \frac{1-\alpha}{M(\alpha)} \mu_i^n + \frac{\alpha}{M(\alpha)} \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \mu_i^j d\tau, \tag{3.20} $$

$$ = \frac{1-\alpha}{M(\alpha)} \mu_i^n + \frac{\alpha}{M(\alpha)} \sum_{j=0}^{n-1} \mu_i^j \int_{t_j}^{t_{j+1}} d\tau, \tag{3.21} $$

$$ = \frac{1-\alpha}{M(\alpha)} \mu_i^n + \frac{\alpha}{M(\alpha)} \sum_{j=0}^{n-1} \mu_i^j (t_{j+1} - t_j), \tag{3.22} $$

$$= \frac{1-\alpha}{M(\alpha)}\mu_i^n + \frac{\alpha}{M(\alpha)}\sum_{j=0}^{n-1}\mu_i^j \Delta t. \tag{3.23}$$

3.2.3 Numerical Approximation to Atangana-Baleanu (AB) Derivative in Caputo sense

Due to the complexity of the geological environments through which groundwater flow and transport takes place, there is a need for the application of a suitable differential operator that will account for these complexities. Recently, Atangana and Baleanu proposed a new fractional derivative based on the generalized Mittag-Leffler function. This new fractional operator is called the Atangana-Baleanu derivative and incorporates both the non-singular and non-local kernels. Since this new version of derivative has been very successful in the solution of real world problems, therefore, this paper also aims at utilizing the benefits of the AB derivative to solve problems related to advection and dispersion.

The new operator of AB in the sense of Caputo is given as:

$${}^{ABC}_{\ a}D_t^{\alpha}\big(f(t_n)\big) = \frac{AB(\alpha)}{1-\alpha}\int_0^{t_n}\frac{d}{d\tau}f(\tau)E_{\alpha}\left[-\alpha\frac{(t_n-\tau)^{\alpha}}{1-\alpha}\right]d\tau. \tag{3.24}$$

The numerical approximation of AB derivative in the sense of Caputo is presented below, n is a positive integer, and the subdivisions of time intervals are also given as:

Let, $0 = t_0 \leq t_1 \leq t_2 \ldots \leq t_{n-1} \leq t_n \leq \Delta t = t_k - t_{k-1}$

$${}^{ABC}_{\ a}D_t^{\alpha}\big(f(t_n)\big) = \frac{AB(\alpha)}{1-\alpha}\int_0^{t_n}\frac{d}{d\tau}f(\tau)E_{\alpha}\left[-\alpha\frac{(t_n-\tau)^{\alpha}}{1-\alpha}\right]d\tau, \tag{3.25}$$

$$= \frac{AB(\alpha)}{1-\alpha}\sum_{k=0}^{n-1}\int_{t_k}^{t_{k+1}}\frac{f(t_{k+1})-f(t_k)}{\Delta t}E_{\alpha}\left[-\alpha\frac{(t_n-\tau)^{\alpha}}{1-\alpha}\right]d\tau, \tag{3.26}$$

$$= \frac{AB(\alpha)}{1-\alpha}\sum_{k=0}^{n-1}\frac{f(t_{k+1})-f(t_k)}{\Delta t}\int_{t_k}^{t_{k+1}}E_{\alpha}\left[-\alpha\frac{(t_n-\tau)^{\alpha}}{1-\alpha}\right]d\tau, \tag{3.27}$$

$$= \frac{AB(\alpha)}{1-\ \alpha}\sum_{k=0}^{n-1}\frac{f(t_{k+1})-f(t_k)}{\Delta t}\Big\{(t_n-\ t_{k+1})E_{\alpha,2}\Big[\frac{\alpha}{1-\alpha}(t_n-\ t_{k+1})\Big] \tag{3.28}$$

$$-\ (t_n-\ t_k)E_{\alpha,2}\Big[\frac{\alpha}{1-\alpha}(t_n-\ t_k)\Big]\Big\},$$

$$= \frac{AB(\alpha)}{1-\ \alpha}\sum_{k=0}^{n}\frac{f(t_{k+1})-f(t_k)}{\Delta t}\,\Phi\delta_{n,k}^{\alpha}, \tag{3.29}$$

Where,

$$\Phi\delta_{n,k}^{\alpha} = (t_n-t_{k+1})E_{\alpha,2}\Big[\frac{\alpha}{1-\alpha}(t_n-t_{k+1})\Big]-(t_n-t_k)E_{\alpha,2}\Big[\frac{\alpha}{1-\alpha}(t_n-t_k)\Big].$$

The Atangana-Baleanu fractional integral can be presented as follows:

If, $f \in C^2[0,\mathrm{T}]$

Then,

$${}_{0}^{AB}I_t^{\alpha}\big(f(t_k)\big) = \frac{1-\alpha}{AB(\alpha)}f(t_k) + \frac{\alpha(\Delta t)^{\alpha}}{AB(\alpha)\Gamma(\alpha+1)}\sum_{j=0}^{k-1}{b_j}^{\alpha}\,\frac{f\big(t_{k-j}\big)+f\big(t_{k-j+1}\big)}{2}+R_{k,\alpha}, \tag{3.30}$$

Where,

$\left|R_{k,\alpha}\right| \le Kt_k^{\alpha}\tau, k = 1,2,3,\dots,n$ and $b_j^{\alpha} = (j+1)^{\alpha}-j^{\alpha}, j = 0,1,2,3,\dots n.$

Therefore, the Atangana-Baleanu integral is approximated using discretization approach as:

$${}_{0}^{AB}I_t^{\alpha}\mu(x,t) = \frac{1-\alpha}{AB(\alpha)}\mu(x,t)+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^t \mu(x,\tau)(t-\tau)^{\alpha-1}d\tau. \tag{3.31}$$

At (x_i, t_n) we have:

$$ {}^{AB}_{0}I^{\alpha}_{t}\mu(x_i,t_n) = \frac{1-\alpha}{AB(\alpha)}\mu(x_i,t_n) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^t \mu(x_i,\tau)(t_n-\tau)^{\alpha-1}\,d\tau, \tag{3.32} $$

$$ = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\int_{t_j}^{t_{j+1}} \mu_i^j (t_n-\tau)^{\alpha-1}\,d\tau, \tag{3.33} $$

$$ = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\int_{t_j}^{t_{j+1}} (t_n-\tau)^{\alpha-1}\,d\tau, \tag{3.34} $$

Let$y=(t_n-\tau), y=\left(t_n-t_{j+1}\right), y=\left(t_n-t_j\right)$ *and* $y=dy=-d\tau \Rightarrow d\tau=-dy$

Then,

$$ {}^{AB}_{0}I^{\alpha}_{t}\mu(x_i,t_n) = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\int_{t_n-t_j}^{t_n-t_{j+1}} y^{\alpha-1}\,(-dy), \tag{3.35} $$

For any variable, $-\int_a^b f(x)dx = \int_b^a f(x)dx$

Therefore,

$$ {}^{AB}_{0}I^{\alpha}_{t}\mu(x_i,t_n) = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\int_{t_n-t_{j+1}}^{t_n-t_j} y^{\alpha-1}\,dy, \tag{3.36} $$

$$ = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\int_{t_n-t_{j+1}}^{t_n-t_j} \frac{y^{(\alpha-1)+1}}{(\alpha-1)+1}, \tag{3.37} $$

$$ = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j y^{\alpha}\Big|_{t_n-t_{j+1}}^{t_n-t_j}, \tag{3.38} $$

$$ = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\left\{\left(t_n-t_j\right)^{\alpha}-\left(t_n-t_{j+1}\right)^{\alpha}\right\}, \tag{3.39} $$

If $t=\Delta t,\ t_j=j\Delta t,\ t_n=n\Delta t,\ t_n-t_j=n\Delta t-j\Delta t,\ t_n-t_{j+1}=n\Delta t-(j+1)\Delta t$

$$ {}^{AB}_{0}I^{\alpha}_{t}\mu(x_i,t_n) = \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\left\{\left(\Delta t(n-j)\right)^{\alpha}-\left(\Delta t(n-j-1)\right)^{\alpha}\right\}, \tag{3.40} $$

$$= \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\{(\Delta t)^\alpha((n-j)^\alpha - (n-j-1)^\alpha)\}, \tag{3.41}$$

$$= \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha(\Delta t)^{\alpha-1}}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n-1}\mu_i^j\{(n-j)^\alpha - (n-j-1)^\alpha\}, \tag{3.42}$$

$$= \frac{1-\alpha}{AB(\alpha)}\mu_i^n + \frac{\alpha(\Delta t)^{\alpha}}{AB(\alpha)\Gamma(\alpha+1)}\sum_{j=0}^{n-1}\mu_i^j\{(n-j)^\alpha - (n-j-1)^\alpha\} + \tilde{R}_{n,\alpha}, \tag{3.43}$$

Where,

$$\tilde{R}_{n,\alpha} = \sum_{j=0}^{n-1}\int_{t_j}^{t_{j+1}} \frac{f(y)+f\left(t_{j+1}\right)}{(t_n-y)^{1-\alpha}}dy.$$

3.3 NUMERICAL SOLUTION OF THE NEW MODEL WITH FRACTIONAL OPERATORS

The previous section is based on the numerical approximations of the well-known fractional derivatives and their integrals. The numerical approximation to the solutions of ordinary differential equations are normally achieved through application of numerical methods for ordinary differential equations (Süli, 2014). The most widely applied methods when presenting the approximated solutions to the initial value problem for ordinary differential equations are the Adams methods, which are based on approximating the integral by means of a polynomial integration within the intervals, say (t_n, t_{n+1}) (Peinado *et al*., 2010). In addition, there exists two types of Adamsmethods, being the explicit and the implicitAdams-Bashforth (AB) methods. These methods are derived from the fundamental theorem of calucus by means of polynomial interpolation in the Lagrange form.In this section, we apply the AB approach based on the Caputo, Caputo-Fabrizio and the Atangana-Baleanu fractional derivative to solve the advection-dispersion transport.

3.3.1 Numerical Solution of the New Model with Caputo Fractional Derivative

The following modified advection-dispersion transport equation is expressed in terms of Caputo fractional operator:

$$ {}_{0}^{C}D_t^{\alpha} C(x,t) = \hat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda\hat{R}C(x,t), \tag{3.44}$$

Where the terms on the right hand side can be replaced by the function, $f\big(x,t,C(x,t)\big)$ such that:

$$ \hat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda\hat{R}C(x,t) = f\big(x,t,C(x,t)\big), \tag{3.45}$$

Therefore, we consider the following non-linear fractional ordinary equation:

$$ {}_{0}^{C}D_t^{\alpha} C(x,t) = f\big(x,t,C(x,t)\big), \tag{3.46}$$

or

$$ f\big(x,t,C(x,t)\big) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-\tau)^{\alpha-1} f'(\tau)\,d\tau, \tag{3.47}$$

When applying the fundamental theorem of calculus to eq. (3.47), we obtain:

$$ C(x,t) - C(x,0) = \frac{1}{\Gamma(2-\alpha)}\int_0^t (t-\tau)^{\alpha-1} f\big(x,\tau,C(x,\tau)\big)\,d\tau, \tag{3.48}$$

We then consider at point (t_{n+1}), where n = 0, 1, 2, 3 . . ., now the equation above is reformulated as follows:

$$ C_i^{n+1} - C_i^0 = \frac{1}{\Gamma(2-\alpha)}\int_0^{t_{n+1}} (t_{n+1}-\tau)^{\alpha-1} f\big(x_i,\tau,C(x_i,\tau)\big)\,d\tau, \tag{3.49}$$

$$= \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} (t_{n+1}-\tau)^{\alpha-1} f\big(x_i, \tau, C(x_i,\tau)\big)\, d\tau, \tag{3.50}$$

When we approximate of the function $f\big(x_i, \tau, C(x_i,\tau)\big)$ within the interval $[t_j, t_{j+1}]$ using the Lagrange Polynomial method, the following equation is obtained:

$$P_j(\tau) = \frac{\tau - t_{j-1}}{t_j - t_{j-1}} f\big(x_i, t_j, C_i^j\big) - \frac{\tau - t_j}{t_j - t_{j-1}} f\big(x_i, t_{j-1}, C_i^{j-1}\big), \tag{3.51}$$

We can now substitute with $P_j(\tau)$, into eq. (3.50) as follows:

$$C_i^{n+1} = C_i^0 + \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} (t_{n+1}-\tau)^{\alpha-1} P_j(\tau)\, d\tau, \tag{3.52}$$

Therefore,

$$\begin{aligned} C_i^{n+1} = C_i^0 + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^{n} \Big[& f\big(x_i, t_j, C_i^j\big)\{(n-j+1)^{\alpha}(n-j+2+\alpha) \\ & - (n-j)^{\alpha}(n-j+2+2\alpha)\} \\ & - f\big(x_i, t_{j-1}, C_i^{j-1}\big)\{(n-j+1)^{\alpha+1} - (n-j)^{\alpha}(n-j+1+\alpha)\}\Big]. \end{aligned} \tag{3.53}$$

Let us recall the function $f\big(x, t, C(x,t)\big)$, presented earlier as:

$$\widehat{D}\, \frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\, \frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t) = f\big(x, t, C(x,t)\big), \tag{3.54}$$

Then,

$$f\big(x_i, t_j, C_i^j\big) = \widehat{D}\, \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{(\Delta x)^2} - \hat{v}\, \frac{C_{i+1}^j - C_{i-1}^j}{\Delta x} - \lambda \hat{R} C_i^j, \tag{3.55}$$

$$f\big(x_i, t_{j-1}, C_i^{j-1}\big) = \widehat{D}\, \frac{C_{i+1}^{j-1} - 2C_i^{j-1} + C_{i-1}^{j-1}}{(\Delta x)^2} - \hat{v}\, \frac{C_{i+1}^{j-1} - C_{i-1}^{j-1}}{\Delta x} - \lambda \hat{R} C_i^{j-1}, \tag{3.56}$$

Rewriting eq. (3.53) by substituting with the results of the functions obtained in eqs. (3.55) and (3.56), we then have the following form of equation:

$$
\begin{aligned}
C_i^{n+1} = C_i^0 + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^{n} \Bigg[& \Bigg(\widehat{D} \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{(\Delta x)^2} - \hat{v} \frac{C_{i+1}^j - C_{i-1}^j}{\Delta x} \\
& - \lambda \hat{R} C_i^j \Bigg) \{(n-j+1)^\alpha (n-j+2+\alpha) - (n-j)^\alpha (n-j+2+2\alpha)\} \\
& - \Bigg(\widehat{D} \frac{C_{i+1}^{j-1} - 2C_i^{j-1} + C_{i-1}^{j-1}}{(\Delta x)^2} - \hat{v} \frac{C_{i+1}^{j-1} - C_{i-1}^{j-1}}{\Delta x} \\
& - \lambda \hat{R} C_i^{j-1} \Bigg) \{(n-j+1)^{\alpha+1} - (n-j)^\alpha (n-j+1+\alpha)\} \Bigg].
\end{aligned} \tag{3.57}
$$

3.3.2 Numerical Solution of the New Model with Caputo-Fabrizio Fractional Derivative

We recall from eq. (2.19) where the terms on the right hand side can be replaced by the function, $f\big(x,t,C(x,t)\big)$ such that:

$$\widehat{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v} \frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t) = f\big(x,t,C(x,t)\big). \tag{3.58}$$

We then consider the following non-linear fractional equation expressed in terms of the Caputo-Fabrizio fractional operator ${}_{0}^{CF}D_t^\alpha$, as:

$${}_{0}^{CF}D_t^\alpha C(x,t) = f\big(x,t,C(x,t)\big), \tag{3.59}$$

or,

$$f\big(x,t,C(x,t)\big) = \frac{M(\alpha)}{1-\alpha} \int_0^t f'(\tau) \exp\left[-\alpha \frac{t-\tau}{1-\alpha}\right] d\tau. \tag{3.60}$$

By utilizing the fundamental theorem of calculus, the above equation becomes:

$$\mu(x,t) - \mu(x,0) = \frac{1-\alpha}{M(\alpha)} f\big(x,t,C(x,t)\big) + \frac{\alpha}{M(\alpha)} \int_0^t f\big(x,\tau,C(x,\tau)\big)\, d\tau, \tag{3.61}$$

We consider at a given point (x_i, t_{n+1}), where n = 0, 1, 2, 3. . ., then the above equation is reformulated as follows:

$$\mu(x_i, t_{n+1}) = \mu(x_i, 0) + \frac{1-\alpha}{M(\alpha)} f\big(x_i, t_n, C(x_i, t_n)\big) + \frac{\alpha}{M(\alpha)} \int_0^{t_{n+1}} f\big(x_i, \tau \;\; C(x_i, \tau)\big)\, d\tau, \tag{3.62}$$

At a point (x_i, t_n),

$$\mu(x_i, t_n) = \mu(x_i, 0) + \frac{1-\alpha}{M(\alpha)} f\big(x_i, t_{n-1}, C(x_i, t_{n-1})\big) + \frac{\alpha}{M(\alpha)} \int_0^{t_n} f\big(x_i, \tau \;\; C(x_i, \tau)\big)\, d\tau, \tag{3.63}$$

By subtracting eq. (3.63) from eq. (3.62), the following is obtained:

$$\begin{aligned} \mu_i^{n+1} - \mu_i^n &= \frac{1-\alpha}{M(\alpha)} [f(x_i, t_n, C_i^n) - f(x_i, t_{n-1}, C_i^{n-1})] \\ &+ \frac{\alpha}{M(\alpha)} \int_{t_n}^{t_{n+1}} f\big(x_i, \tau, C(x_i, \tau)\big) d\tau, \end{aligned} \tag{3.64}$$

$$\begin{aligned} \mu_i^{n+1} &= \mu_i^n + \frac{1-\alpha}{M(\alpha)} [f(x_i, t_n, C_i^n) - f(x_i, t_{n-1}, C_i^{n-1})] \\ &+ \frac{\alpha}{M(\alpha)} \left[\frac{3}{2} \Delta t f(x_i, t_n, C_i^n) - \frac{\Delta t}{2} f(x_i, t_{n-1}, C_i^{n-1})\right]. \end{aligned} \tag{3.65}$$

Apply the Caputo-Fabrizio integral operator discretization to the solution of the modified advection-dispersion equation. First, let us recall the modified advection-dispersion equation to be used in the numerical solution, given as:

$${}_{0}^{CF}D_t^{\alpha} C(x,t) = \widehat{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v} \frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t). \tag{3.66}$$

Let us remember that,

$$\widehat{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v} \frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t) = f\big(x, t, C(x,t)\big). \tag{3.67}$$

Replacing $\mu_i^{n+1}$by $C_i^{n+1}$and μ_i^n by C_i^n in eq. (3.65) yields the following equation:

$$C_i^{n+1} = C_i^n + \frac{1-\alpha}{M(\alpha)}[f(x_i, t_n, C_i^n) - f(x_i, t_{n-1}, C_i^{n-1})] + \frac{\alpha}{M(\alpha)}\left[\frac{3}{2}\Delta t f(x_i, t_n, C_i^n) - \frac{\Delta t}{2} f(x_i, t_{n-1}, C_i^{n-1})\right], \tag{3.68}$$

At this point, the functions $f(x_i, t_n, C_i^n)$ and $f(x_i, t_{n-1}, C_i^{n-1})$ from eq. (3.68) can be presented as:

$$f(x_i, t_n, C_i^n) = \widehat{D}\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} - \hat{v}\frac{C_{i+1}^n - C_{i-1}^n}{\Delta x} - \lambda \hat{R} C_i^n, \tag{3.69}$$

$$f(x_i, t_{n-1}, C_i^{n-1}) = \frac{C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}}{(\Delta x)^2} - \hat{v}\frac{C_{i+1}^{n-1} - C_{i-1}^{n-1}}{\Delta x} - \lambda \hat{R} C_i^{n-1}, \tag{3.70}$$

Substituting with the results of the functions, then the new model is presented as follows based on the discretized Caputo-Fabrizio integral operator:

$$\begin{aligned} C_i^{n+1} = C_i^n &+ \frac{1-\alpha}{M(\alpha)}\left\{\left(\widehat{D}\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} - \hat{v}\frac{C_{i+1}^n - C_{i-1}^n}{\Delta x} - \lambda \hat{R} C_i^n\right)\right. \\ &\left. - \left(\widehat{D}\frac{C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}}{(\Delta x)^2} - \hat{v}\frac{C_{i+1}^{n-1} - C_{i-1}^{n-1}}{\Delta x} - \lambda \hat{R} C_i^{n-1}\right)\right\} \\ &+ \frac{\alpha}{M(\alpha)}\left\{\frac{3\Delta t}{2}\left(\widehat{D}\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} - \hat{v}\frac{C_{i+1}^n - C_{i-1}^n}{\Delta x} - \lambda \hat{R} C_i^n\right)\right. \\ &\left. - \frac{\Delta t}{2}\left(\widehat{D}\frac{C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}}{(\Delta x)^2} - \hat{v}\frac{C_{i+1}^{n-1} - C_{i-1}^{n-1}}{\Delta x} - \lambda \hat{R} C_i^{n-1}\right)\right\}. \end{aligned} \tag{3.71}$$

3.3.3 Numerical Solution of the New Model with Atangana-Baleanu Fractional Derivative Caputo sense

Let us consider the following non-linear fractional equation expressed in terms of Atangana-Baleanu fractional derivative in a Caputo sense (ABC).

$${}_{0}^{ABC}D_t^{\alpha} C(x,t) = f\big(x, t, C(x,t)\big), \tag{3.72}$$

or

$$f\big(x,t,C(x,t)\big) = \frac{AB(\alpha)}{1-\alpha}\int_0^t f'(\tau)E_\alpha\left[-\alpha\frac{(t-\tau)^\alpha}{1-\alpha}\right]d\tau. \tag{3.73}$$

Applying the fundamental theorem of calculus to the above eq. (3.73) yields:

$$\begin{aligned} &C(x,t)-C(x,0)\\ &=\frac{1-\alpha}{AB(\alpha)}f\big(x,t,C(x,t)\big)\\ &+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^t (t-\tau)^{\alpha-1}f\big(x,\tau,C(x,\tau)\big)\,d\tau. \end{aligned} \tag{3.74}$$

We then consider at point (t_{n+1}), where n = 0, 1, 2, 3, . . ., then the above equation is reformulated as:

$$\begin{aligned} C_i^{n+1}-C_i^0 &= \frac{1-\alpha}{AB(\alpha)}f(x_i,t_n,C_i^n)\\ &+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^{t_{n+1}}(t_{n+1}-\tau)^{\alpha-1}f\big(x_i,\tau,C(x_i,\tau)\big)\,d\tau, \end{aligned} \tag{3.75}$$

$$=\frac{1-\alpha}{AB(\alpha)}f(x_i,t_n,C_i^n)+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n}\int_{t_j}^{t_{j+1}}(t_{n+1}-\tau)^{\alpha-1}f\big(x_i,\tau,C(x_i,\tau)\big)\,d\tau, \tag{3.76}$$

We now apply the Lagrange Polynomial method to approximate the function $f\big(x_i,\tau,C(x_i,\tau)\big)$ within the interval $\left[t_j,t_{j+1}\right]$, and obtain:

$$P_j(\tau)=\frac{\tau-t_{j-1}}{t_j-t_{j-1}}f\big(x_i,t_j,C_i^j\big)-\frac{\tau-t_j}{t_j-t_{j-1}}f\big(x_i,t_{j-1},C_i^{j-1}\big), \tag{3.77}$$

Substituting with $P_j(\tau)$ in eq. (3.76), we obtain:

$$C_i^{n+1}-C_i^0=\frac{1-\alpha}{AB(\alpha)}f(x_i,t_n,C_i^n)+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=0}^{n}\int_{t_j}^{t_{j+1}}P_j(\tau)(t-\tau)^{\alpha-1}d\tau, \tag{3.78}$$

Then, the following form of equation is generated:

$$C_i^{n+1} = C_i^0 + \frac{1-\alpha}{AB(\alpha)} f(x_i, t_n, C_i^n)$$
$$+ \frac{(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha+2)} \sum_{j=0}^{n} \Big[f\big(x_i, t_j, C_i^j\big)\{(n-j+1)^\alpha (n-j+2+\alpha)$$
$$- (n-j)^\alpha (n-j+2+2\alpha)\}$$
$$- f\big(x_i, t_{j-1}, C_i^{j-1}\big)\{(n-j+1)^{\alpha+1} - (n-j)^\alpha (n-j+1+\alpha)\}\Big]. \tag{3.79}$$

Let us recall, based on our modified advection-dispersion equation, that the function $f\big(x, t, C(x,t)\big)$ is expressed as follows:

$$f\big(x, t, C(x,t)\big) = \hat{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v} \frac{\partial C(x,t)}{\partial x} - \lambda \hat{R} C(x,t), \tag{3.80}$$

Therefore,

$$f\big(x_i, t_j, C_i^j\big) = \hat{D} \frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{(\Delta x)^2} - \hat{v} \frac{C_{i+1}^j - C_{i-1}^j}{\Delta x} - \lambda \hat{R} C_i^j, \tag{3.81}$$
$$f\big(x_i, t_{j-1}, C_i^{j-1}\big) = \hat{D} \frac{C_{i+1}^{j-1} - 2C_i^{j-1} + C_{i-1}^{j-1}}{(\Delta x)^2} - \hat{v} \frac{C_{i+1}^{j-1} - C_{i-1}^{j-1}}{\Delta x} - \lambda \hat{R} C_i^{j-1}, \tag{3.82}$$
$$f(x_i, t_n, C_i^n) = \hat{D} \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} - \hat{v} \frac{C_{i+1}^n - C_{i-1}^n}{\Delta x} - \lambda \hat{R} C_i^n, \tag{3.83}$$

Equation (3.79) can now be written by substituting with the results of the functions in eqs. (3.81), (3.82) and (3.83), we then have the following:

$$
\begin{aligned}
C_i^{n+1} = C_i^0 &+ \frac{1-\alpha}{AB(\alpha)}\left[\widehat{D}\,\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} - \hat{v}\,\frac{C_{i+1}^n - C_{i-1}^n}{\Delta x} - \lambda\hat{R}C_i^n\right] \\
&+ \frac{(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha+2)}\sum_{j=0}^{n}\Bigg[\Bigg(\widehat{D}\,\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{(\Delta x)^2} - \hat{v}\,\frac{C_{i+1}^j - C_{i-1}^j}{\Delta x} \\
&- \lambda\hat{R}C_i^j\Bigg)\{(n-j+1)^\alpha(n-j+2+\alpha) - (n-j)^\alpha(n-j+2+2\alpha)\} \\
&- \Bigg(\widehat{D}\,\frac{C_{i+1}^{j-1} - 2C_i^{j-1} + C_{i-1}^{j-1}}{(\Delta x)^2} - \hat{v}\,\frac{C_{i+1}^{j-1} - C_{i-1}^{j-1}}{\Delta x} \\
&- \lambda\hat{R}C_i^{j-1}\Bigg)\{(n-j+1)^{\alpha+1} - (n-j)^\alpha(n-j+1+\alpha)\}\Bigg].
\end{aligned} \tag{3.84}
$$

CHAPTER 4: NUMERICAL STABILITY ANALYSIS OF THE NEW MODEL USING VON NEUMANN METHOD

4.1 INTRODUCTION

In this section, the conditions for stability of numerical schemes for the new generated groundwater transport model is analyzed using Von Neumann stability analysis. The Von Neumann stability method is also referred to as the Fourier's method. The British Researchers Crank and Nicolson invented this method at Los Alamos National in 1947. This method has been in operation since its development and is still in use to date. Analysis for stability is very essential because during discretization of partial differential equations (PDEs), numerical errors are likely to be generated hence the need for stability analysis (Delahaies, 2012). Von Neumann method is mostly employed to investigate the stability of finite difference schemes in relation to solutions of PDEs. A finite difference scheme is said to be stable if the associated error remains constant or decreases with time throughout the entire process of computation. On the other hand, when the generated error increases with time, then the scheme becomes unstable. Note that, the numerical scheme is said to be stable if $|\xi| \leq 1$, and unstable if $|\xi| > 1$.

The von Neumann method is based on the decay of errors into Fourier series. Consequently, the Fourier expansion can be presented in terms of space as follows:

$$\rho(x,t) = \sum_{f} \hat{\rho}(t)\, exp(ik_m x). \tag{4.1}$$

For von Neumann stability analysis, we assume the following:

$$\varepsilon_i^{n+1} = \hat{\rho}_{n+1} e^{ik_m x}, \tag{4.2}$$

$$\varepsilon_i^{n} = \hat{\rho}_{n} e^{ik_m x}, \tag{4.3}$$

$$\varepsilon_{i+1}^{n} = \hat{\rho}_{n} e^{ik_m (x+\Delta x)}, \tag{4.4}$$

$$\varepsilon_{i-1}^{n} = \hat{\rho}_n e^{ik_m(x-\Delta x)}, \tag{4.5}$$

$$\varepsilon_{i}^{n-1} = \hat{\rho}_{n-1} e^{ik_m x}, \tag{4.6}$$

$$\varepsilon_{i+1}^{n-1} = \hat{\rho}_{n-1} e^{ik_m(x+\Delta x)}, \tag{4.7}$$

$$\varepsilon_{i-1}^{n-1} = \hat{\rho}_{n-1} e^{ik_m(x-\Delta x)}. \tag{4.8}$$

4.1.1 Stability analysis of the new numerical scheme for solution of PDEs derived in terms of Caputo-Fabrizio fractional derivative

In this section, we present the condition of stability to our discretized advection-dispersion transport equation (eq. 3.71) in the case of Caputo-Fabrizio fractional order derivative. The approach employed is the Von Neumann stability analysis.

Let us recall our discretized eq. (3.71) given as:

$$\begin{aligned} C_i^{n+1} = C_i^n &+ \frac{1-\alpha}{M(\alpha)}\left\{\left(\widehat{D}\,\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} - \hat{v}\,\frac{C_{i+1}^n - C_{i-1}^n}{\Delta x} - \lambda\hat{R}C_i^n\right)\right. \\ &\left.- \left(\widehat{D}\,\frac{C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}}{(\Delta x)^2} - \hat{v}\,\frac{C_{i+1}^{n-1} - C_{i-1}^{n-1}}{\Delta x} - \lambda\hat{R}C_i^{n-1}\right)\right\} \\ &+ \frac{\alpha}{M(\alpha)}\left\{\frac{3\Delta t}{2}\left(\widehat{D}\,\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} - \hat{v}\,\frac{C_{i+1}^n - C_{i-1}^n}{\Delta x} - \lambda\hat{R}C_i^n\right)\right. \\ &\left.- \frac{\Delta t}{2}\left(\widehat{D}\,\frac{C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}}{(\Delta x)^2} - \hat{v}\,\frac{C_{i+1}^{n-1} - C_{i-1}^{n-1}}{\Delta x} - \lambda\hat{R}C_i^{n-1}\right)\right\}, \end{aligned} \tag{4.9}$$

and assume that,

$$\frac{\widehat{D}}{(\Delta x)^2} = a, \qquad \frac{\hat{v}}{\Delta x} = b, \qquad \lambda\hat{R} = z, \qquad \frac{1-\alpha}{M(\alpha)} = f, \qquad \frac{\alpha}{M(\alpha)} = g, \qquad \frac{3\Delta t}{2} = h, \qquad \frac{\Delta t}{2} = k.$$

Therefore, substituting with these variables into eq. (4.9), we obtain:

$$
\begin{aligned}
C_i^{n+1} = C_i^n &+ f\{[a(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - b(C_{i+1}^n - C_{i-1}^n) - zC_i^n] \\
&- [a(C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}) - b(C_{i+1}^{n-1} - C_{i-1}^{n-1}) - zC_i^{n-1}]\} \\
&+ g\{h[a(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - b(C_{i+1}^n - C_{i-1}^n) - zC_i^n] \\
&- k[a(C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}) - b(C_{i+1}^{n-1} - C_{i-1}^{n-1}) - zC_i^{n-1}]\}.
\end{aligned} \tag{4.10}
$$

Further numerical solution by collection of the like terms and simplification to the above equation becomes:

$$
\begin{aligned}
C_i^{n+1} = C_i^n&[(1 - 2af - zf)] + f[a(C_{i+1}^n + C_{i-1}^n) - b(C_{i+1}^n - C_{i-1}^n)] \\
&+ C_i^{n-1}[-(-2af - zf)] - f[a(C_{i+1}^{n-1} + C_{i-1}^{n-1}) - b(C_{i+1}^{n-1} - C_{i-1}^{n-1})] \\
&+ C_i^n[(-2agh - zgh)] + g[ah(C_{i+1}^n + C_{i-1}^n) - bh(C_{i+1}^n - C_{i-1}^n)] \\
&+ C_i^{n-1}[-(-2agk - zgk)] \\
&- g[ak(C_{i+1}^{n-1} + C_{i-1}^{n-1}) - bk(C_{i+1}^{n-1} - C_{i-1}^{n-1})].
\end{aligned} \tag{4.11}
$$

We consider the above-simplified eq. (4.11) and plug eqs. (4.2) to (4.8) as follows:

$$
\begin{aligned}
\hat{\rho}_{n+1}e^{ik_mx} = (1 - 2af - zf)&\hat{\rho}_n e^{ik_mx} + af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} \\
&- bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} + (2af + zf)\hat{\rho}_{n-1}e^{ik_mx} \\
&- af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}e^{ik_mx} \\
&+ bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}e^{ik_mx} - (2agh + zgh)\hat{\rho}_n e^{ik_mx} \\
&+ agh\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} - bgh\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} \\
&+ (2agk + zgk)\hat{\rho}_{n-1}e^{ik_mx} - agk\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}e^{ik_mx} \\
&+ bgk\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}e^{ik_mx}.
\end{aligned} \tag{4.12}
$$

Dividing both sides of eq. (4.12) by e^{ik_mx} yields the following:

$$
\begin{aligned}
\hat{\rho}_{n+1} = {} & (1-2af-zf)\hat{\rho}_n + af\left(e^{ik_m\Delta x}+e^{-ik_m\Delta x}\right)\hat{\rho}_n - bf\left(e^{ik_m\Delta x}-e^{-ik_m\Delta x}\right)\hat{\rho}_n \\
& + (2af+zf)\hat{\rho}_{n-1} - af\left(e^{ik_m\Delta x}+e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1} \\
& + bf\left(e^{ik_m\Delta x}-e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1} - (2agh+zgh)\hat{\rho}_n \\
& + agh\left(e^{ik_m\Delta x}+e^{-ik_m\Delta x}\right)\hat{\rho}_n - bgh\left(e^{ik_m\Delta x}-e^{-ik_m\Delta x}\right)\hat{\rho}_n \\
& + (2agk+zgk)\hat{\rho}_{n-1} - agk\left(e^{ik_m\Delta x}+e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1} \\
& + bgk\left(e^{ik_m\Delta x}-e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}.
\end{aligned} \tag{4.13}
$$

If,

$$
e^{ik_m\Delta x} = \cos(k_m\Delta x) + i\sin(k_m\Delta x), \tag{4.14}
$$

and,

$$
e^{-ik_m\Delta x} = \cos(k_m\Delta x) - i\sin(k_m\Delta x). \tag{4.15}
$$

Then, by further simplification in eq. (4.13), we obtain:

$$
\begin{aligned}
\hat{\rho}_{n+1} = {} & (1-2af-zf)\hat{\rho}_n + af(2\cos(k_m\Delta x))\hat{\rho}_n - bf(2i\sin(k_m\Delta x))\hat{\rho}_n \\
& + (2af+zf)\hat{\rho}_{n-1} - af(2\cos(k_m\Delta x))\hat{\rho}_{n-1} + bf(2i\sin(k_m\Delta x))\hat{\rho}_{n-1} \\
& - (2agh+zgh)\hat{\rho}_n + agh(2\cos(k_m\Delta x))\hat{\rho}_n - bgh(2i\sin(k_m\Delta x))\hat{\rho}_n \\
& + (2agk+zgk)\hat{\rho}_{n-1} - agk(2\cos(k_m\Delta x))\hat{\rho}_{n-1} \\
& + bgk(2i\sin(k_m\Delta x))\hat{\rho}_{n-1}.
\end{aligned} \tag{4.16}
$$

By simplifying and factorizing, we obtain the following:

$$
\begin{aligned}
\hat{\rho}_{n+1} = {} & [1 - zf - 2af(1-\cos(k_m\Delta x)) - bf(2i\sin(k_m\Delta x)) - zgh \\
& - 2agh(1-\cos(k_m\Delta x)) - bgh(2i\sin(k_m\Delta x))]\hat{\rho}_n \\
& + [zf + 2af(1-\cos(k_m\Delta x)) + bf(2i\sin(k_m\Delta x)) + zgk \\
& + 2agk(1-\cos(k_m\Delta x)) + bgk(2i\sin(k_m\Delta x))]\hat{\rho}_{n-1}.
\end{aligned} \tag{4.17}
$$

We can further simplify as follows:

$$\hat{\rho}_{n+1} = \Big[1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\Big]\hat{\rho}_n + \Big[zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2i\sin(k_m\Delta x)) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right) + bgk(2i\sin(k_m\Delta x))\Big]\hat{\rho}_{n-1}. \tag{4.18}$$

Let us suppose that:

$$A = \Big[1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\Big],$$

and,

$$B = \Big[zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2i\sin(k_m\Delta x)) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right) + bgk(2i\sin(k_m\Delta x))\Big].$$

Then, eq. (4.18) can be written as:

$$\hat{\rho}_{n+1} = A\hat{\rho}_n + B\hat{\rho}_{n-1}. \tag{4.19}$$

From eq. (4.18), when $n = 0$ we have:

$$\hat{\rho}_1 = A\hat{\rho}_0$$

$$\hat{\rho}_1 = \Big[1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\Big]\hat{\rho}_0. \tag{4.20}$$

By rearranging, we get:

$$\frac{\hat{\rho}_1}{\hat{\rho}_0} = \Big[1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\Big]. \tag{4.21}$$

Thus, we find the stability condition for which:

$$\left|\frac{\hat{\rho}_1}{\hat{\rho}_0}\right| < 1. \tag{4.22}$$

Which implies that:

$$\left|\frac{\hat{\rho}_1}{\hat{\rho}_0}\right| = |A| < 1, \qquad |A| < 1. \tag{4.23}$$

Let us recall that:

$$A = \Big[1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\Big]$$

Therefore, by applying the absolute value of a complex number, where we assume that $s = a + ib$ and $|s| = \sqrt{a^2 + b^2}$. We now have:

$$|A| = \sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2}, \tag{4.24}$$

We can also rewrite the above equation that:

$$\left|1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\right| = \sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2}, \tag{4.25}$$

Thus,

$$|A| = \sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m \Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m \Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2} < 1, \tag{4.26}$$

Therefore, we can infer that $|\hat{\rho}_1| < |\hat{\rho}_0|$ when:

$$\sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m \Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m \Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2} < 1. \tag{4.27}$$

We again recall from eq. (4.18), that:

$$B = \left[zf + 4af\sin^2\left(\frac{k_m \Delta x}{2}\right) + bf(2i\sin(k_m\Delta x)) + zgk + 4agk\sin^2\left(\frac{k_m \Delta x}{2}\right) + bgk(2i\sin(k_m\Delta x))\right]$$

Then,

$$|B| = \sqrt{\left(zf + 4af\sin^2\left(\frac{k_m \Delta x}{2}\right) + zgk + 4agk\sin^2\left(\frac{k_m \Delta x}{2}\right)\right)^2 + (2bf\sin(k_m\Delta x) + 2bgk\sin(k_m\Delta x))^2}, \tag{4.28}$$

Similarly,

$$\left|zf + 4af\sin^2\left(\frac{k_m \Delta x}{2}\right) + bf(2i\sin(k_m\Delta x)) + zgk + 4agk\sin^2\left(\frac{k_m \Delta x}{2}\right) + bgk(2i\sin(k_m\Delta x))\right| = \sqrt{\left(zf + 4af\sin^2\left(\frac{k_m \Delta x}{2}\right) + zgk + 4agk\sin^2\left(\frac{k_m \Delta x}{2}\right)\right)^2 + (2bf\sin(k_m\Delta x) + 2bgk\sin(k_m\Delta x))^2}. \tag{4.29}$$

$\forall\, n > 0$, we assume that:

$$|\hat{\rho}_n| < |\hat{\rho}_0| \Rightarrow \left|\frac{\hat{\rho}_n}{\hat{\rho}_0}\right| < 1$$

Using the above assumption, we can prove that:

$$|\hat{\rho}_{n+1}| < |\hat{\rho}_0| \Rightarrow \left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < 1,$$

Thus,

$$|\hat{\rho}_{n+1}| = |A\hat{\rho}_n + B\hat{\rho}_{n-1}|$$

$$\begin{aligned}|\hat{\rho}_{n+1}| = \Bigg|\hat{\rho}_n \Bigg(& 1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh \\ & - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\Bigg) \\ & + \hat{\rho}_{n-1}\Bigg(zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2i\sin(k_m\Delta x)) + zgk \\ & + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right) + bgk(2i\sin(k_m\Delta x))\Bigg)\Bigg|,\end{aligned} \tag{4.30}$$

Which means that,

$$|\hat{\rho}_{n+1}| \leq |A||\hat{\rho}_n| + |B||\hat{\rho}_{n-1}|$$

$$\begin{aligned}&|\hat{\rho}_{n+1}| \\ &\leq \sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2}|\hat{\rho}_n| \\ &+ \sqrt{\left(zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + (2bf\sin(k_m\Delta x) + 2bgk\sin(k_m\Delta x))^2}|\hat{\rho}_{n-1}|.\end{aligned} \tag{4.31}$$

By applying the inductive hypothesis, we suppose that:

$$|\hat{\rho}_n| < 0 \text{ and } |\hat{\rho}_{n-1}| < |\hat{\rho}_0|$$

$$|\hat{\rho}_{n+1}| < |A||\hat{\rho}_0| + |B||\hat{\rho}_0|, \tag{4.32}$$

$$|\hat{\rho}_{n+1}| < |\hat{\rho}_0|\left(\sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2}\right) + |\hat{\rho}_0|\left(\sqrt{\left(zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + (2bf\sin(k_m\Delta x) + 2bgk\sin(k_m\Delta x))^2}\right).$$

By factorization, we can infer that:

$$|\hat{\rho}_{n+1}| < |\hat{\rho}_0|(|A| + |B|),$$

$$|\hat{\rho}_{n+1}| < |\hat{\rho}_0|\left(\sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2} + \sqrt{\left(zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + (2bf\sin(k_m\Delta x) + 2bgk\sin(k_m\Delta x))^2}\right). \tag{4.33}$$

We further have:

$$\left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < |A| + |B|,$$

$$\left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < \sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2} + \sqrt{\left(zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + (2bf\sin(k_m\Delta x) + 2bgk\sin(k_m\Delta x))^2}. \tag{4.34}$$

Remember that:

$$\left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < 1$$

This also implies that:

$$|A| + |B| < 1,$$

$$\left|\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - bf(2i\sin(k_m\Delta x)) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right) - bgh(2i\sin(k_m\Delta x))\right)\right| + \left|+\left(zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2i\sin(k_m\Delta x)) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right) + bgk(2i\sin(k_m\Delta x))\right)\right| < 1, \tag{4.35}$$

Similarly,

$$\sqrt{\left(1 - zf - 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zgh - 4agh\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 - \left(2bf\sin(k_m\Delta x) + 2bgh\sin(k_m\Delta x)\right)^2} + \sqrt{\left(zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + zgk + 4agk\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + (2bf\sin(k_m\Delta x) + 2bgk\sin(k_m\Delta x))^2} < 1. \tag{4.36}$$

Therefore, we conclude that, under this condition our numerical method is conditionally stable.

4.1.2 Stability analysis of the new numerical scheme for solution of PDEs derived in terms of Atangana-Baleanu fractional derivative in Caputo sense

This section presents the analysis of stability condition to our discretized advection-dispersion transport equation (eq. 3.84) in the case of Atangana-Baleanu fractional order derivative in Caputo sense. The method of approach employed to test for stability is the Von Neumann stability method.

Consider the transport equation below expressed in terms of Atangana-Baleanu fractional derivative in the sense of Caputo as:

$$ {}^{ABC}_{0}D_t^{\alpha} C(x,t) = \widehat{D}\frac{\partial^2 C(x,t)}{\partial x^2} - \hat{v}\frac{\partial C(x,t)}{\partial x} - \lambda\hat{R}C(x,t). $$

Therefore, we recall our discretized eq. (3.84) that:

$$ \begin{aligned} C_i^{n+1} = C_i^n &+ \frac{1-\alpha}{AB(\alpha)}\left[\widehat{D}\frac{(C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1})}{(\Delta x)^2} - \hat{v}\frac{(C_{i+1}^{n+1} - C_{i-1}^{n+1})}{\Delta x} - \lambda\hat{R}C_i^{n+1}\right] \\ &- \frac{1-\alpha}{AB(\alpha)}\left[\widehat{D}\frac{(C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n})}{(\Delta x)^2} - \hat{v}\frac{(C_{i+1}^{n} - C_{i-1}^{n})}{\Delta x} - \lambda\hat{R}C_i^{n}\right] \\ &+ \frac{(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha)}\left[\widehat{D}\frac{(C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n})}{(\Delta x)^2} - \hat{v}\frac{(C_{i+1}^{n} - C_{i-1}^{n})}{\Delta x}\right. \\ &\left. - \lambda\hat{R}C_i^{n}\right](n-j+1)^\alpha(n-j+2+\alpha) - (n-j)^\alpha(n-j+2+2\alpha) \\ &- \frac{(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha)}\left[\widehat{D}\frac{(C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1})}{(\Delta x)^2} - \hat{v}\frac{(C_{i+1}^{n-1} - C_{i-1}^{n-1})}{\Delta x}\right. \\ &\left. - \lambda\hat{R}C_i^{n-1}\right](n-j+1)^{\alpha+1} - (n-j)^\alpha(n-j+1+\alpha). \end{aligned} \tag{4.37} $$

From the above equation, we then assume that:

$$ \begin{gathered} \frac{\widehat{D}}{(\Delta x)^2} = a, \qquad \frac{\hat{v}}{\Delta x} = b, \qquad \lambda\hat{R} = z, \qquad \frac{1-\alpha}{AB(\alpha)} = f, \qquad \frac{(\Delta t)^\alpha}{AB(\alpha)\Gamma(\alpha)} = g, \\ \delta_n^{\alpha,1} = (n-j+1)^\alpha(n-j+2+\alpha) - (n-j)^\alpha(n-j+2+2\alpha), \\ \delta_n^{\alpha,2} = (n-j+1)^{\alpha+1} - (n-j)^\alpha(n-j+1+\alpha) \end{gathered} $$

Therefore, substituting with these variables into eq. (4.37) gives:

$$ \begin{aligned} C_i^{n+1} = C_i^n &+ f[a(C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}) - b(C_{i+1}^{n+1} - C_{i-1}^{n+1}) - zC_i^{n+1}] \\ &- f[a(C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n}) - b(C_{i+1}^{n} - C_{i-1}^{n}) - zC_i^{n}] \\ &+ g[a(C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n}) - b(C_{i+1}^{n} - C_{i-1}^{n}) - zC_i^{n}]\delta_n^{\alpha,1} \\ &- g[a(C_{i+1}^{n-1} - 2C_i^{n-1} + C_{i-1}^{n-1}) - b(C_{i+1}^{n-1} - C_{i-1}^{n-1}) - zC_i^{n-1}]\delta_n^{\alpha,2}. \end{aligned} \tag{4.38} $$

Simplification of the above eq. (4.38) gives:

$$\begin{aligned}
C_i^{n+1} &= C_i^n(1+2af+zf) - af(C_{i+1}^n + C_{i-1}^n) + bf(C_{i+1}^n - C_{i-1}^n) \\
&\quad - C_i^n(2ag+zg)\delta_n^{\alpha,1} + ag\delta_n^{\alpha,1}(C_{i+1}^n + C_{i-1}^n) - bg\delta_n^{\alpha,1}(C_{i+1}^n - C_{i-1}^n) \\
&\quad - C_i^{n+1}(2af+zf) + af(C_{i+1}^{n+1} + C_{i-1}^{n+1}) - bf(C_{i+1}^{n+1} - C_{i-1}^{n+1}) \\
&\quad + C_i^{n-1}(2ag+zg)\delta_n^{\alpha,2} - ag\delta_n^{\alpha,2}(C_{i+1}^{n-1} + C_{i-1}^{n-1}) \\
&\quad + bg\delta_n^{\alpha,2}(C_{i+1}^{n-1} - C_{i-1}^{n-1}).
\end{aligned} \tag{4.39}$$

For Von Neumann stability analysis, we utilize the assumptions from eqs. (4.2) to (4.8) and plug into eq. (4.39) to obtain the following:

$$\begin{aligned}
\hat{\rho}_{n+1}e^{ik_mx} &= (1+2af+zf)\hat{\rho}_n e^{ik_mx} - af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} \\
&\quad + bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} - \left(2ag\delta_n^{\alpha,1} + zg\delta_n^{\alpha,1}\right)\hat{\rho}_n e^{ik_mx} \\
&\quad + ag\delta_n^{\alpha,1}\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} \\
&\quad - bg\delta_n^{\alpha,1}\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_n e^{ik_mx} - (2af+zf)\hat{\rho}_{n+1}e^{ik_mx} \\
&\quad + af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_{n+1}e^{ik_mx} \\
&\quad - bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_{n+1}e^{ik_mx} + \left(2ag\delta_n^{\alpha,2} + zg\delta_n^{\alpha,2}\right)\hat{\rho}_{n-1}e^{ik_mx} \\
&\quad - ag\delta_n^{\alpha,2}\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}e^{ik_mx} \\
&\quad + bg\delta_n^{\alpha,2}\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}e^{ik_mx}.
\end{aligned} \tag{4.40}$$

Dividing both sides of eq. (4.40) by e^{ik_mx} yields the following:

$$\begin{aligned}
\hat{\rho}_{n+1} &= (1+2af+zf)\hat{\rho}_n - af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_n + bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_n \\
&\quad - \left(2ag\delta_n^{\alpha,1} + zg\delta_n^{\alpha,1}\right)\hat{\rho}_n + ag\delta_n^{\alpha,1}\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_n \\
&\quad - bg\delta_n^{\alpha,1}\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_n - (2af+zf)\hat{\rho}_{n+1} \\
&\quad + af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_{n+1} - bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_{n+1} \\
&\quad + \left(2ag\delta_n^{\alpha,2} + zg\delta_n^{\alpha,2}\right)\hat{\rho}_{n-1} - ag\delta_n^{\alpha,2}\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1} \\
&\quad + bg\delta_n^{\alpha,2}\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\hat{\rho}_{n-1}.
\end{aligned} \tag{4.41}$$

By factorization and simplification, we obtain the following:

$$
\begin{aligned}
\hat{\rho}_{n+1} = \Big[&(1 + 2af + zf) - af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right) + bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right) \\
&- \left(2ag\delta_n^{\alpha,1} + zg\delta_n^{\alpha,1}\right) + ag\delta_n^{\alpha,1}\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right) \\
&- bg\delta_n^{\alpha,1}\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\Big]\hat{\rho}_n \\
&+ \Big[\left(2ag\delta_n^{\alpha,2} + zg\delta_n^{\alpha,2}\right) - ag\delta_n^{\alpha,2}\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right) \\
&+ bg\delta_n^{\alpha,2}\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\Big]\hat{\rho}_{n-1} \\
&- \Big[(2af + zf) - af\left(e^{ik_m\Delta x} + e^{-ik_m\Delta x}\right) \\
&+ bf\left(e^{ik_m\Delta x} - e^{-ik_m\Delta x}\right)\Big]\hat{\rho}_{n+1}.
\end{aligned}
\tag{4.42}
$$

If,

$$e^{ik_m\Delta x} = \cos(k_m\Delta x) + i\sin(k_m\Delta x), \tag{4.43}$$

and,

$$e^{-ik_m\Delta x} = \cos(k_m\Delta x) - i\sin(k_m\Delta x). \tag{4.44}$$

Then further simplification yields:

$$
\begin{aligned}
\hat{\rho}_{n+1} = \Big[&(1 + 2af + zf) - af(2\cos(k_m\Delta x)) + bf(2isin(k_m\Delta x)) \\
&- \left(2ag\delta_n^{\alpha,1} + zg\delta_n^{\alpha,1}\right) + ag\delta_n^{\alpha,1}(2\cos(k_m\Delta x)) \\
&- bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\Big]\hat{\rho}_n \\
&+ \Big[\left(2ag\delta_n^{\alpha,2} + zg\delta_n^{\alpha,2}\right) - ag\delta_n^{\alpha,2}(2\cos(k_m\Delta x)) \\
&+ bg\delta_n^{\alpha,2}(2isin(k_m\Delta x))\Big]\hat{\rho}_{n-1} \\
&- \Big[(2af + zf) - af(2\cos(k_m\Delta x)) + bf\delta_n^{\alpha,1}(2isin(k_m\Delta x))\Big]\hat{\rho}_{n+1}.
\end{aligned}
\tag{4.45}
$$

By factorizing, we have:

$$\begin{aligned}\hat{\rho}_{n+1} = \big[&1 + zf - 2af(1-\cos(k_m\Delta x)) + bf(2isin(k_m\Delta x)) + zg\delta_n^{\alpha,1}\\
&- 2ag\delta_n^{\alpha,1}(1-\cos(k_m\Delta x)) - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\big]\hat{\rho}_n\\
&+ \big[zg\delta_n^{\alpha,2} + 2ag\delta_n^{\alpha,2}(1-\cos(k_m\Delta x)) + bg\delta_n^{\alpha,2}(2isin(k_m\Delta x))\big]\hat{\rho}_{n-1}\\
&- [zf + 2af(1-\cos(k_m\Delta x)) + bf(2isin(k_m\Delta x))]\hat{\rho}_{n+1}.\end{aligned} \tag{4.46}$$

We further have:

$$\begin{aligned}\hat{\rho}_{n+1} = &\left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1}\right.\\
&\left.- 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\right]\hat{\rho}_n\\
&+ \left[zg\delta_n^{\alpha,2} + 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2} + bg\delta_n^{\alpha,2}(2isin(k_m\Delta x))\right]\hat{\rho}_{n-1}\\
&- \left[zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))\right]\hat{\rho}_{n+1},\end{aligned} \tag{4.47}$$

and,

$$\begin{aligned}&\left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))\right]\hat{\rho}_{n+1}\\
&= \left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1}\right.\\
&\left.- 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\right]\hat{\rho}_n\\
&+ \left[zg\delta_n^{\alpha,2} + 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2} + bg\delta_n^{\alpha,2}(2isin(k_m\Delta x))\right]\hat{\rho}_{n-1}.\end{aligned} \tag{4.48}$$

From the above equation when $n = 0$, we have:

$$\begin{aligned}&\left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))\right]\hat{\rho}_1\\
&= \left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1}\right.\\
&\left.- 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\right]\hat{\rho}_0.\end{aligned} \tag{4.49}$$

Let us suppose that:

$$A_m = \left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))\right],$$

and,

$$B_m = \left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\right].$$

Therefore, we can present eq. (4.49) as:

$$\hat{\rho}_1 A_m = \hat{\rho}_0 B_m. \tag{4.50}$$

Thus, we can find the condition for which:

$$\left|\frac{\hat{\rho}_1}{\hat{\rho}_0}\right| < 1. \tag{4.51}$$

Which implies that:

$$\left|\frac{\hat{\rho}_1}{\hat{\rho}_0}\right| = \left|\frac{B_m}{A_m}\right| < 1. \tag{4.52}$$

Let us recall that:

$$A_m = \left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))\right],$$

and,

$$B_m = \left[1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\right].$$

Therefore, we can express $\left|\frac{B_m}{A_m}\right|$ as follows:

$$\left|\frac{1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))}{1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))}\right|. \quad (4.53)$$

By applying the absolute value of a complex number, where we assume that $s = a + ib$ and $|s| = \sqrt{a^2 + b^2}$. Thus, we now have:

$$|A_m| = \sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + \left(2bfsin(k_m\Delta x)\right)^2}, \quad (4.54)$$

and,

$$|B_m| = \sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2 + \left(2bf\,sin(k_m\Delta x) - 2bg\delta_n^{\alpha,1}\,sin(k_m\Delta x)\right)^2}. \quad (4.55)$$

Which means that:

$$\left|\frac{1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))}{1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))}\right| = \frac{\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2 + \left(2bf\,sin(k_m\Delta x) - 2bg\delta_n^{\alpha,1}\,sin(k_m\Delta x)\right)^2}}{\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + \left(2bfsin(k_m\Delta x)\right)^2}}. \quad (4.56)$$

Therefore, $\left|\frac{B_m}{A_m}\right| < 1$ is presented as:

$$\left|\frac{B_m}{A_m}\right| = \frac{\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2 + \left(2bf\,sin(k_m\Delta x) - 2bg\delta_n^{\alpha,1}\,sin(k_m\Delta x)\right)^2}}{\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + \left(2bfsin(k_m\Delta x)\right)^2}} < 1. \quad (4.57)$$

Simplifying,

$$\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)-zg\delta_n^{\alpha,1}-4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2+\left(2bf\,sin(k_m\Delta x)-2bg\delta_n^{\alpha,1}\,sin(k_m\Delta x)\right)^2}$$
$$<\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2+\left(2bf sin(k_m\Delta x)\right)^2}. \tag{4.58}$$

We recall eq. (4.46) and suppose that:

$$C_m=\left[zg\delta_n^{\alpha,2}+4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}+bg\delta_n^{\alpha,2}(2isin(k_m\Delta x))\right],$$

Then,

$$|C_m|=\sqrt{\left(zg\delta_n^{\alpha,2}+4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}\right)^2+\left(bg\delta_n^{\alpha,2}(2sin(k_m\Delta x))\right)^2}. \tag{4.59}$$

Similarly,

$$\left|zg\delta_n^{\alpha,2}+4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}+bg\delta_n^{\alpha,2}(2isin(k_m\Delta x))\right|$$
$$=\sqrt{\left(zg\delta_n^{\alpha,2}+4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}\right)^2+\left(bg\delta_n^{\alpha,2}(2sin(k_m\Delta x))\right)^2}. \tag{4.60}$$

Therefore, eq. (4.46) can be presented as:

$$\hat{\rho}_{n+1}A_m=\hat{\rho}_nB_m+\hat{\rho}_{n-1}C_m. \tag{4.61}$$

$\forall\, n>0$, we assume that:

$$|\hat{\rho}_n|<|\hat{\rho}_0|\Longrightarrow\left|\frac{\hat{\rho}_n}{\hat{\rho}_0}\right|<1,$$

Using the above assumption, we can prove that:

$$\left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < 1,$$

Thus,

$$|\hat{\rho}_{n+1}||A_m| = |\hat{\rho}_n B_m + \hat{\rho}_{n-1} C_m|,$$

$$\begin{aligned}
&|\hat{\rho}_{n+1}|\left|1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x))\right| \\
&= \left|\hat{\rho}_n\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) + bf(2isin(k_m\Delta x)) - zg\delta_n^{\alpha,1}\right.\right. \\
&\left. - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1} - bg\delta_n^{\alpha,1}(2isin(k_m\Delta x))\right) \\
&\left. + \hat{\rho}_{n-1}\left(zg\delta_n^{\alpha,2} + 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2} + bg\delta_n^{\alpha,2}(2isin(k_m\Delta x))\right)\right|.
\end{aligned} \tag{4.62}$$

Which means that:

$$|\hat{\rho}_{n+1}||A_m| \leq |\hat{\rho}_n||B_m| + |\hat{\rho}_{n-1}||C_m|,$$

$$\begin{aligned}
&|\hat{\rho}_{n+1}|\left(\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + \left(2bfsin(k_m\Delta x)\right)^2}\right) \\
&\leq |\hat{\rho}_n|\left(\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2 + \left(2bf\,sin(k_m\Delta x) - 2bg\delta_n^{\alpha,1}\,sin(k_m\Delta x)\right)^2}\right) \\
&+ |\hat{\rho}_{n-1}|\left(\sqrt{\left(zg\delta_n^{\alpha,2} + 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}\right)^2 + \left(bg\delta_n^{\alpha,2}(2sin(k_m\Delta x))\right)^2}\right).
\end{aligned} \tag{4.63}$$

By applying the inductive hypothesis, we suppose that:

$$|\hat{\rho}_n| < 0 \text{ and } |\hat{\rho}_{n-1}| < |\hat{\rho}_0|$$

$$|\hat{\rho}_{n+1}||A_m| < |\hat{\rho}_0||B_m| + |\hat{\rho}_0||C_m|, \tag{4.64}$$

$$
\begin{aligned}
&|\hat{\rho}_{n+1}|\left(\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2+\left(2bf sin(k_m\Delta x)\right)^2}\right)\\
&\le |\hat{\rho}_0|\left(\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)-zg\delta_n^{\alpha,1}-4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2+\left(2bf\, sin(k_m\Delta x)-2bg\delta_n^{\alpha,1}\, sin(k_m\Delta x)\right)^2}\right)\\
&+|\hat{\rho}_0|\left(\sqrt{\left(zg\delta_n^{\alpha,2}+4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}\right)^2+\left(bg\delta_n^{\alpha,2}(2sin(k_m\Delta x))\right)^2}\right).
\end{aligned}
$$

By factorization, we have:

$$
|\hat{\rho}_{n+1}||A_m| < |\hat{\rho}_0|(|B_m|+|C_m|),
$$

$$
\begin{aligned}
&|\hat{\rho}_{n+1}|\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2+\left(2bf sin(k_m\Delta x)\right)^2}\\
&< |\hat{\rho}_0|\left(\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)-zg\delta_n^{\alpha,1}-4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2+\left(2bf\, sin(k_m\Delta x)-2bg\delta_n^{\alpha,1}\, sin(k_m\Delta x)\right)^2}\right.\\
&\left.+\sqrt{\left(zg\delta_n^{\alpha,2}+4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}\right)^2+\left(bg\delta_n^{\alpha,2}(2sin(k_m\Delta x))\right)^2}\right).
\end{aligned}
\tag{4.65}
$$

We further have:

$$
\left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < \frac{|B_m|+|C_m|}{|A_m|}, \tag{4.66}
$$

$$
\left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < \frac{\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)-zg\delta_n^{\alpha,1}-4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2+\left(2bf\, sin(k_m\Delta x)-2bg\delta_n^{\alpha,1}\, sin(k_m\Delta x)\right)^2}+\sqrt{\left(zg\delta_n^{\alpha,2}+4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}\right)^2+\left(bg\delta_n^{\alpha,2}(2sin(k_m\Delta x))\right)^2}}{\sqrt{\left(1+zf+4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2+\left(2bf sin(k_m\Delta x)\right)^2}}.
$$

Remember that:

$$
\left|\frac{\hat{\rho}_{n+1}}{\hat{\rho}_0}\right| < 1,
$$

Which also implies that:

$$\frac{|B_m| + |C_m|}{|A_m|} < 1, \tag{4.67}$$

$$\frac{\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right) - zg\delta_n^{\alpha,1} - 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,1}\right)^2 + \left(2bf\, sin(k_m\Delta x) - 2bg\delta_n^{\alpha,1}\, sin(k_m\Delta x)\right)^2} + \sqrt{\left(zg\delta_n^{\alpha,2} + 4ag\sin^2\left(\frac{k_m\Delta x}{2}\right)\delta_n^{\alpha,2}\right)^2 + \left(bg\delta_n^{\alpha,2}(2sin(k_m\Delta x))\right)^2}}{\sqrt{\left(1 + zf + 4af\sin^2\left(\frac{k_m\Delta x}{2}\right)\right)^2 + \left(2bfsin(k_m\Delta x)\right)^2}}$$

$$< 1.$$

We can therefore conclude that, under this condition our numerical method is conditionally stable.

CHAPTER 5: NUMERICAL SIMULATIONS

Modeling real world problem requires three major steps including observation, analysis and prediction. The last two steps are performed within the framework of mathematical models, where observed facts are converted into a mathematical equation or set of mathematical equations. To perform the analysis, one needs to solve such mathematical problem using either analytical methods which normally provide exact solutions however, when the model is highly nonlinear, analytical methods are replaced by numerical methods. Numerical methods are now able to provide an approximate solution of the model. In the previous chapter, we presented some application of new numerical methods to solve the new model of groundwater flow with stochastic coefficients. The stability analysis was performed to guarantee the accuracy of the method.

In this section, we present the numerical simulations of the new suggested method for modeling advection and dispersion transport problems via ABC derivative with different alpha values used. The figures are plotted using the MATLAB software and the numerical simulations via this software are portrayed from figures 3 to 22. The simulations depict change in contaminant concentration with respect to time and distance within a preferential flow path. To perform the simulation, we consider the following theoretical parameters $0.2<D<2$, $0.4<V<2$, the following initial condition is considered c(0,0)=1000, we consider the boundary condition to following exponential decay law with respect to time, and consider a fixed decay rate of 0.9. For each set of dispersion we consider the normal distribution as its statistical representation. Since the subsurface is concerned and heterogeneity, one will expect a cross-over behavior in transport distribution. To account for this crossover, we chose to simulate the model with the Atangana-Baleanu fractional derivative as this derivative was found to be a powerful mathematical operator able to capture crossover from waiting time distribution to probability distribution. In general, we are aware that within a geological formation with heterogeneity, the pollution path always follow the non-Gaussian distribution. This also allow us not to simulate with Caputo-Fabrizio to avoid steady state situation.

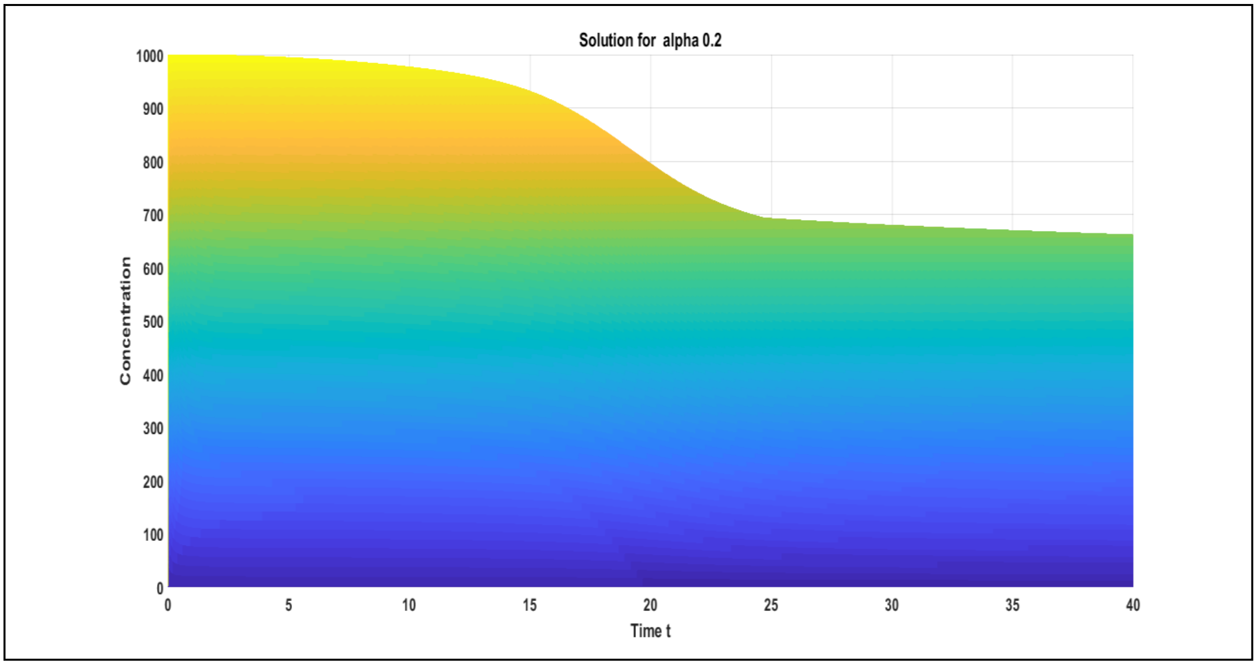

Figure 3: Numerical Simulation for contaminant concentration with respect to time using ABC, for α = 0.2

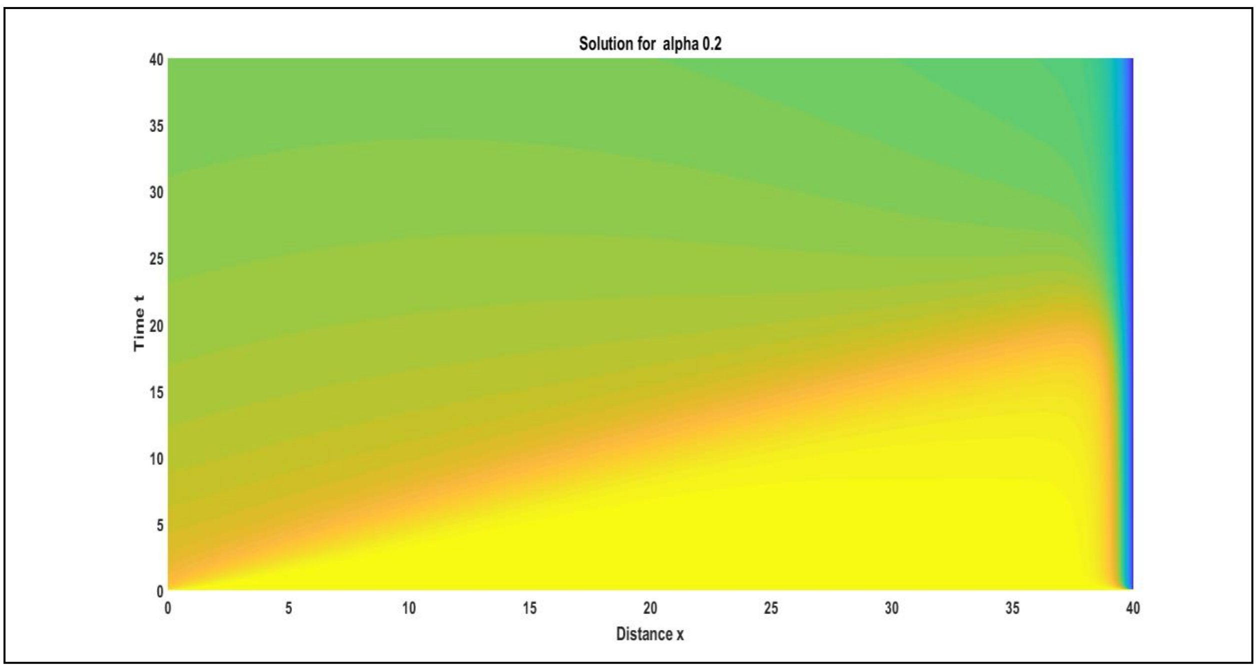

Figure 4: Numerical Simulation for contaminant concentration within a preferential flow path using ABC derivative, for α =0.2

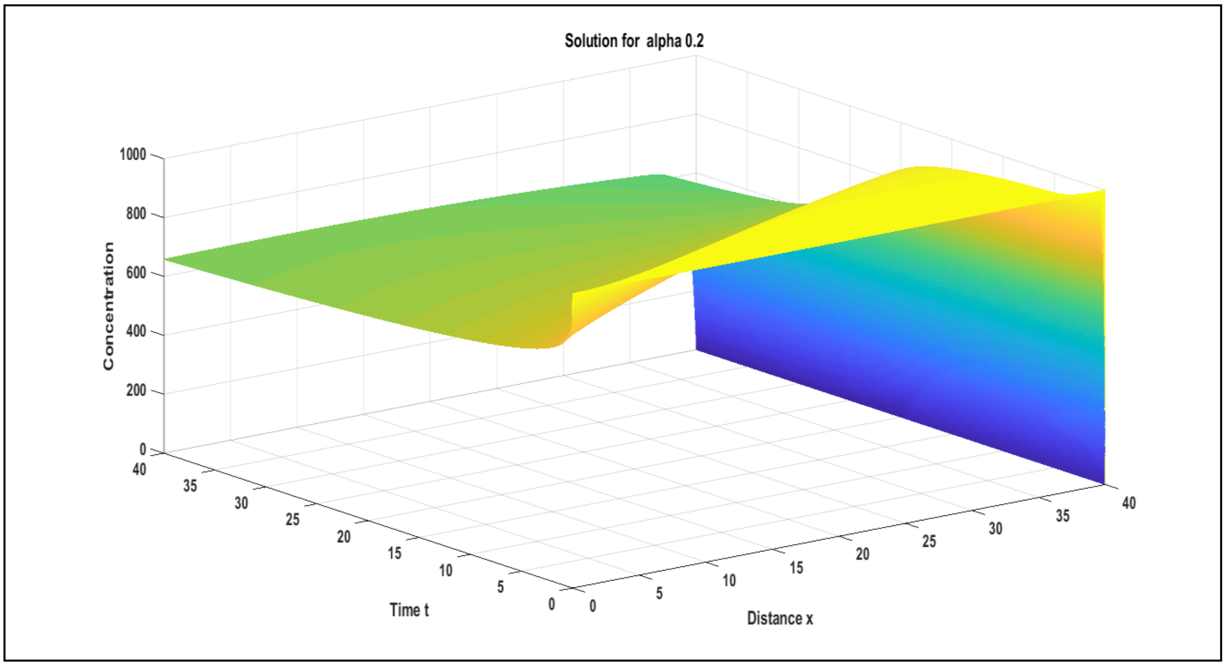

Figure 5: Numerical presentation for a contaminant concentration with respect to time and distance using ABC derivative, for α =0.2

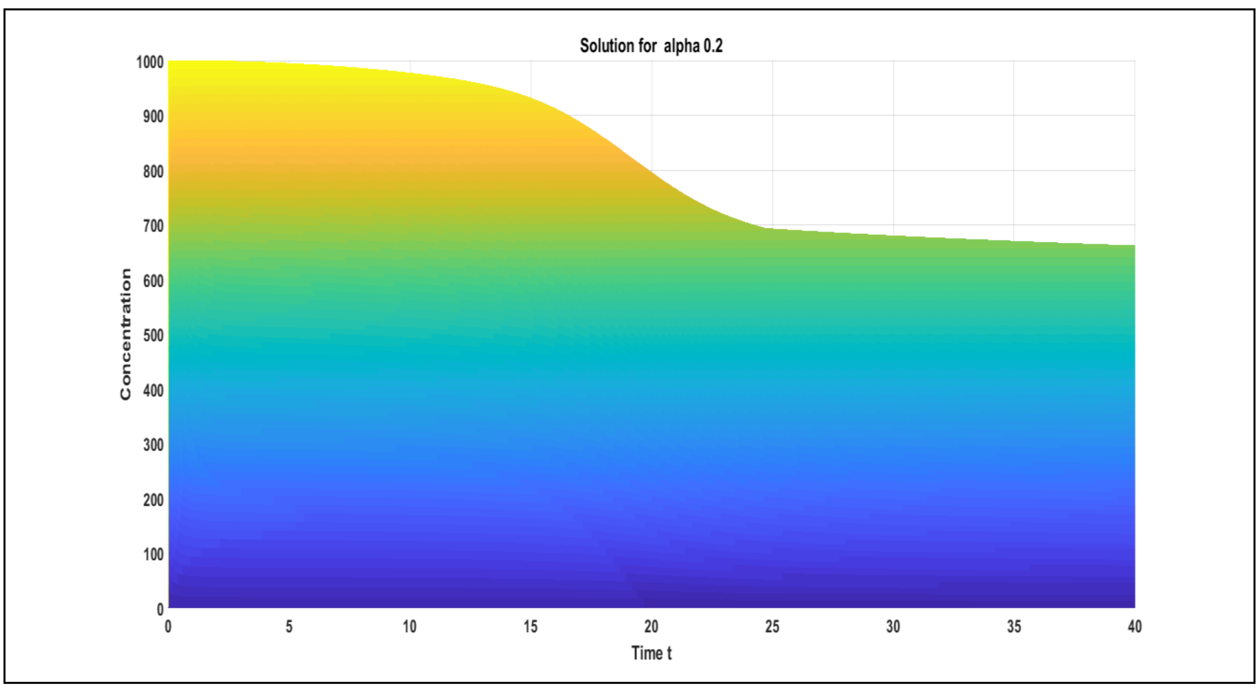

Figure 6: Numerical Simulation for contaminant concentration with respect to time using ABC derivative, for α = 0.2

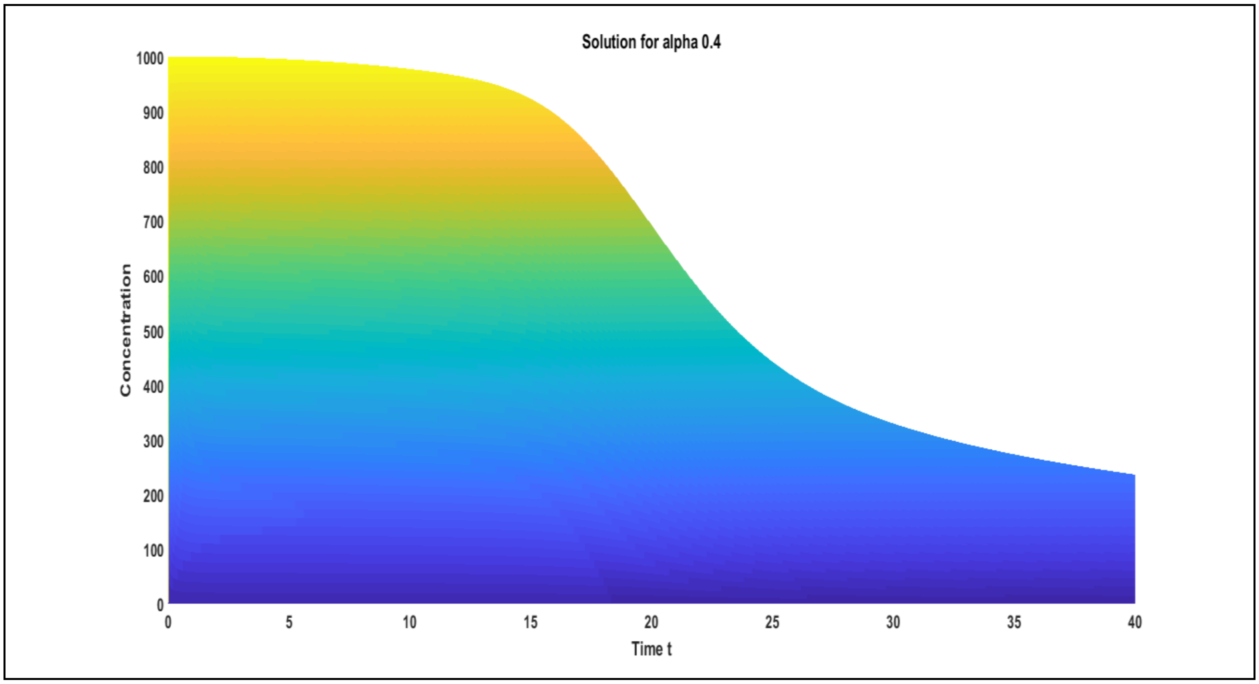

Figure 7: Numerical Simulation for concentration with respect to time using ABC derivative, for α = 0.4

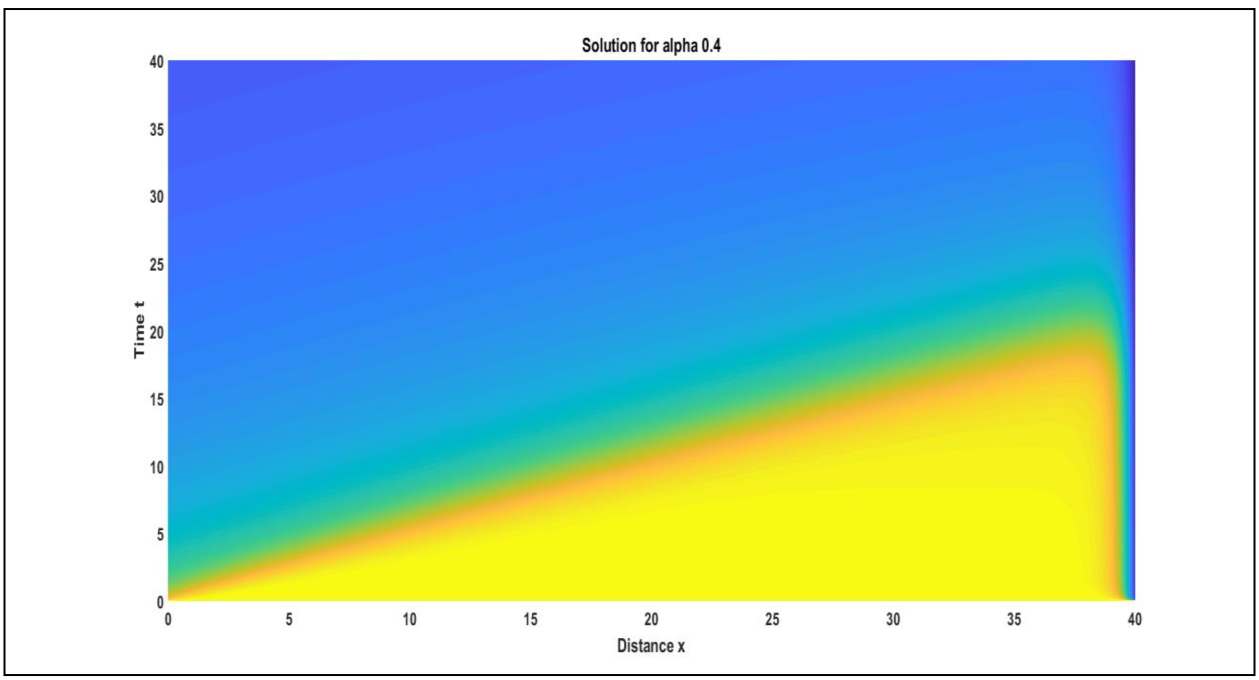

Figure 8: Numerical Simulation for contaminant concentration within a preferential flow paths using ABC derivative, α =0.4

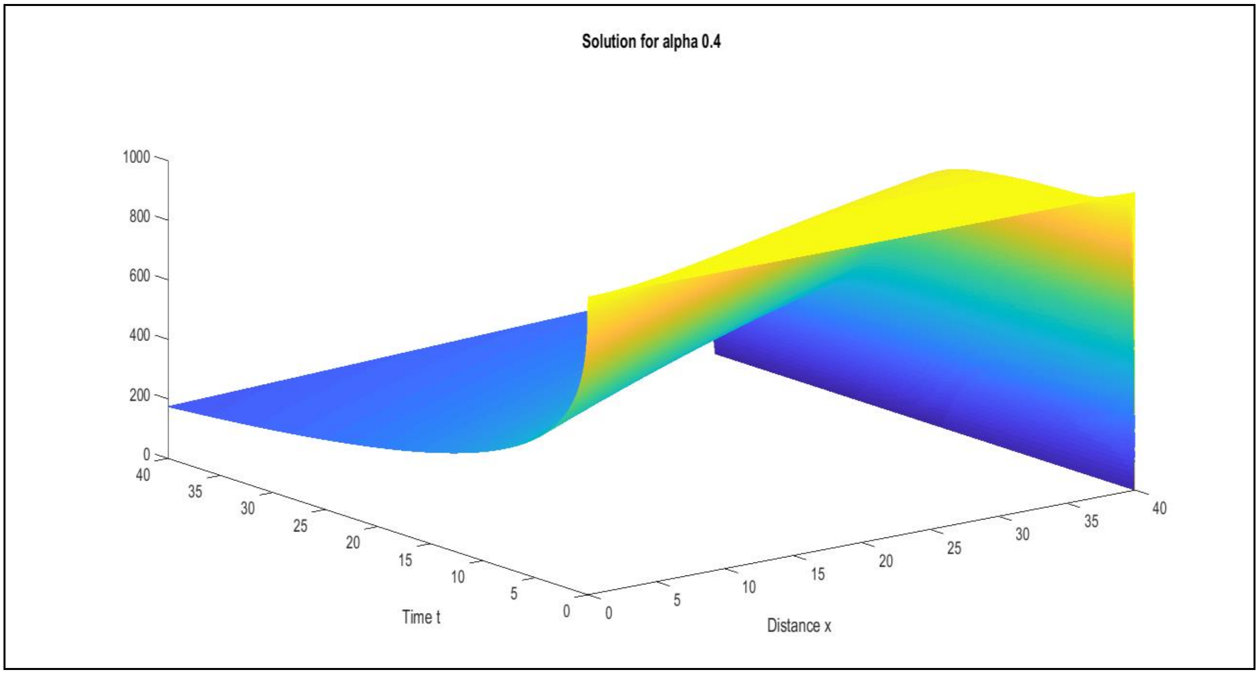

Figure 9: Numerical presentation for a contaminant concentration with respect to time and distance using ABC derivative, α = 0.4

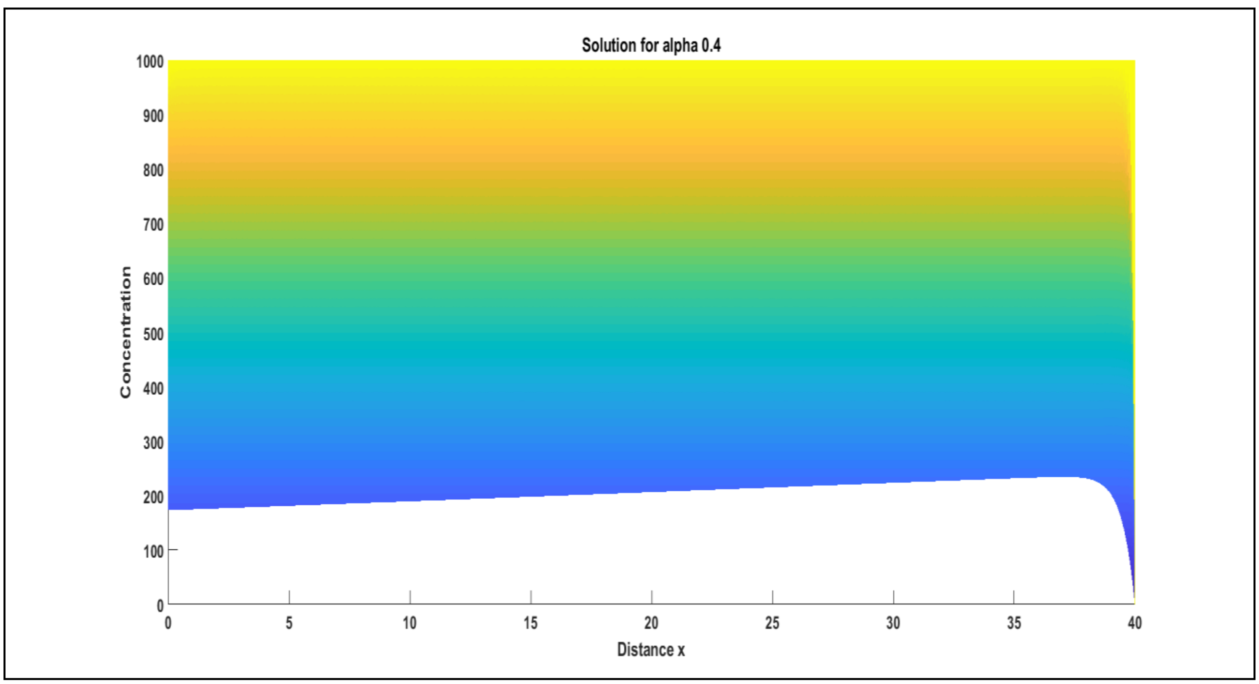

Figure 10: Numerical presentation for a contaminant concentration with respect to distance using ABC derivative, α = 0.4

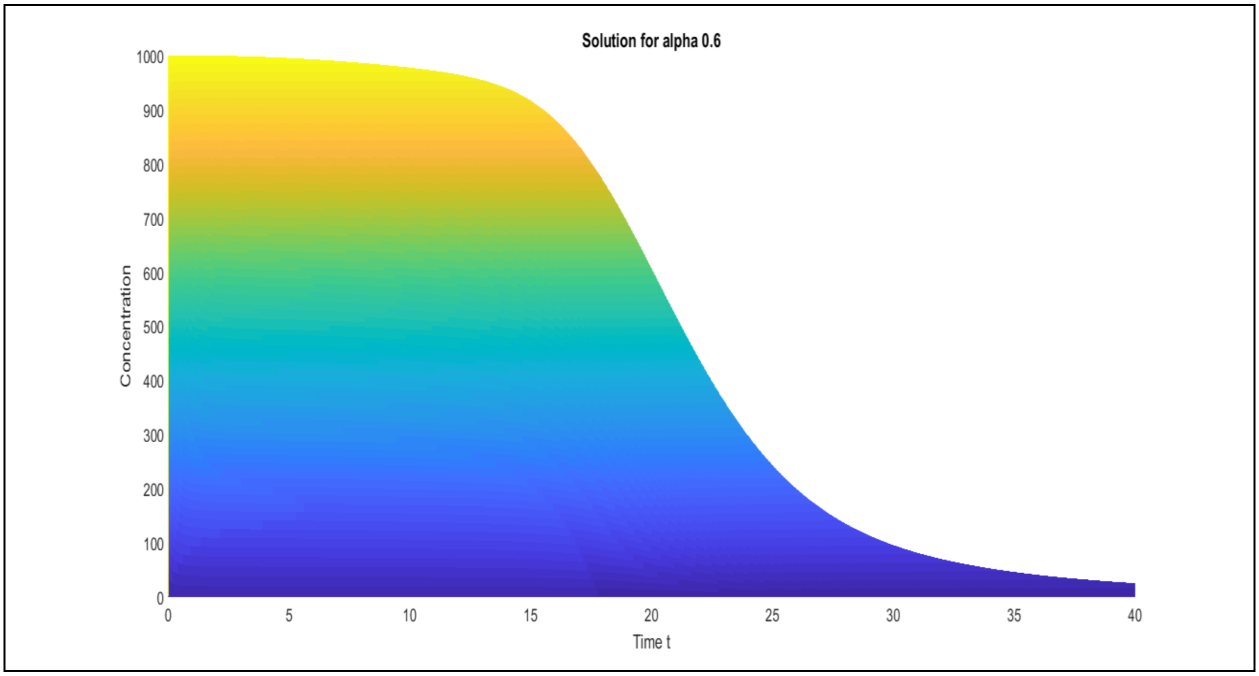

Figure 11: Numerical presentation for a contaminant concentration with respect to time using ABC derivative, $\alpha = 0.6$

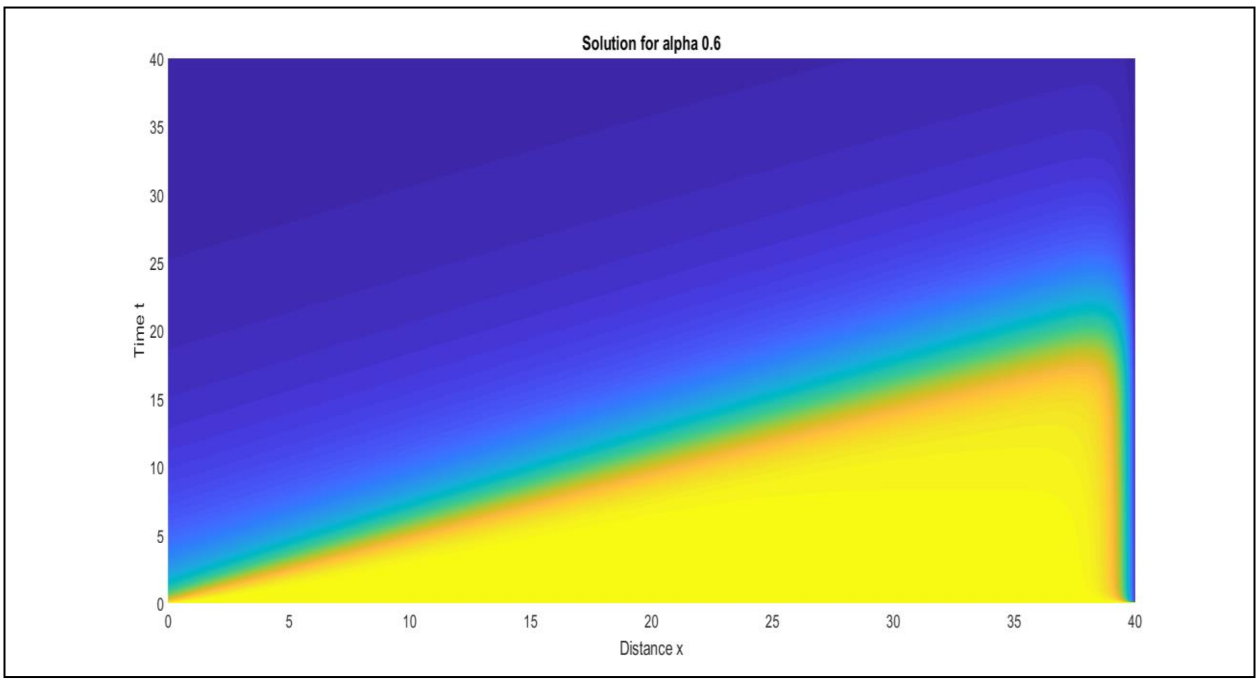

Figure 12: Numerical Simulation for contaminant concentration within a preferential flow path with respect to time and space using ABC derivative, $\alpha = 0.6$

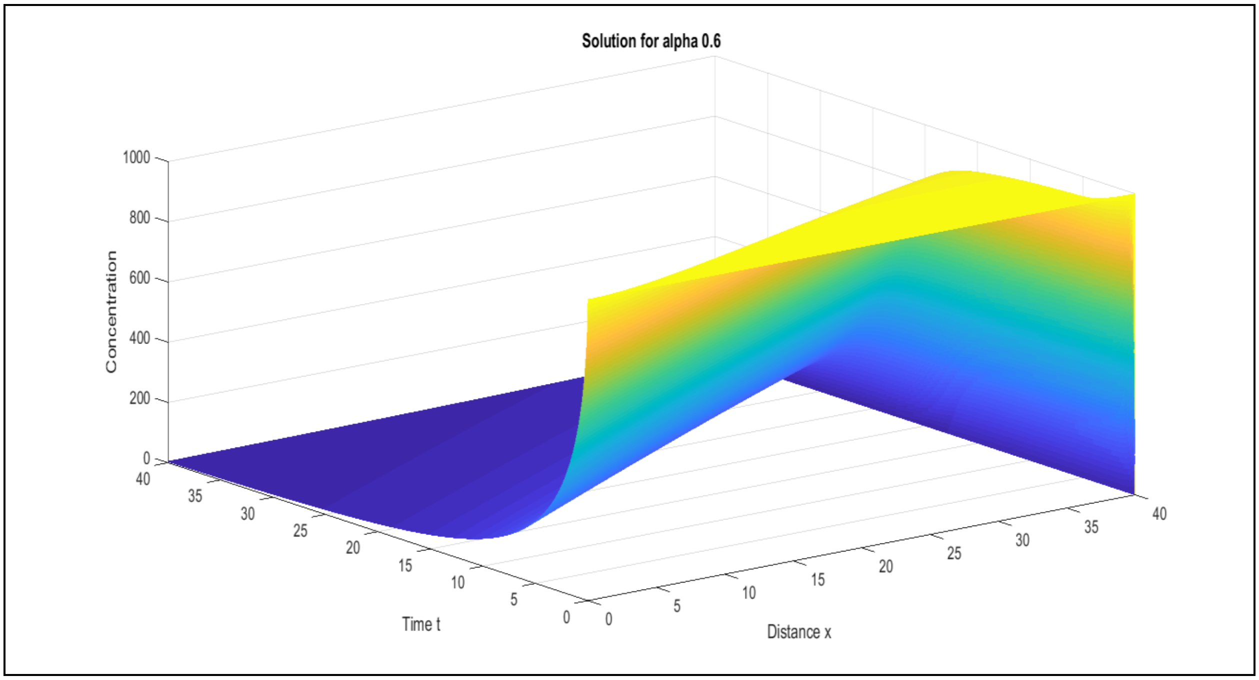

Figure 13: Numerical presentation for a contaminant concentration with respect to time and distance using ABC derivative, α = 0.6

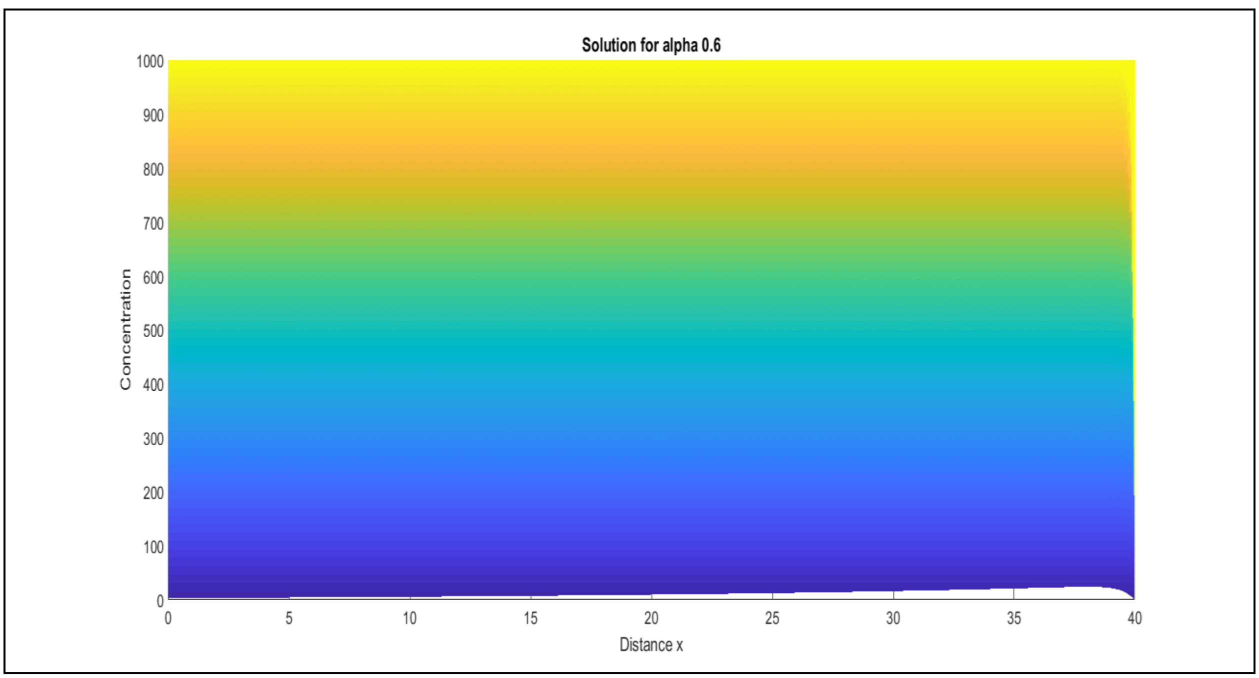

Figure 14: Numerical presentation for a contaminant concentration with respect to distance using ABC derivative, α = 0.6

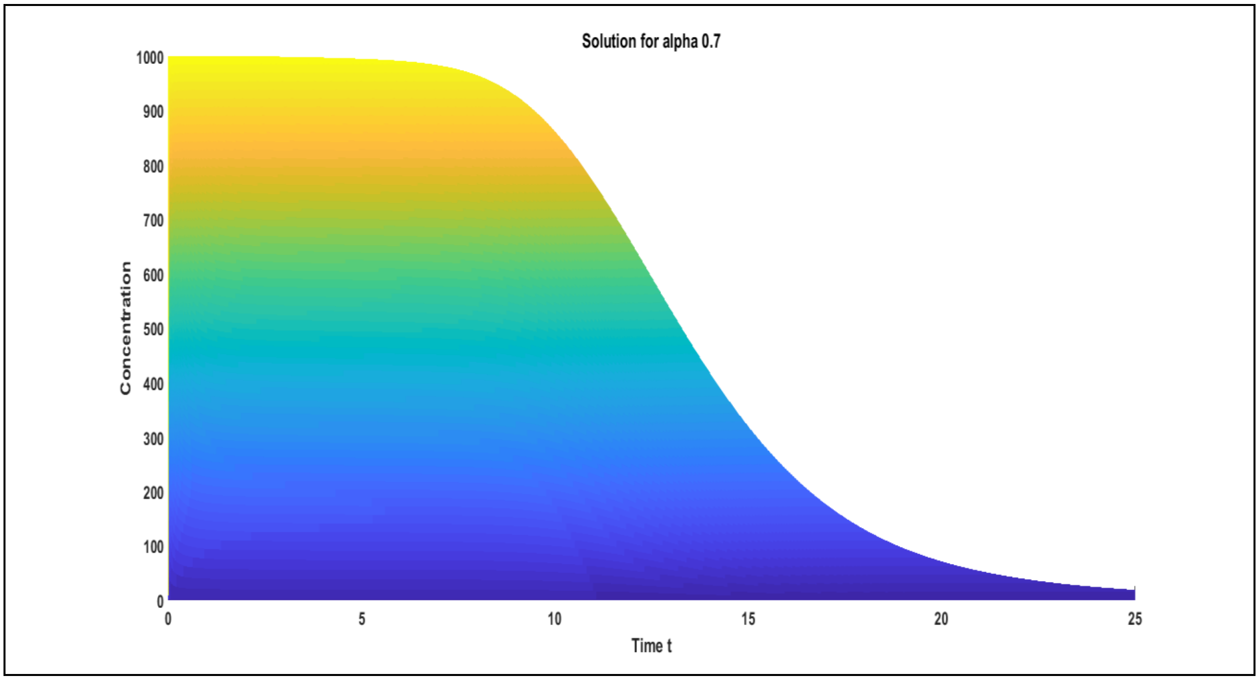

Figure 15: Numerical presentation for a contaminant concentration with respect to time using ABC derivative, α = 0.7

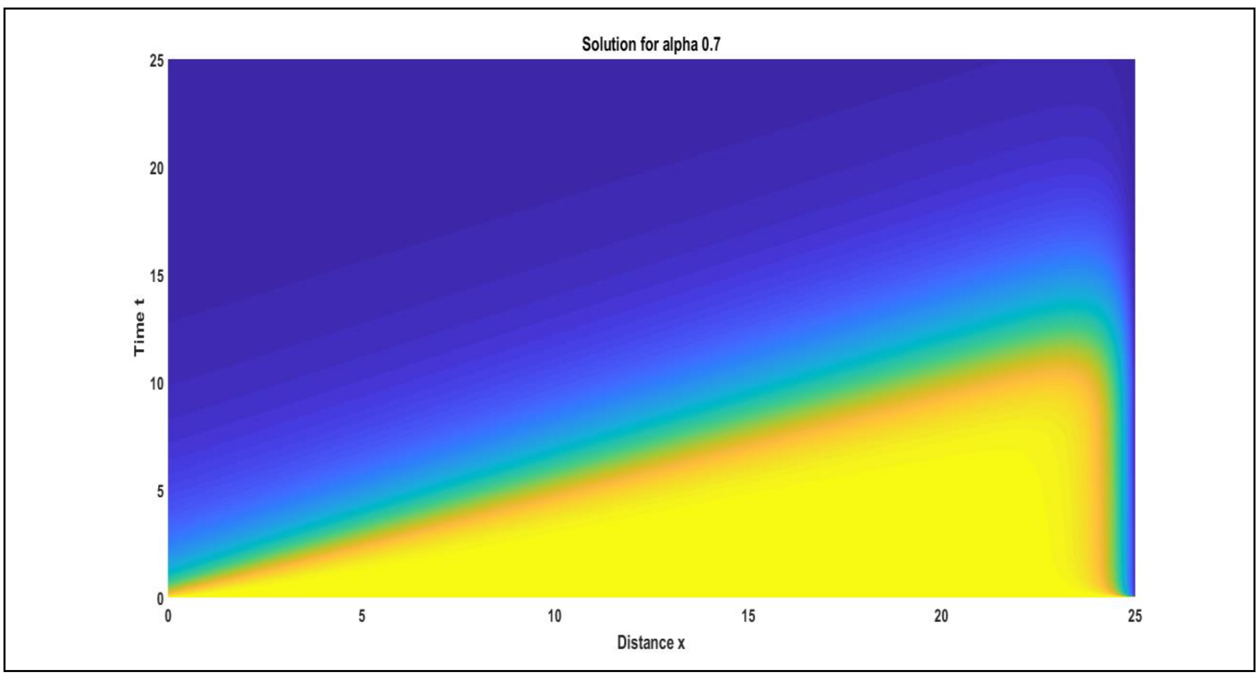

Figure 16: Numerical Simulation for contaminant transport within a preferential flow path with respect to time and space using ABC derivative, α = 0.7

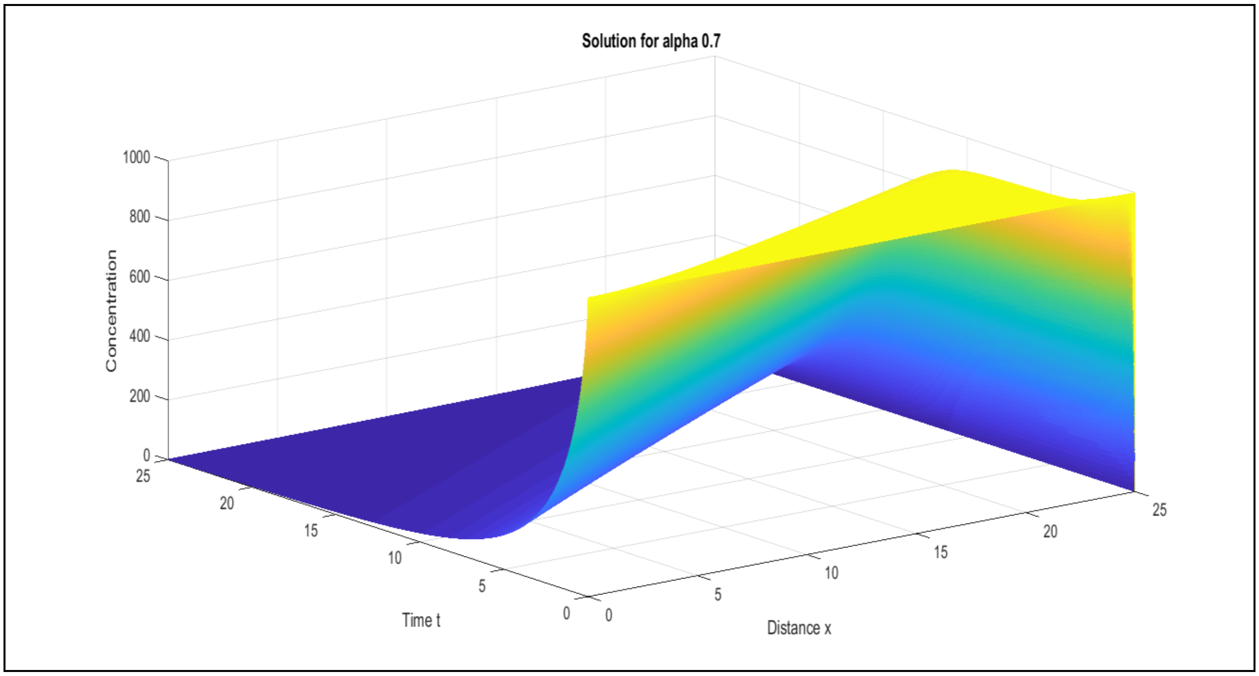

Figure 17: Numerical presentation for a contaminant concentration with respect to time and distance using ABC derivative, $\alpha = 0.7$

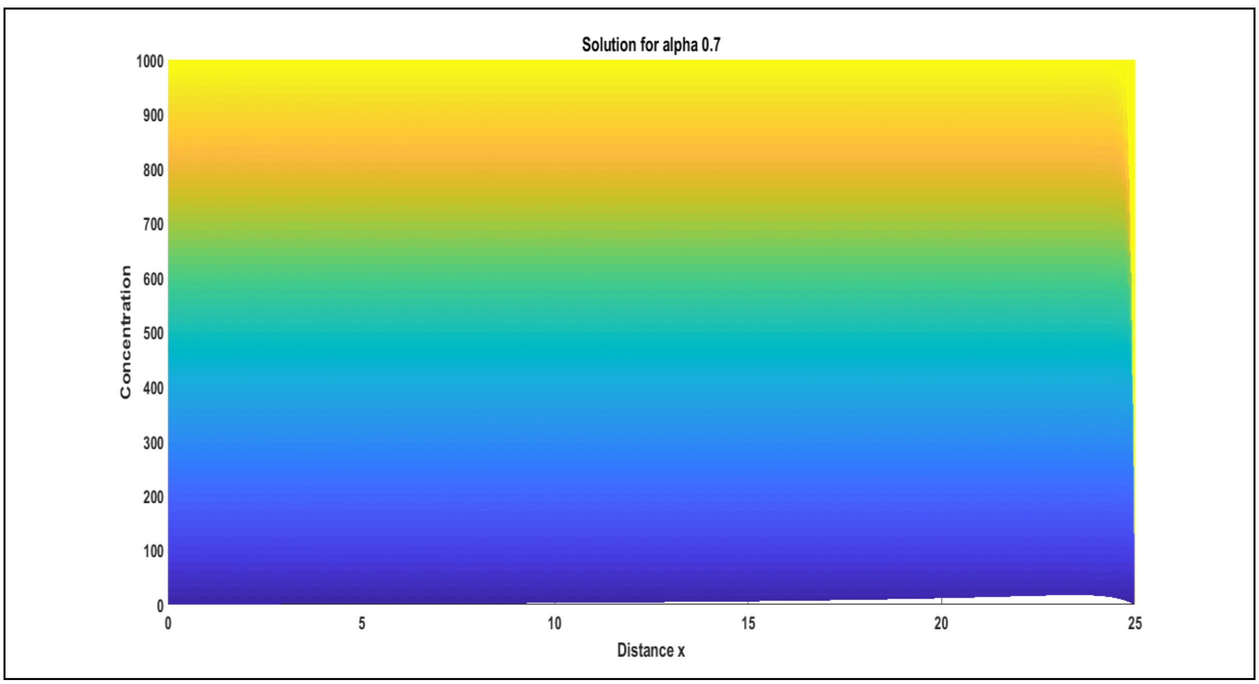

Figure 18: Numerical presentation for a contaminant concentration with respect to distance using ABC derivative, $\alpha = 0.7$

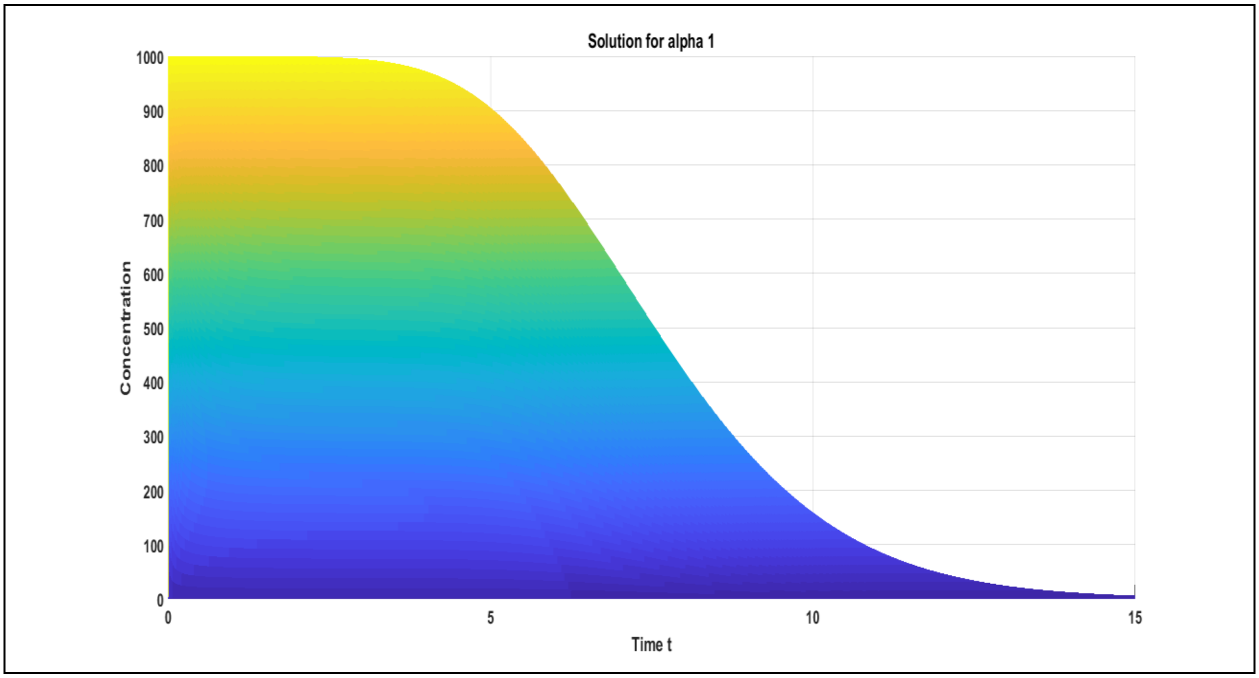

Figure 19: Numerical presentation for a contaminant concentration with respect to time using ABC derivative, α = 1

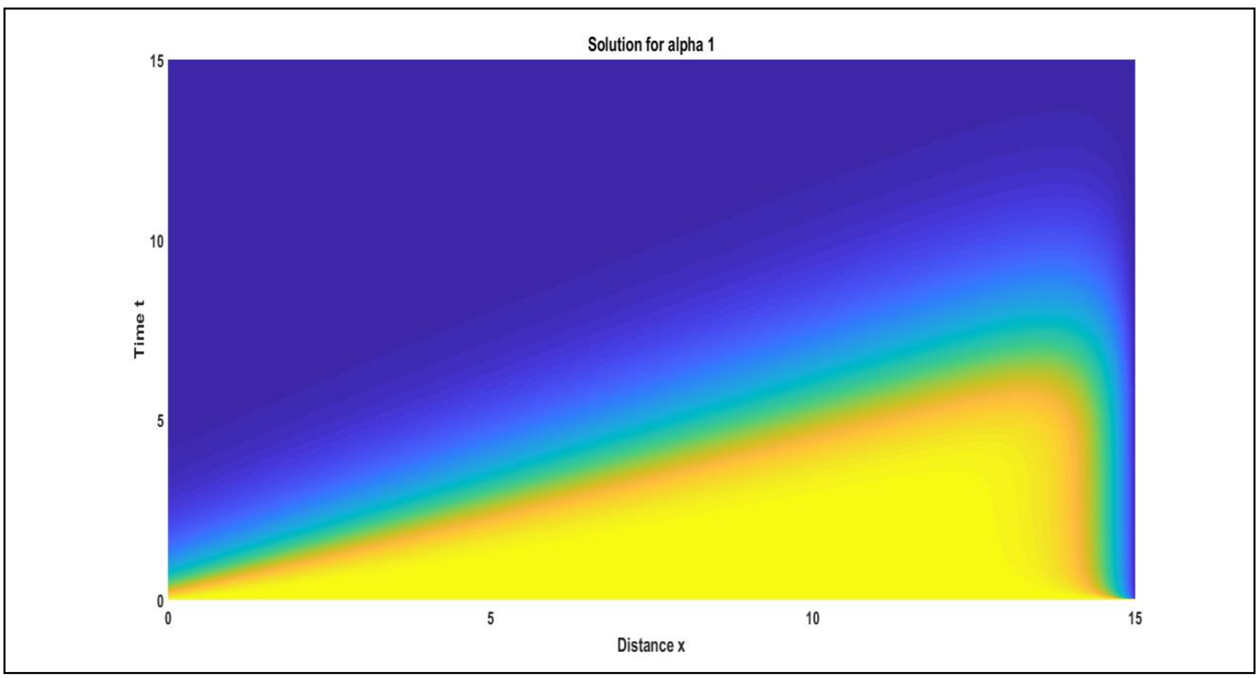

Figure 20: Numerical Simulation for contaminant transport within a preferential flow path with respect to time and space using ABC derivative, α = 1

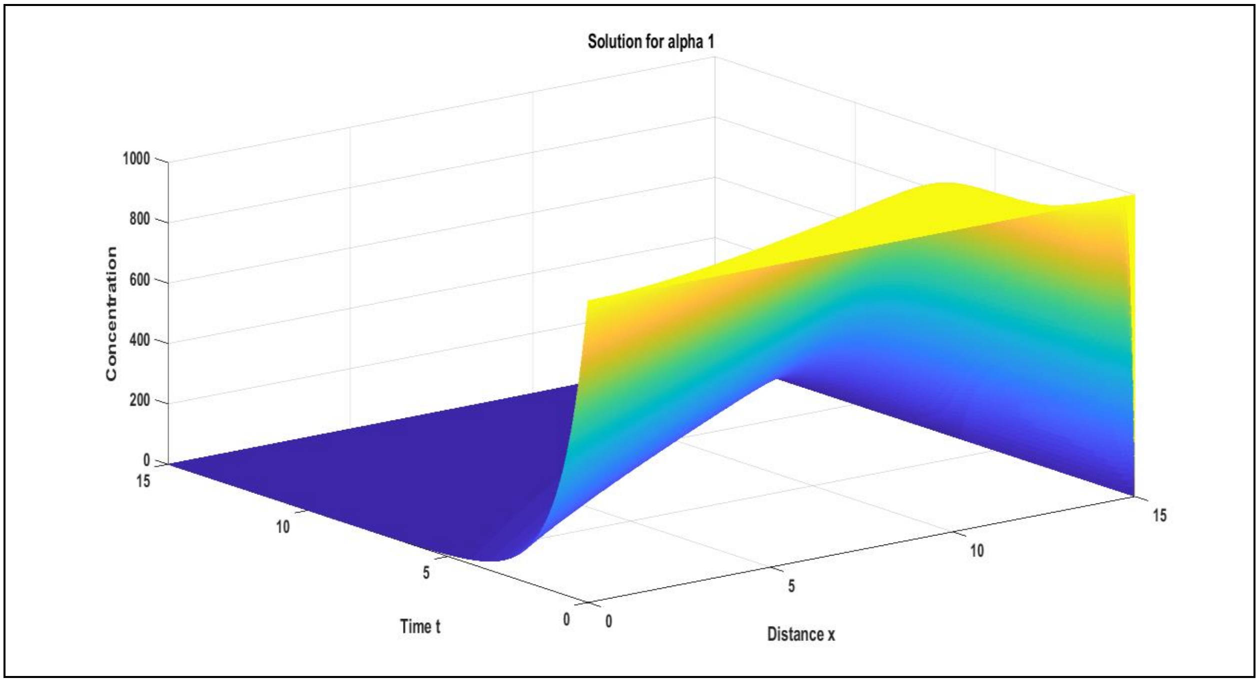

Figure 21: Numerical Simulation for contaminant concentration with respect to time and space using ABC derivative, α = 1

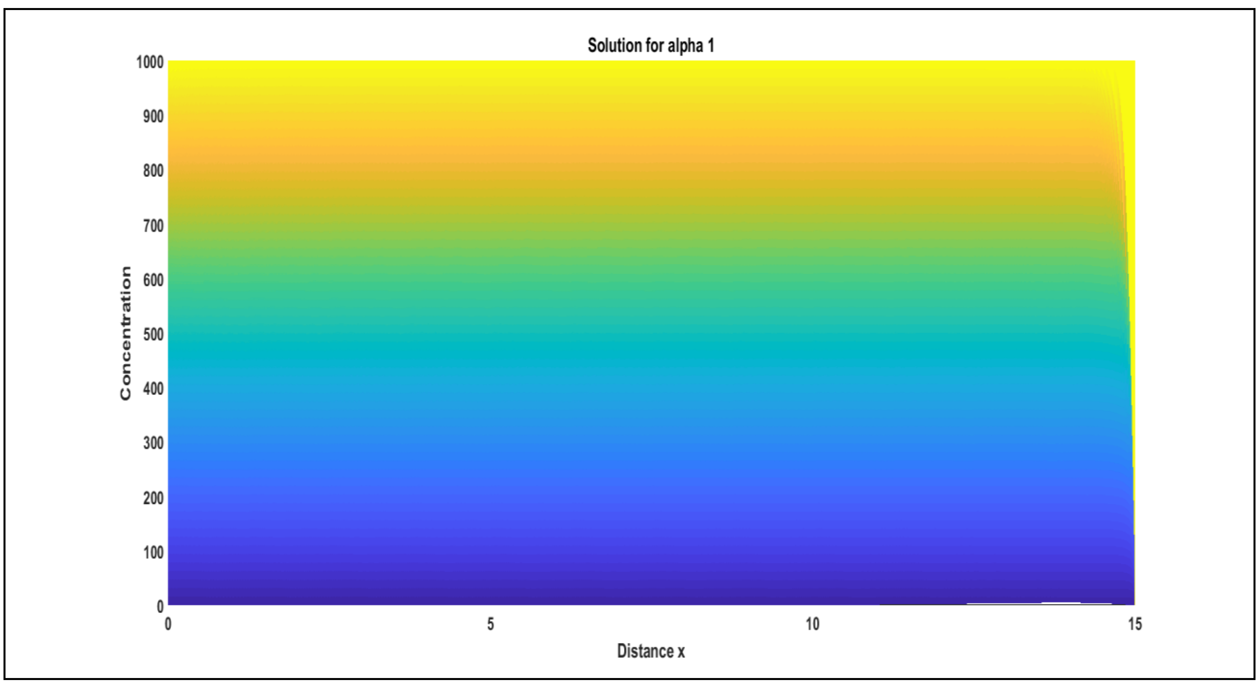

Figure 22: Numerical presentation for a contaminant concentration with respect to distance using ABC derivative, α = 1

5.1 RESULTSAND DISCUSSIONS

From the numerical simulations presented in the previous section, it can be seen that the results depict the behavior of certain real world situation in which the contaminant concentration changes with respect to time and space. This also indicates that the presence of heterogeneity with the aquifer systems has an impact on the groundwater velocity and dispersion of pollution. From the above figures 3, 5, 6, 10, 14 and 18, we observe the gradual decrease of the contaminant concentration with time. That is, in high values of alpha the pollution concentration decreases within a short time as compared to low alpha values. This means that, increasing or decreasing the scale factor has a direct influence on the concentration of pollution. The numerical simulations also show that there is a crossover from Gauss to non-Gaussian probability distribution. This is true for field scale observations because heterogeneity does exist in groundwater systems, and has an influence on groundwater velocity variability which also leads to dispersion of a pollutant. Thus, the above figures depict a normal distributions at some point but as the pollution travels with respect to time and distance, then we observe a change to non-Gaussian distribution. This is the main reason why the Atangana-Baleanu fractional derivative was used as it can capture these crossovers.

Therefore, the new theorem here is that classical differential operators can only be used be to model homogeneous groundwater systems. However, in reality groundwater systems are not homogeneous, but are characterized by heterogeneity. We therefore conclude that, fractional differential operators must be used to model natural groundwater systems because they can capture heterogeneity. The numerical simulations obviously show that the fractional order the differential operator can replicate very accurately the fast, slow and normal flow depending on the value of the used alpha. Another important fact is that the concept of arithmetic average used in groundwater problems is not suitable as it gives exaggerated results. We suggest geometric means if all the same are different from zero.

CONCLUSION

Modeling groundwater flow behavior using mathematical equations has always been a challenge as it requires a detailed understanding about the geologic formation through which groundwater moves. This remains a tricky challenge because the response and geological formation through which groundwater moves is invisible and can change with time and space. Some literature however, assumes that the aquifer parameters are constant at every point within the geological formation. Nevertheless, such assumptions become practically invalid because the subsurface is characterized by heterogeneity and aquifer parameters are not known with certainty. It is therefore very preferable to capture such uncertainties and heterogeneities using the concept of stochastic modeling. Stochastic models are very useful for providing predictions in situations where little information on aquifer parameters is available. Also, stochastic approach is used to estimate the variability of aquifer parameters of interest in a statistical framework, where a given constant coefficient is converted into a distribution. Thus, a stochastic approach has the ability to capture some physical processes with statistical setting. Nonetheless, some models fail to provide reliable groundwater flow estimates due to their inability to account for the heterogeneity, viscoelasticity and memory effect. The concept of differentiation is therefore very suitable to model different types of geological formations. For example, literature proves that the Atangana-Baleanu fractional derivative which is based on the Mittag-Leffler function is fit for application in various types of geological formations including the homogeneous, heterogeneous and viscoelastic subsurfaces. The Caputo fractional operator which utilizes the power function is very suitable for application in elastic and homogeneous subsurfaces, while the Caputo-Fabrizio fractional derivative which is based on the exponential law is suitable for modeling heterogeneous subsurfaces. Accordingly, the aim of this study was to combine the concept of non-local differential and integral operators with the stochastic approach because both concepts are capable to model complexity in real-world problems. In addressing the main, a new numerical scheme was developed using the Adams-Bashforth method to generate a new solution of modeling groundwater flow problems. Then, the condition for stability was tested using the Von Neumann stability analysis method. Lastly, numerical simulations were also presented.

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