# DEVELOPMENT OF A FRACTAL ADVECTION-DISPERSION EQUATION AND NEW NUMERICAL SCHEMES FOR THE CLASSICAL, FRACTAL AND FRACTIONAL ADVECTION-DISPERSION TRANSPORT EQUATIONS

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# DECLARATION

I, Amy Allwright, hereby declare that the dissertation hereby submitted by me to the Institute for Groundwater Studies in the Faculty of Natural and Agricultural Sciences at the University of the Free State, in fulfilment of the degree of Doctoral Scientiae, is my own independent work. It has not previously been submitted by me to any other institution of higher education. In addition, I declare that all sources cited have been acknowledged by means of a list of references.

I furthermore cede copyright of the dissertation and its contents in favour of the University of the Free State.

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Amy Allwright (2010083661)

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My heavenly Father, who has given me everything I needed to complete this thesis. You have been a constant presence through all the trials and highlights. Your hand has guided this endeavour from the beginning to the end, and all the glory is Yours.

# ABSTRACT

Groundwater is a vital source of fresh water to many people across the globe, but it is prone to contamination by human activities. In the last few decades, great strides have been made in legislation protecting and controlling the quality of groundwater, creating awareness of potential groundwater contamination and the importance of prevention and mitigation. The accurate representation of contaminant movement within a groundwater system is important, because misrepresentation could increase the environmental impact due to inadequate mitigation or remediation measures. However, groundwater transport is particularly complex due to the inherent heterogeneity of aquifers. Where, predicting the movement of contaminants within groundwater systems, especially in fractured systems, is prone to discrepancies between modelled and observed. There are two general approaches to improve the simulation of groundwater transport: develop the physical characterisation of the heterogeneous system, or redefine the formulation of the governing equations. The focus of this research is to advance the simulation of groundwater transport by examining the formulation of the governing advection-dispersion equation. To achieve this aim, improved numerical approximation schemes for the classical advection-dispersion equation are developed, fractal and fractional derivatives are incorporated into the formulation, and fractional and fractal derivatives are combined.

Augmented upwind finite difference numerical approximation schemes, which are better suited for advection-dominated systems, are applied to the solution of the classical advection-dispersion equation for fractured groundwater systems. The simulation of anomalous transport in fractured aquifer systems is improved by providing a fractal advection-dispersion equation with numerical integration and approximation methods for solution. The fractal advection-dispersion equation is proven to simulate superdiffusion and subdiffusion by varying the fractal dimension, without explicit characterisation of fractures or preferential pathways. To improve the governing equation for groundwater transport modelling, the Caputo and Atangana-Baleanu in Caputo sense (ABC) fractional derivatives are applied to the advection-dispersion equation with a focus on the advection term to account for *anomalous advection*. Appropriate numerical approximation methods for the fractional advection-dispersion equations are provided and analysed for stability requirements. A fractional-fractal advection-dispersion equation is developed to provide an efficient non-local, in both space and time, modelling tool. The fractional-fractal model provides a flexible tool to model anomalous diffusion, where the fractional order controls the breakthrough curve peak, and the fractal dimension controls the position of the peak and tailing effect. These two controls potentially provide the tools to improve the representation of anomalous breakthrough curves that cannot be described by the classical model.

A modest step is taken forward to advance the use of fractional calculus, achieve the collective mission of resolving the difference between modelled and observed, and to increase the comprehension and management of natural systems.

Academic journal articles published from thesis:

Allwright, A. and Atangana, A. (2018). Fractal advection-dispersion equation for groundwater transport in fractured aquifers with self-similarities. *The European Physical Journal Plus*, 133(2), 48. Impact factor 2.240.

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Book chapter from thesis (published):

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Academic journal articles from thesis (submitted):

Fractional-fractal advection-dispersion model: simulation of a dual non-local system for anomalous transport in fractured systems

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# 1 INTRODUCTION

Real world systems are complex, by definition a complexity by which any one method is not able to capture all the nuances of that system. It is this that compels science to improve and continuously strive for new methods and approaches, ever endeavouring to reconcile the difference between modelled and observed.

Simulating transport with the advection-dispersion equation is a real world problem, where the general discrepancy between modelled and observed is particularly large. This discrepancy lead to the development of the term anomalous diffusion (non-Fickian diffusion), especially when using traditional methods. In groundwater systems, this discrepancy can be attributed to the highly heterogeneous nature of aquifer systems, especially in fractured systems; and the understanding on which the governing equation was formulated upon. Therefore, the solution of this problem from a groundwater perspective logically involves either improving the characterisation of heterogeneity in the system, and/or improving the formulation of the governing equation.

Improving the characterisation of heterogeneity has been historically topical; from some of the first comprehensive groundwater books (Freeze and Cherry, 1979) up to the present. In 2015, the *MADE challenge for groundwater transport in highly heterogeneous aquifers: insights from 30 years of modelling and characterisation at the field scale and promising future directions* was held to assess the progress made from the original tracer series at the Macrodispersion Experiment, in the late 1980s to 1990s, which sparked the consideration of new approaches for solute transport in highly heterogeneous media (Gómez-Hernández et al., 2017). While extensive research has been done to improve the characterisation of heterogeneity, ranging from new measurement devices, new parameter estimate methods, to discrete fracture network models, the challenge of how best to characterise a heterogeneous system, to incorporate that heterogeneity into a model, and to simulate transport within that system, remains.

On the other hand, from the perspective of improving the formulation of the governing equation, numerous non-local approaches have been applied, ranging from multiple-rate mass transfer method and rate-limited mass transfer, stochastic averaging, continuous-time random walk, to fractal and fractional differential equations (Koch and Brady, 1988; Schumer et al., 2003a; Schumer et al., 2003b and b; Berkowitz et al., 2006; Singha et al., 2007; Zhang et al., 2009; Neuman and Tartakovsky, 2009; Zhang et al., 2013; Sun et al., 2014).

For this research, the latter approach will be perused, where the formulation of the advection-dispersion equation can be improved to better simulate groundwater transport without a detailed characterisation of the heterogeneity of a system, especially a fractured aquifer system.

## 1.1 Anomalous diffusion and transport in heterogeneous systems

The traditional advection-dispersion equation is used to describe the transport of non-reactive contaminants or tracers, which is founded on an analogy to Fick's Law of diffusion. Non-Fickian transport or diffusion, also termed anomalous diffusion, is any transport that is not adequately described by the traditional advection-dispersion equation. Anomalous transport can be defined by non-Gaussian leading or trailing tails of a plume or break-through curve from a point source, or nonlinear growth of the centered second moment. Subdivisions of anomalous diffusion include superdiffusion and subdiffusion, superdiffusion is characterised by a growth rate faster than linear growth (i.e. faster movement found in preferential flow pathways), and subdiffusion is characterised by a growth rate slower than linear growth (i.e. slower movement in low-permeability zones) (Zhang et al., 2009; Neuman and Tartakovsky, 2009; Zhang et al., 2013; Sun et al., 2014).

Anomalous diffusion is not anomalous in the traditional sense of the word, but rather a term coined to describe natural phenomena that cannot be modelled accurately using traditional modelling approaches and equations (Klafter and Sokolov, 2005). Examples of anomalous diffusion range from signalling of biological cells to foraging behaviour of animals, from the operation of photocopier machines to transport of contaminants in groundwater. Anomalous diffusion in fractured groundwater systems have been well documented (Liu et al., 2004; Klafter and Sokolov, 2005; Meerschaert et al., 2008; Pablo et al., 2009; Cello et al., 2009). Yang et al. (2012) considered two-phase flow in fractured media with an adaptive circle fitting interface, where the fractured system modelled producing highly irregular contaminant plume (Figure 1-1).

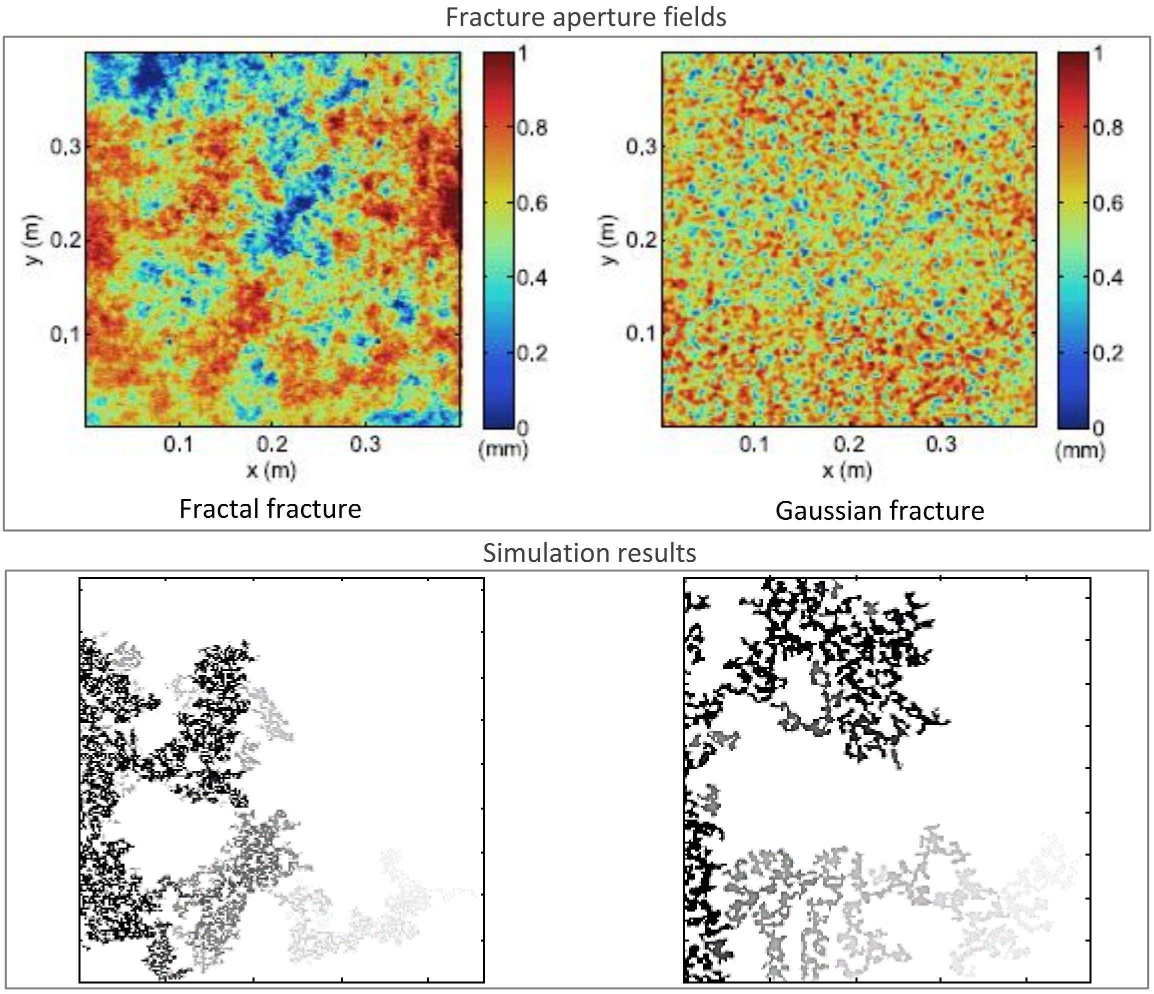


**Figure 1-1 Aperture fields measured by fractal fractures and Gaussian fractures (top), and the associated simulation results (bottom). Modified from Yang et al. (2012).**

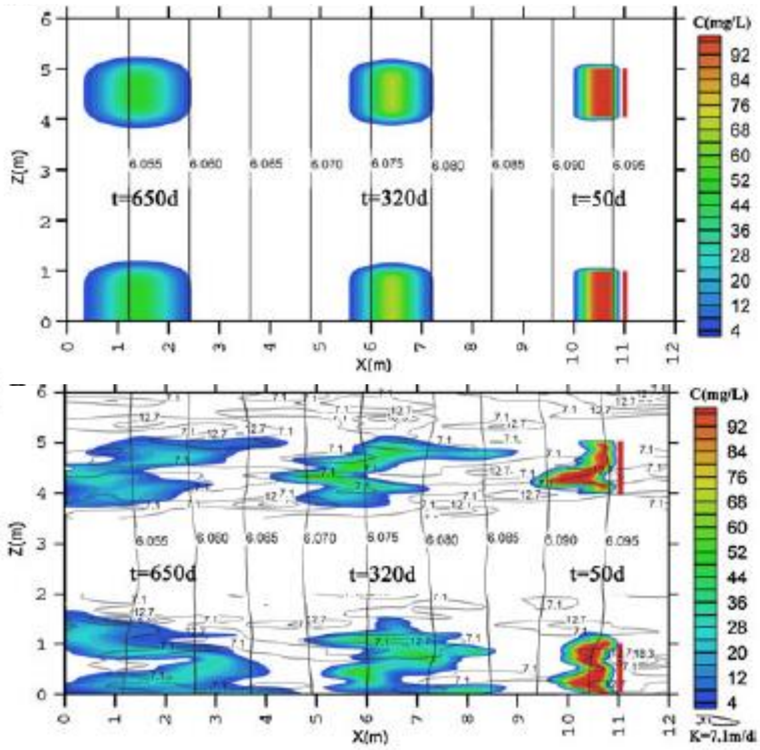


**Figure 1-2 Simulated hydraulic head contours and plume migration for a homogeneous aquifer (top) and for a heterogeneous aquifer (bottom). Modified from Qin et al. (2013).**

The resulting contaminant movement shows the potentially complex transport patterns in fractured media. The influence of heterogeneity on transport in groundwater was considered by Qin et al. (2013), where the transport of a solute within a dipping heterogeneous, confined aquifer is used to determine plume shapes under the various conditions (Figure 1-2). Figure 1-2 illustrates the potential influence heterogeneity has on the transport of contaminants within the subsurface, and highlights the importance of correctly including this aspect to ensure the correct prediction of contaminant movement for remediation and mitigation.

The main limitation in accurately predicting the movement of contaminants in groundwater is that spatial heterogeneity will never completely be characterised, regardless of the amount of data collected (Gómez-Hernández et al., 2016). Thus, investigating the reformulation of the governing equation to simulate variable transport without a complete characterisation of the system is a valid pursuit.

## 1.2 Non-local approaches

Numerous non-local approaches exist and have been applied to the problem of anomalous diffusion, as discussed. For this research, specific non-local approaches will be considered, including fractal and fractional derivatives.

### 1.2.1 Fractal geometry and derivative

Geometry is traditionally considered rigid, because classical geometry is unable to define the shape of a cloud, mountain or coastline. These natural phenomena and objects do not conform to the Euclid or standard geometry of smooth spheres, cones, circles and straight lines. Mandelbrot (1982) found that nature exhibits a higher-degree of irregularity and fragmentation when compared to standard geometry, where it can actually be considered a different level of complexity altogether. Mandelbrot (1982) describes these irregular and fragmented patterns by identifying a family of shapes termed fractals, forming the foundation for fractal geometry, and the fractal derivative (Figure 1-3). The term fractal was selected by Mandelbrot (1982) for the original Latin meaning, "to break, to create irregular fragments, describing a general fragmented and irregular nature (Mandelbrot, 1982; Le Méhauté, 1991; West, *et al*., 2012).

Fractal geometry is based on the principle that irregular objects in nature tend to exhibit inherent patterns that repeat themselves at different scales, termed *self-similarity*. Field observations have demonstrated that multiple length-scales exist in a variety of naturally fractured media (Acuna and Yortsos, 1995; Shokri et al., 2016). Shokri et al. (2016) document natural fracture networks that demonstrate fractal geometries (Figure 1-4). Fractal heterogeneity is not spatially periodic, but rather exhibit a pattern that is independent of the scale of observation (Wheatcraft and Tyler, 1988).

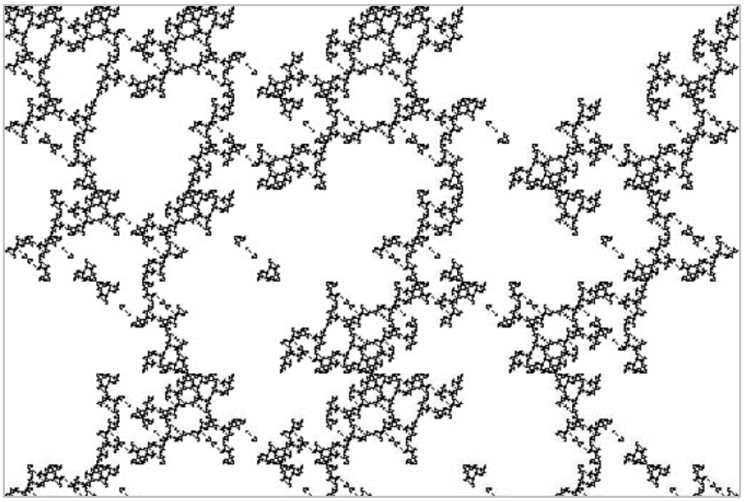

**Figure 1-3 Example of a fractal geometry with self-similarity. Modified after Mandelbrot (1982).**

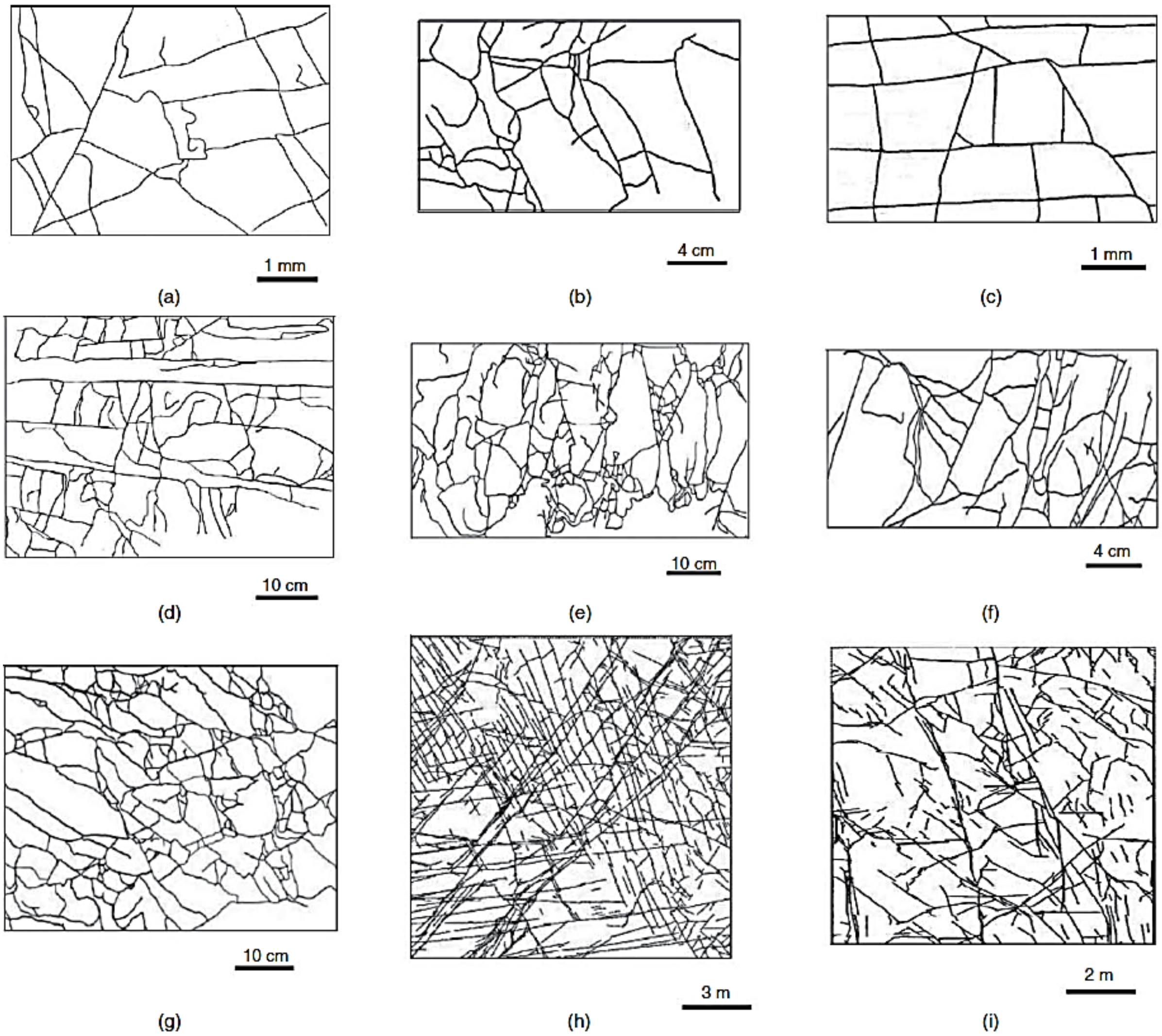


**Figure 1-4 Natural fracture networks demonstrating fractal geometries. Taken from Shokri et al. (2016).**

Developments in the theory of fractal geometry have resulted in numerous applications, to many branches of science, especially to problems stemming from unstable phenomena (Acuna and Yortsos, 1995; Rocco and West, 1999; Schumer et al., 2003b; Chen, 2006; Santizo, 2012; Liang et al., 2016). Fractal geometry incorporates the complexity of the natural system by describing an object by the repetition of a given algorithmic rule or pattern over a multitude of separate length scales. Fractured-rock aquifers have proven to be an appropriate candidate for a fractal description (Acuna and Yortsos, 1995), and the ability of a fractal geometry to describe complexity on different scales provides the ability to potentially describe scale-dependent dispersivity. Currently available transport models for fractured systems are not able to capture the property of *self-similarity* found in fractured systems.

In response to the current limitations of groundwater transport modelling in fractured systems, a fractal groundwater advection-dispersion transport equation is deemed an appropriate and worthwhile investigation. A fractal advection-dispersion equation has the potential to simulate the full range of observed non-Fickian behaviour, from subdiffusion to superdiffusion, which is related to the well-established fractal model for fractured systems, without the detailed characterisation of the heterogeneity of the system. A fractal in space advection-dispersion equation has not been developed before, and therefore will be considered in this research.

### 1.2.2 Fractional derivative

Complexity from the perspective of fractional calculus is explored by West (2016), where fractional differential equations are one approach to improve the simulation of real world problems. Fractional calculus is not a new topic, having its original inception in the late 1600s, but the application of fractional derivations to practical problems has steadily increased since the 1970s.

The inception of fractional calculus has its roots in the relationship between Leibniz and L'Hopital, where Leibniz ignited an idea within L'Hopital that has gone on to diversify knowledge. L'Hopital posed the seemingly inapt question, what would happen if the derivative order were a fraction? Leibniz's famous response was "it will lead to a paradox from which one day useful consequences will be drawn". Perhaps, Leibniz should have paid greater attention to the seemingly inapt question at the time because; the non-integer fractional derivative has proven to be exceptionally useful (Oldham and Spanier, 1974).

From this original conversation, the practical application was only realised much later and resisted direct application for many years. Oldham and Spanier (1974) found the earliest systematic studies on the fractional derivative were performed by Liouville (1832), Riemann (1953), and Holmgren (1864), although Euler (1730) and Lagrange (1772) made even earlier contributions, as cited by Oldham and Spanier (1974) (Debnath, 2004; Loverro, 2004; Petráš, 2010; Herrmann, 2011; Tarasov, 2013).

Fractional calculus can be described as an extension of the concept of a derivative operator from an integer order ($n$) to an arbitrary order ($\alpha$) (Herrmann, 2011):

$$\frac{d^n}{dx^n} \rightarrow \frac{d^\alpha}{dx^\alpha}$$

where,

$\alpha$ denotes a non-integer order that is a real, complex value or even a complex-valued function $\alpha = \alpha(x,t)$.

The fractional advection-dispersion equation was first developed by Benson (1998), and an application demonstrated by Benson et al. (2000) (Figure 1-5). In an experiment, Benson et al. (2000) demonstrated an anomalous diffusion system and the inadequacy of the Fickian or traditional equation to model the measured concentrations. Furthermore, by incorporating the fractional derivative and adjusting the fractional order ($\alpha$), a model can be developed to improve the representation of the system.

With the endeavour to continually improve simulation methods, a progression of fractional derivative definitions have been developed over the years, with definitions including Riemann-Liouville, Caputo, Caputo-Fabrizio, and the latest Atangana-Baleanu (Oldham and Spanier, 1974; Herrmann, 2011; Li et al., 2011; Atangana and Baleanu, 2016). Following on from the work performed by Tateishi et al. (2017), which found that the new fractional derivatives could be effective in modelling anomalous diffusion, the new fractional derivatives are applied to the advection-dispersion equation to model not only anomalous diffusion, but potentially *anomalous advection* in the form of preferential pathways in fractures within the groundwater system.

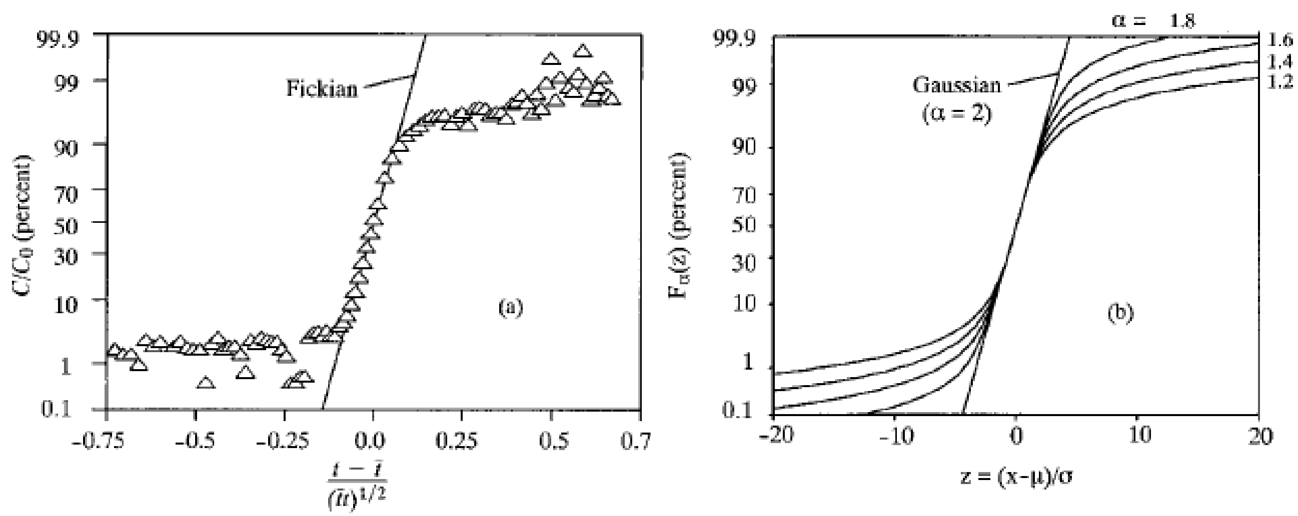


**Figure 1-5 Measured concentration outputs from an experiment performed by Benson et al. (2000) and the predicted concentration by the traditional Fickian approach (top). The fractional models generated by varying the fractional order ($\alpha$) to better represent the experimental system (bottom). Taken from Benson et al. (2000).**

## 1.3 Aims and objectives

The aim of this research is to improve the simulation of groundwater transport in fractured system using the advection-dispersion equation, following the approach of reformulation of the governing equation. The objectives are sub-divided between improvements for the local advection-dispersion equation, fractal advection-dispersion equation, and fractional advection-dispersion equation.

### 1.3.1 Local advection-dispersion equation

The objectives for this research to improve the simulation using the local advection-dispersion equation includes:

- Identify numerical approximation methods for the specific advection-dominated fracture systems
- Consider possible improvements to the numerical approximation scheme
- Evaluate the developed schemes in terms of stability and computational times

### 1.3.2 Fractal advection-dispersion equation

The objectives for this research for using a fractal advection-dispersion equation includes:

- Investigate the use of the fractal derivative for fractured groundwater systems and previous applications
- Develop an improved fractal advection-dispersion equation
- Investigate numerical solution methods for the new equation
- Evaluate the developed schemes in terms of stability
- Perform simulations to test the validity of the equation to fractured systems

### 1.3.3 Fractional advection-dispersion equation

The objectives for application of a new fractional advection-dispersion equation includes:

- Develop a fractional advection-dispersion equation specifically for fractured systems using the new derivatives
- Investigate numerical solution methods for the new equation
- Evaluate the developed schemes in terms of stability
- Perform simulations to test the validity of the equation to fractured systems

### 1.3.4 Fractional-fractal advection-dispersion equation

The objectives for the development of a fractional-fractal advection-dispersion equation includes:

- Consider the need and implications of developing a fractional-fractal advection-dispersion equation
- Develop a fractional-fractal advection-dispersion equation
- Perform simulations to test the validity of the equation to fractured systems

## 1.4 Structure of thesis

The structure of the thesis is designed as follows:

**Chapter 1 Introduction**

The rationale for the current research is explained, each aspect is briefly introduced, and the aims and objectives are defined.

**Chapter 2 Classical advection-dispersion equation**

Augmented upwind numerical schemes are developed to better simulate groundwater transport in advection-dominated fractured systems. The numerical schemes are evaluated for stability and computational times for a simple one-dimensional problem.

**Chapter 3 Fractal advection-dispersion equation**

A fractal advection-dispersion equation for fractured groundwater systems is developed, along with numerical approximation methods. A generic transport problem is simulated to test the validity of the fractal advection-dispersion equation to fractured groundwater transport.

**Chapter 4 Fractional derivatives: singular and non-singular**

An overview of fractional calculus in the form of the functions required for the definition of fractional integrals and derivatives, fundamental fractional derivative definitions, and an analysis of the kernels associated with each fractional definition.

**Chapter 5 and 6 Fractional advection-dispersion equations**

New fractional advection-dispersion equations are developed with the Caputo and Atangana-Baleanu fractional derivative definitions. The advection-dominated numerical schemes are applied and tested for stability. Some simulations of fractional systems are investigated.

**Chapter 7 Fractional-Fractal advection-dispersion equation**

Considering the developed fractal in space advection-dispersion equation, and the fractional advection-dispersion equation, a fractional-fractal advection-dispersion equation is conceptualised. The developed equation is simulated in a simple transport problem to determine the meaning of fractional-fractal and evaluate the fractal dimension and fractional order.

**Chapter 8 Discussion**

A critical discussion of the research performed and outcomes are provided.

**Chapter 9 Conclusions**

The main findings and outcomes from the performed research are presented.

**References**

**Appendices**

# 2 CLASSICAL ADVECTION-DISPERSION EQUATION

The advection-dispersion equation is infamously challenging to solve, due to the simultaneous presence of two processes, namely advection and hydrodynamic dispersion. Additionally, in complex groundwater systems, applying an analytical solution of the advection-dispersion equation is often unsuccessful and thus numerical techniques are usually applied. There are numerous numerical techniques available, yet often the stability criteria are stringent; and oscillations and numerical dispersion are frequently found. Advection-dominated solute transport is often the cause for the numerical instabilities, where the advection-dispersion equation approximates to a hyperbolic-type partial differential equation, and numerical approximation methods become prone to these problems in this environment. To address these common numerical instabilities, an upwind numerical scheme can serve to correct these problems by damping responses to produce a more realistic solution in both heat transfer and fluid flow simulations (Hirt et al., 1975; Gray and Pinder, 1976; Patankar, 1980; Busnaina et al., 1991; Baptista et al., 1995; Ewing and Wang, 2001; Witek et al., 2008; Company et al., 2009; Aswin et al., 2015; Appadu et al., 2016; Kajishima and Taira, 2016).

Upwind numerical schemes have been applied to finite difference and finite element methods. For the finite difference method, it is common to make use of the upwind scheme to approximate the advective terms of the advection-dispersion equation by applying first-order one-sided (flow direction-biased) differences (Diersch, 2014). However, for finite element methods, the first order upwinding creates strong smearing effects and is rarely used (Kuzmin, 2010). For this investigation, the traditional and augmented upwind schemes are applied for the finite difference method.

Several authors have investigated the upwind scheme for the numerical solution of the advection-dispersion equation, or the more general form the convection-dispersion equation (Busnaina et al., 1991; Vested et al., 1992; Lazarov et al., 1996; Appadu et al., 2016). For instance, upstream weighting is often applied to finite element methods, where an element upstream of a node is weighted more heavily than the element located downstream, namely the Petrov-Galerkin finite element method (Sun and Yeh, 1983; Diersch, 2014). In Computational Fluid Dynamics (CFD), the flux-vector splitting upwind scheme splits the advective term into two fluxes to both represent both a positive and negative wave direction (Van Leer, 1982; Lomax at al., 2013). Applying aspects from the finite element upstream weighting and the CFD flux-splitting methods, a weighted upwind-downwind finite difference scheme is developed and investigated for groundwater transport simulations.

To improve the solution of the classical advection-dispersion equation for fractured groundwater systems, the traditional finite difference upwind scheme is reviewed and then applied, along with augmented upwind schemes, to the advection-dispersion equation. The traditional explicit and implicit schemes, as well as the Crank-Nicolson scheme, are developed and analysed for numerical stability to form a base of comparison. Two new numerical approximation schemes are considered, namely a Crank-Nicolson scheme that is only applied for the advection term, and a weighted upwind-downwind scheme. These newly developed schemes are analysed for numerical stability and compared to the traditional schemes.

## 2.1 Upwind finite difference scheme for local operator

Upwind schemes discretise hyperbolic partial differential equations with a finite differencing biased in the direction determined by the sign of the groundwater velocity, thus applying a solution-sensitive approach to simulate the direction of movement in a flow field (Courant et al., 1952; Ewing and Wang, 2001).

The movement of the particle or contaminant is towards the negative direction (left), when the vector term ($a$) is negative; and when the vector term ($a$) is positive, the movement of the particle or contaminant is towards the positive direction (right). Considering a one-dimensional derivative of a function $f(u)$ with a directional vector ($a$):

$$a\frac{\partial f(u)}{\partial x} \tag{2-1}$$

The first-order upwind scheme (explicit) numerical approximation is:

$$a\frac{u_i^n - u_{i-1}^n}{\Delta x} \qquad for\ a > 0 \tag{2-2}$$

$$a\frac{u_{i+1}^n - u_i^n}{\Delta x} \qquad for\ a < 0 \tag{2-3}$$

Thus, for a positive direction (upwind side) vector term backward differences are applied, and for the negative direction (downwind side) vector term forward differences are applied.

The first-order upwind finite difference scheme (implicit) numerical approximation is:

$$a\frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} \qquad for\ a > 0 \tag{2-4}$$

$$a\frac{u_{i+1}^{n+1} - u_i^{n+1}}{\Delta x} \qquad for\ a < 0 \tag{2-5}$$

Upwind methods eliminate undesirable oscillations, yet may have other related shortcomings, especially in terms of accuracy (Diersch, 2014). Thus, an upwind scheme is a compromise between accuracy and stability. Ewing and Wang (2001) found the upwind finite difference scheme to eliminate artificial oscillations in the classical finite difference method solutions, and to provide more stable solutions for complex multiphase and multicomponent flow systems. The upwind finite difference scheme can be expressed as a second-order approximation for the one-dimensional advection-dispersion equation with a modified diffusion $D(1 + (Pe/2)(1 - Cr))$, where $Pe$ is the Peclet number and $Cr$ is the Courant number (Ewing and Wang, 2001). Ewing and Wang (2001) further confirm the warning by Diersch (2014) where the upwind finite difference scheme introduces excessive numerical diffusion and the numerical solutions are dependent upon grid orientation.

Summary of the key benefits and limitations for the upwind scheme (Diersch, 2014):

Benefits:

- Finite difference and finite element numerical approximation methods are prone to create artificial oscillations in advection-dominated problems, but upwinding can stabilise the solution to obtain more realistic solutions (albeit less accurate) (Diersch, 2014)
- Upwind methods improve the efficiency of numerical solutions and reduce the need for extremely fine meshes (Diersch, 2014)

Limitations:

- The artificial damping measures by upwinding may suppress other issues in the model such as limitations in the spatial and temporal discretization (Diersch, 2014)

- Diffusion is artificially increased in dependence on the chosen mesh, and considered dependent on the mesh geometry, yet can still be considered accurate where the numerical diffusion is significantly less than the physical diffusion (Diersch, 2014)

In summary, the upwind scheme is a powerful tool that has benefits for numerical stability. Yet, this tool should be applied with an understanding of the limitations, and the compromise on accuracy appropriately compensated for with numerical stability.

## 2.2 Upwind finite difference schemes for the classical advection-dispersion equation

The first-order upwind scheme is applied to the classical advection-dispersion equation for numerical approximation. Considering the one-dimensional advection-dispersion equation:

$$\frac{\partial c}{\partial t} + v_x \frac{\partial c}{\partial x} - D_L \frac{\partial^2 c}{\partial x^2} = 0 \tag{2-6}$$

The first-order upwind scheme for the classical advection-dispersion equation finite difference approximation influences the advection term, where backward or forward differences are considered depending on the direction of the transporting velocity.

The traditional explicit and implicit schemes, as well as the Crank-Nicolson scheme, are developed and analysed for numerical stability to form a comparison base. Two new numerical approximation schemes are proposed, namely a Crank-Nicolson scheme where only for the advection term is applied, and a weighted upwind-downwind scheme. The numerical stability for the newly developed schemes are evaluated to validate their use in solving the advection-dispersion equation.

### 2.2.1 Explicit upwind

An explicit first-order upwind finite difference scheme for the one-dimensional advection-dispersion equation uses a one-sided finite difference in the upstream direction to approximate the advection term in the advection-dispersion equation and can be expressed as follows (assuming $v > 0$) (Ewing and Wang, 2001):

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + v_x \frac{c_i^n - c_{i-1}^n}{\Delta x} - D_L \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2} = 0 \tag{2-7}$$

Rearranging,

$$\left(\frac{1}{\Delta t}\right) c_i^{n+1} = \left(\frac{1}{\Delta t} - \frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}\right) c_i^n + \left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) c_{i-1}^n + \left(\frac{D_L}{(\Delta x)^2}\right) c_{i+1}^n$$

Simplifying by using constants $a_1$, $b_1$, $c_1$, and $d_1$

$$a_1 c_i^{n+1} = b_1 c_i^n + c_1 c_{i-1}^n + d_1 c_{i+1}^n \tag{2-8}$$

where,

$$a_1 = \frac{1}{\Delta t}$$
$$b_1 = \frac{1}{\Delta t} - \frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}$$
$$c_1 = \frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}$$
$$d_1 = \frac{D_L}{(\Delta x)^2}$$

Equation (2-8) is the explicit upwind finite difference approximation of the one-dimensional advection-dispersion equation.

### 2.2.2 Implicit upwind

The implicit formulation of the first-order upwind finite difference scheme for the one-dimensional advection-dispersion equation is:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + v_x \frac{c_i^{n+1} - c_{i-1}^{n+1}}{\Delta x} - D_L \frac{c_{i+1}^{n+1} - 2c_i^{n+1} + c_{i-1}^{n+1}}{(\Delta x)^2} = 0 \qquad (2\text{-}9)$$

Rearranging,

$$\left(\frac{1}{\Delta t} + \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right) c_i^{n+1} = \left(\frac{1}{\Delta t}\right) c_i^n + \left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) c_{i-1}^{n+1} + \left(\frac{D_L}{(\Delta x)^2}\right) c_{i+1}^{n+1}$$

Simplifying by using constants $a_1$, $e_1$, $c_1$, and $d_1$

$$e_1 c_i^{n+1} = a_1 c_i^n + c_1 c_{i-1}^{n+1} + d_1 c_{i+1}^{n+1} \qquad (2\text{-}10)$$

where,

$$e_1 = \frac{1}{\Delta t} + \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}$$

Equation (2-10) is the implicit upwind finite difference approximation of the one-dimensional advection-dispersion equation.

### 2.2.3 Upwind Crank-Nicolson scheme

Upwind and Crank-Nicolson schemes were compared in terms of accuracy and numerical dispersion by Karahan (2006). The Crank-Nicolson scheme was found to be more accurate and reduced numerical dispersion, and for this reason, a combination of these two schemes is investigated here. The Crank-Nicolson scheme applied for the first-order upwind finite difference scheme approximation for the advection-dispersion equation

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \begin{bmatrix} 0.5\left(v_x \dfrac{c_i^n - c_{i-1}^n}{\Delta x} - D_L \dfrac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2}\right) \\ +0.5\left(v_x \dfrac{c_i^{n+1} - c_{i-1}^{n+1}}{\Delta x} - D_L \dfrac{c_{i+1}^{n+1} - 2c_i^{n+1} + c_{i-1}^{n+1}}{(\Delta x)^2}\right) \end{bmatrix} = 0 \qquad (2\text{-}11)$$

Expanding and rearranging,

$$\left(\frac{1}{\Delta t}+0.5\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_i^{n+1}=\left(\frac{1}{\Delta t}-0.5\frac{v_x}{\Delta x}-\frac{D_L}{(\Delta x)^2}\right)c_i^n$$
$$+0.5\left(\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_{i-1}^n+0.5\left(\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_{i-1}^{n+1}+0.5\left(\frac{D_L}{(\Delta x)^2}\right)c_{i+1}^n+0.5\left(\frac{D_L}{(\Delta x)^2}\right)c_{i+1}^{n+1} \quad (2\text{-}12)$$

Simplifying by using constants $f_1, g_1, h_1$, and $j_1$

$$f_1c_i^{n+1}=g_1c_i^n+h_1c_{i-1}^n+h_1c_{i-1}^{n+1}+j_1c_{i+1}^n+j_1c_{i+1}^{n+1} \quad (2\text{-}13)$$

where,

$$f_1=\frac{1}{\Delta t}+0.5\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}$$
$$g_1=\frac{1}{\Delta t}-0.5\frac{v_x}{\Delta x}-\frac{D_L}{(\Delta x)^2}$$
$$h_1=0.5\left(\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)$$
$$j_1=0.5\left(\frac{D_L}{(\Delta x)^2}\right)$$

Equation (2-13) is the upwind Crank-Nicolson finite difference approximation of the one-dimensional advection-dispersion equation.

### 2.2.4 Upwind advection Crank-Nicolson scheme

The Crank-Nicolson scheme applied only for advection term of the advection-dispersion equation for the first-order upwind finite difference scheme approximation

$$\frac{c_i^{n+1}-c_i^n}{\Delta t}+\left[0.5\left(v_x\frac{c_i^n-c_{i-1}^n}{\Delta x}\right)+0.5\left(v_x\frac{c_i^{n+1}-c_{i-1}^{n+1}}{\Delta x}\right)\right]-D_L\frac{c_{i+1}^n-2c_i^n+c_{i-1}^n}{(\Delta x)^2}=0 \quad (2\text{-}14)$$

Expanding and rearranging,

$$\frac{c_i^{n+1}}{\Delta t}-\frac{c_i^n}{\Delta t}+0.5v_x\frac{c_i^n}{\Delta x}-0.5v_x\frac{c_{i-1}^n}{\Delta x}+0.5v_x\frac{c_i^{n+1}}{\Delta x}-0.5v_x\frac{c_{i-1}^{n+1}}{\Delta x}-D_L\frac{c_{i+1}^n}{(\Delta x)^2}+D_L\frac{2c_i^n}{(\Delta x)^2}-D_L\frac{c_{i-1}^n}{(\Delta x)^2}=0$$

Simplifying,

$$\left(\frac{1}{\Delta t}+0.5\frac{v_x}{\Delta x}\right)c_i^{n+1}=\left(\frac{1}{\Delta t}-0.5\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}\right)c_i^n+\left(0.5\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_{i-1}^n+\left(\frac{D_L}{(\Delta x)^2}\right)c_{i+1}^n$$
$$+\left(0.5\frac{v_x}{\Delta x}\right)c_{i-1}^{n+1}$$

Simplifying by using constants $k_1$, $l_1$, $h_1$, $d_1$ and $o_1$

$$k_1c_i^{n+1}=l_1c_i^n+m_1c_{i-1}^n+d_1c_{i+1}^n+o_1c_{i-1}^{n+1} \quad (2\text{-}15)$$

where,

$$k_1=\frac{1}{\Delta t}+0.5\frac{v_x}{\Delta x}$$

$$l_1 = \frac{1}{\Delta t} - 0.5\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}$$
$$m_1 = 0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}$$
$$o_1 = 0.5\frac{v_x}{\Delta x}$$

Equation (2-15) is the upwind advection Crank-Nicolson finite difference approximation of the one-dimensional advection-dispersion equation.

### 2.2.5 Explicit upwind-downwind weighted scheme

Considering both the upwind and downwind direction for the advection term for the first-order upwind finite difference scheme approximation (explicit), where the ratio of upwind to downwind is controlled by $\theta$, where $0 \leq \theta \leq 1$:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \left[\theta\left(v_x\frac{c_i^n - c_{i-1}^n}{\Delta x}\right) + (1-\theta)\left(v_x\frac{c_{i+1}^n - c_i^n}{\Delta x}\right)\right] - D_L\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2} = 0 \qquad (2\text{-}16)$$

Expanding and rearranging,

$$\frac{c_i^{n+1}}{\Delta t} - \frac{c_i^n}{\Delta t} + \theta v_x\frac{c_i^n}{\Delta x} - \theta v_x\frac{c_{i-1}^n}{\Delta x} + (1-\theta)v_x\frac{c_{i+1}^n}{\Delta x} - (1-\theta)v_x\frac{c_i^n}{\Delta x} - D_L\frac{c_{i+1}^n}{(\Delta x)^2} + D_L\frac{2c_i^n}{(\Delta x)^2} - D_L\frac{c_{i-1}^n}{(\Delta x)^2} = 0$$

Simplifying,

$$\left(\frac{1}{\Delta t}\right)c_i^{n+1} = \left(\frac{1}{\Delta t} - \theta\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}\right)c_i^n + \left(\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right)c_{i-1}^n + \left(\frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}\right)c_{i+1}^n$$

Simplifying by using constants $a_1$, $p_1$, $q_1$, and $r_1$

$$a_1 c_i^{n+1} = p_1 c_i^n + q_1 c_{i-1}^n + r_1 c_{i+1}^n \qquad (2\text{-}17)$$

where,

$$p_1 = \frac{1}{\Delta t} - \theta\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}$$
$$q_1 = \theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}$$
$$r_1 = \frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}$$

Equation (2-17) is the explicit upwind-downwind weighted finite difference approximation of the one-dimensional advection-dispersion equation.

### 2.2.6 Implicit upwind-downwind weighted scheme

Now for the implicit formulation, the upwind and downwind direction, where the ratio of upwind to downwind is controlled by $\theta$, where $0 \leq \theta \leq 1$:

$$\frac{c_i^{n+1}-c_i^n}{\Delta t}+\left[\theta\left(v_x\frac{c_i^{n+1}-c_{i-1}^{n+1}}{\Delta x}\right)+(1-\theta)\left(v_x\frac{c_{i+1}^{n+1}-c_i^{n+1}}{\Delta x}\right)\right]-D_L\frac{c_{i+1}^{n+1}-2c_i^{n+1}+c_{i-1}^{n+1}}{(\Delta x)^2}=0 \quad (2\text{-}18)$$

Expanding and rearranging,

$$\frac{c_i^{n+1}}{\Delta t}-\frac{c_i^n}{\Delta t}+\theta v_x\frac{c_i^{n+1}}{\Delta x}-\theta v_x\frac{c_{i-1}^{n+1}}{\Delta x}+(1-\theta)v_x\frac{c_{i+1}^{n+1}}{\Delta x}-(1-\theta)v_x\frac{c_i^{n+1}}{\Delta x}$$
$$-D_L\frac{c_{i+1}^{n+1}}{(\Delta x)^2}+D_L\frac{2c_i^{n+1}}{(\Delta x)^2}-D_L\frac{c_{i-1}^{n+1}}{(\Delta x)^2}=0$$

Simplifying,

$$\left(\frac{1}{\Delta t}+\theta\frac{v_x}{\Delta x}-(1-\theta)\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}\right)c_i^{n+1}$$
$$=\left(\frac{1}{\Delta t}\right)c_i^n+\left(\theta\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_{i-1}^{n+1}+\left(\frac{D_L}{(\Delta x)^2}-(1-\theta)\frac{v_x}{\Delta x}\right)c_{i+1}^{n+1}$$

Simplifying by using constants $v_1$, $a_1$, $q_1$, and $r_1$

$$v_1c_i^{n+1}=a_1c_i^n+q_1c_{i-1}^{n+1}+r_1c_{i+1}^{n+1} \quad (2\text{-}19)$$

where,

$$v_1=\frac{1}{\Delta t}+\theta\frac{v_x}{\Delta x}-(1-\theta)\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}$$

Equation (2-19) is the implicit upwind-downwind weighted finite difference approximation of the one-dimensional advection-dispersion equation.

## 2.3 Numerical stability analysis

A finite difference scheme is considered stable if the errors incurred at a discrete time step are not propagated throughout the simulation. Assuming a Fourier expansion in space,

$$c(x,t)=\sum_n \hat{c}\,(t)\exp(ik_mx) \quad (2\text{-}20)$$

where,

$$c_i^{n+1}=\hat{c}_{n+1}e^{ik_mx}$$
$$c_i^n=\hat{c}_ne^{ik_mx}$$
$$c_{i-1}^{n+1}=\hat{c}_{n+1}e^{ik_m(x-\Delta x)}$$
$$c_{i+1}^{n+1}=\hat{c}_{n+1}e^{ik_m(x+\Delta x)}$$

The recursive numerical stability analysis is performed in two parts, firstly it is proved for a set $\forall\, n>1$,

$$|\hat{c}_n|<|\hat{c}_o| \quad (2\text{-}21)$$

Secondly, making the assumption that $|\hat{c}_n| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_{n+1}| < |\hat{c}_o| \tag{2-22}$$

By examining these two conditions, where the error becomes less over each successive step, the stability criteria for the numerical scheme can be determined (Gnitchogna and Atangana, 2017; Atangana, 2015). This method is applied to investigate the stability of the numerical schemes for the advection-dispersion equation discussed in the previous section.

### 2.3.1 Explicit upwind

The first-order explicit upwind finite difference approximation of the one-dimensional advection-dispersion equation was determined to be (Equation (2-8)), and substituting induction method terms gives,

$$a_1\hat{c}_{n+1}e^{ik_m x} = b_1\hat{c}_n e^{ik_m x} + c_1\hat{c}_n e^{ik_m(x-\Delta x)} + d_1\hat{c}_n e^{ik_m(x+\Delta x)}$$

Multiple out,

$$a_1\hat{c}_{n+1}e^{ik_m x} = b_1\hat{c}_n e^{ik_m x} + c_1\hat{c}_n e^{ik_m x}e^{-i\Delta x km} + d_1\hat{c}_n e^{ik_m x}e^{ik_m\Delta x}$$

Divide by $e^{ik_m x}$,

$$a_1\hat{c}_{n+1} = b_1\hat{c}_n + c_1\hat{c}_n e^{-ik_m\Delta x} + d_1\hat{c}_n e^{ik_m\Delta x} \tag{2-23}$$

The induction numerical stability analysis is performed in two parts; firstly it is proved for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 0$, then

$$a_1\hat{c}_1 = b_1\hat{c}_0 + c_1\hat{c}_0 e^{-ik_m\Delta x} + d_1\hat{c}_0 e^{ik_m\Delta x}$$

Simplifying, and remembering that $a = \frac{1}{\Delta t}$

$$\frac{1}{\Delta t}\hat{c}_1 = \hat{c}_0(b_1 + c_1 e^{-ik_m\Delta x} + d_1 e^{ik_m\Delta x})$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \Delta t(b_1 + c_1 e^{-ik_m\Delta x} + d_1 e^{ik_m\Delta x})$$

A norm is applied,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < \Delta t(|b_1| + \left|c_1 e^{-ik_m\Delta x}\right| + \left|d_1 e^{ik_m\Delta x}\right|)$$

The first condition required, for Equation (2-23), becomes,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, the condition becomes

$$\Delta t(|b_1| + |c_1| + |d_1|) < 1$$

It can be concluded that $|\hat{c}_1| < |\hat{c}_o|$, when

$$\Delta t(|b_1| + |c_1| + |d_1|) < 1$$

The term is expanded using the simplification terms associated with Equation (2-8)

$$\Delta t\left(\left|\frac{1}{\Delta t} - \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|\right) < 1 \tag{2-24}$$

If the assumption is made, where

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} > \frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(\frac{1}{\Delta t} - \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} + \frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}\right) < 1$$

Simplifying,

$$\Delta t\left(\frac{1}{\Delta t} + \frac{4D_L}{(\Delta x)^2}\right) < 1 \tag{2-25}$$

For this numerical scheme, the solution is unstable under this assumption. Considering the nature of the explicit scheme to the use information from the current time step, or initial time step to calculate the next time step thus imposes these restrictions on the solution.

However, considering the situation where the opposite assumption is made,

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} < \frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(-\frac{1}{\Delta t} + \frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2} + \frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}\right) < 1 \tag{2-26}$$

Simplifying,

$$v_x \frac{\Delta t}{\Delta x} < 1 \tag{2-27}$$

This condition corresponds to the Courant-Friedrichs-Lewy (CFL) condition ($C_r$) which is a well-known convergence criterion for the classical advection-dispersion equation when solved using an explicit finite difference numerical approximation method (Courant et al., 1967; Ewing and Wang, 2001).

Therefore, the first-order explicit upwind finite difference approximation of the one-dimensional advection-dispersion equation is stable when:

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} < \frac{v_x}{\Delta x}$$

Thus, the use of information from the current time step, or initial time step to calculate the next time step requires that the ratio of groundwater velocity to the cell size be greater than the inverse of the time step and the ratio of dispersivity to the cell size.

Furthermore for the stability analysis, the assumption that $|\hat{c}_n| < |\hat{c}_o|$ is true for all time steps is made, and the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_{n+1}| < |\hat{c}_o|$$

Rearranging Equation (2-23),

$$\hat{c}_{n+1} = \frac{\left(b_1 + c_1 e^{-ik_m\Delta x} + d_1 e^{ik_m\Delta x}\right)}{a_1}\hat{c}_n$$

Applying a norm on both sides,

$$|\hat{c}_{n+1}| < \frac{\left(|b_1| + \left|c_1 e^{-ik_m\Delta x}\right| + \left|d_1 e^{ik_m\Delta x}\right|\right)}{|a_1|}|\hat{c}_n|$$

Remembering $|e^n| = 1$ and $a = \frac{1}{\Delta t}$, the condition becomes

$$|\hat{c}_{n+1}| < \Delta t(|b_1| + |c_1| + |d_1|)\,|\hat{c}_n|$$

Remembering that it has been proven that for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Thus,

$$|\hat{c}_{n+1}| < \Delta t(|b_1| + |c_1| + |d_1|)\,|\hat{c}_n| < \Delta t(|b| + |c_1| + |d_1|)\,|\hat{c}_o|$$

and, it can be inferred that

$$|\hat{c}_{n+1}| < \Delta t(|b_1| + |c_1| + |d_1|)|\hat{c}_o|$$

Thus, the solution will be stable when,

$$\Delta t(|b_1| + |c_1| + |d_1|) < 1$$

The term is expanded using the simplification terms associated with Equation (2-8)

$$\Delta t\left(\left|\frac{1}{\Delta t} - \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|\right) < 1 \qquad (2\text{-}28)$$

If the assumption is made, where

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} > \frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(\frac{1}{\Delta t} - \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} + \frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}\right) < 1$$

Simplifying, the condition for $|\hat{c}_{n+1}| < |\hat{c}_o|$ is similar to the condition determined for $|\hat{c}_n| < |\hat{c}_o|$, where the explicit scheme is unstable under this assumption. Conversely, consider the complementary assumption,

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} < \frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(-\frac{1}{\Delta t} + \frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2} + \frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}\right) > 1$$

Simplifying,

$$v_x \frac{\Delta t}{\Delta x} < 1 \tag{2-29}$$

Thus, the first-order implicit upwind scheme is conditionally stable under this assumption, and similar to the condition for $|\hat{c}_n| < |\hat{c}_o|$, where the solution is stable under this assumption. The use information from the current time step or initial time step to calculate the next time step requires that the ratio of groundwater velocity to the cell size be greater than the inverse of the time step and the ratio of dispersivity to the cell size.

In summary, the first-order explicit upwind finite difference approximation of the one-dimensional advection-dispersion equation has the following stability criterion (Courant condition) (Equation (2-29)). Under this assumption and condition, the error of the approximation is not propagated throughout the solution, but rather decreases with each time step, as according to the induction method, where for all values of n, $|\hat{c}_{n+1}| < |\hat{c}_o|$.

### 2.3.2 Implicit upwind

The implicit formulation of the first-order upwind finite difference scheme for the one-dimensional advection-dispersion equation was determined to be (Equation (2-10)), and substituting induction method terms gives,

$$e_1\hat{c}_{n+1}e^{ik_m x} = a_1\hat{c}_n e^{ik_m x} + c_1\hat{c}_{n+1}e^{ik_m(x-\Delta x)} + d_1\hat{c}_{n+1}e^{ik_m(x+\Delta x)}$$

Multiple out,

$$e_1\hat{c}_{n+1}e^{ik_m x} = a_1\hat{c}_n e^{ik_m x} + c_1\hat{c}_{n+1}e^{ik_m x}e^{-ik_m\Delta x} + d_1\hat{c}_{n+1}e^{ik_m x}e^{ik_m\Delta x}$$

Divide by $e^{ixkm}$,

$$e_1\hat{c}_{n+1} = a_1\hat{c}_n + c_1\hat{c}_{n+1}e^{-ik_m\Delta x} + d_1\hat{c}_{n+1}e^{ik_m\Delta x} \tag{2-30}$$

The induction numerical stability analysis is performed in two parts, firstly it is proved for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 0$, then

$$e_1\hat{c}_1 = a_1\hat{c}_0 + c_1\hat{c}_1e^{-ik_m\Delta x} + d_1\hat{c}_1e^{ik_m\Delta x}$$

Rearrange,

$$e_1\hat{c}_1 - c_1\hat{c}_1e^{-ik_m\Delta x} - d_1\hat{c}_1e^{ik_m\Delta x} = a_1\hat{c}_0$$

Simplifying, and remembering that $a_1 = \frac{1}{\Delta t}$

$$\hat{c}_1(e_1 - c_1e^{-ik_m\Delta x} - d_1e^{ik_m\Delta x}) = \frac{1}{\Delta t}\hat{c}_0$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{1}{\Delta t(e_1 - c_1e^{-ik_m\Delta x} - d_1e^{ik_m\Delta x})}$$

A norm is applied on both sides,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < \frac{1}{\Delta t(|e_1| + |-c_1e^{-ik_m\Delta x}| + |-d_1e^{ik_m\Delta x}|)}$$

The condition required $|\hat{c}_n| < |\hat{c}_o|$, thus becomes,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, the condition becomes

$$\frac{1}{\Delta t(|e_1| + |c_1| + |d_1|)} < 1$$

It can be concluded that $|\hat{c}_1| < |\hat{c}_o|$, when

$$\Delta t(|e_1| + |c_1| + |d_1|) > 1$$

The term is expanded using the simplification terms associated with Equation (2-10)

$$\Delta t\left(\left|\frac{1}{\Delta t} + \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|\right) > 1 \qquad (2\text{-}31)$$

Simplifying,

$$\frac{2v_x}{\Delta x} + \frac{4D_L}{(\Delta x)^2} > 0 \qquad (2\text{-}32)$$

The condition confirms that the first-order upwind implicit scheme is unconditionally stable.

Secondly, making the assumption that $|\hat{c}_n| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\ n \geq 1$, that

$$|\hat{c}_{n+1}| < |\hat{c}_o|$$

Rearranging Equation (2-30),

$$e_1\hat{c}_{n+1} - c_1\hat{c}_{n+1}e^{-ik_m\Delta x} - d_1\hat{c}_{n+1}e^{ik_m\Delta x} = a_1\hat{c}_n$$

Simplifying,

$$\hat{c}_{n+1} = \frac{a_1}{(e_1 - c_1 e^{-ik_m\Delta x} - d_1 e^{ik_m\Delta x})}\hat{c}_n$$

Applying the norm,

$$|\hat{c}_{n+1}| < \frac{|a_1|}{(|e_1| + |-c_1 e^{-ik_m\Delta x}| + |-d_1 e^{ik_m\Delta x}|)}|\hat{c}_n|$$

Remembering $|e^n| = 1$ and $a_1 = \frac{1}{\Delta t}$, the condition becomes

$$|\hat{c}_{n+1}| < \frac{1}{\Delta t(|e_1| + |c_1| + |d_1|)}|\hat{c}_n|$$

Remembering that it has been proven that for a set $\forall\ n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Thus,

$$|\hat{c}_{n+1}| < \frac{1}{\Delta t(|e_1| + |c_1| + |d_1|)}|\hat{c}_n| < \frac{1}{\Delta t(|e_1| + |c_1| + |d_1|)}|\hat{c}_o|$$

and, it can be inferred that

$$|\hat{c}_{n+1}| < \frac{1}{\Delta t(|e_1| + |c_1| + |d_1|)}|\hat{c}_o|$$

Thus, the solution will be stable when,

$$\frac{1}{\Delta t(|e_1| + |c_1| + |d_1|)} < 1$$

It can be concluded that $|\hat{c}_{n+1}| < |\hat{c}_o|$, when

$$\Delta t(|e_1| + |c_1| + |d_1|) > 1$$

The term is expanded using the simplification terms associated with Equation (2-10)

$$\Delta t\left(\left|\frac{1}{\Delta t} + \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|\right) > 1 \tag{2-33}$$

Simplifying,

$$\frac{2v_x}{\Delta x} + \frac{4D_L}{(\Delta x)^2} > 0 \tag{2-34}$$

The condition for $|\hat{c}_{n+1}| < |\hat{c}_o|$ is similar to the condition determined for $|\hat{c}_n| < |\hat{c}_o|$, where for the first-order implicit upwind scheme is unconditionally stable.

In summary, the first-order implicit upwind finite difference approximation of the one-dimensional advection-dispersion equation is unconditionally stable since under these conditions, the error of the approximation is not propagated throughout the solution, but rather decreases with each time step.

### 2.3.3 Upwind Crank-Nicolson scheme

Crank-Nicolson scheme applied for the first-order upwind finite difference scheme approximation for the advection-dispersion equation was determined to be (Equation (2-13)), and now induction method terms are substituted to facilitate the stability analysis,

$$f_1\hat{c}_{n+1}e^{ik_m x} = g_1\hat{c}_n e^{ik_m x} + h_1\hat{c}_n e^{ik_m(x-\Delta x)} + h_1\hat{c}_{n+1}e^{ik_m(x-\Delta x)} + j_1\hat{c}_n e^{ik_m(x+\Delta x)} + j_1\hat{c}_{n+1}e^{i(x+\Delta x)k_m}$$

Multiple out,

$$f_1\hat{c}_{n+1}e^{ik_m x} = g_1\hat{c}_n e^{ik_m x} + h_1\hat{c}_n e^{ik_m x}e^{-ik_m\Delta x} + h_1\hat{c}_{n+1}e^{ik_m x\Delta}e^{-ik_m\Delta x} + j_1\hat{c}_n e^{ik_m x}e^{ik_m\Delta x} + j_1\hat{c}_{n+1}e^{ik_m x}e^{ik_m\Delta x}$$

Divide by $e^{ik_m x}$,

$$f_1\hat{c}_{n+1} = g_1\hat{c}_n + h_1\hat{c}_n e^{-ik_m\Delta x} + h_1\hat{c}_{n+1}e^{-ik_m\Delta x} + j_1\hat{c}_n e^{ik_m\Delta x} + j_1\hat{c}_{n+1}e^{ik_m\Delta x} \qquad (2\text{-}35)$$

The induction numerical stability analysis is performed in two parts, firstly it is proved for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 0$, then

$$f_1\hat{c}_1 = g_1\hat{c}_0 + h_1\hat{c}_0 e^{-ik_m\Delta x} + h_1\hat{c}_1 e^{-ik_m\Delta x} + j_1\hat{c}_0 e^{ik_m\Delta x} + j_1\hat{c}_1 e^{ik_m\Delta x}$$

Rearrange,

$$f_1\hat{c}_1 - h_1\hat{c}_1 e^{-ik_m\Delta x} - j_1\hat{c}_1 e^{ik_m\Delta x} = g_1\hat{c}_0 + h_1\hat{c}_0 e^{-ik_m\Delta x} + j_1\hat{c}_0 e^{ik_m\Delta x}$$

Simplifying,

$$\hat{c}_1\left(f_1 - h_1 e^{-ik_m\Delta x} - j_1 e^{ik_m\Delta x}\right) = \hat{c}_0\left(g_1 + h_1 e^{-ik_m\Delta x} + j_1 e^{ik_m\Delta x}\right)$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{\left(g_1 + h_1 e^{-ik_m\Delta x} + j_1 e^{ik_m\Delta x}\right)}{\left(f_1 - h_1 e^{-ik_m\Delta x} - j_1 e^{ik_m\Delta x}\right)}$$

A norm is applied,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < \frac{|g_1| + \left|h_1 e^{-ik_m\Delta x}\right| + \left|j_1 e^{ik_m\Delta x}\right|}{|f_1| + \left|-h_1 e^{-ik_m\Delta x}\right| + \left|-j_1 e^{ik_m\Delta x}\right|}$$

The condition required$|\hat{c}_n| < |\hat{c}_o|$, thus becomes:

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, the condition becomes

$$\frac{|g_1| + |h_1| + |j_1|}{|f_1| + |h_1| + |j_1|} < 1$$

The term is expanded using the simplification terms associated with Equation (2-13)

$$\frac{\left|\frac{1}{\Delta t} - 0.5\frac{v_x}{\Delta x} - \frac{D_L}{(\Delta x)^2} + 0.5\left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + 0.5\frac{D_L}{(\Delta x)^2}\right|}{\left|\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + 0.5\left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + 0.5\frac{D_L}{(\Delta x)^2}\right|} < 1$$

Simplifying,

$$\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} > 0 \tag{2-36}$$

The first-order upwind Crank-Nicolson scheme for the advection-dispersion equation is unconditionally stable.

Secondly, making the assumption that $|\hat{c}_n| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_{n+1}| < |\hat{c}_o|$$

Rearranging Equation (2-35),

$$f_1\hat{c}_{n+1} - h_1\hat{c}_{n+1}e^{-ik_m\Delta x} - j_1\hat{c}_{n+1}e^{ik_m\Delta x} = g_1\hat{c}_n + h_1\hat{c}_n e^{-ik_m\Delta x} + j_1\hat{c}_n e^{ik_m\Delta x}$$

Simplifying,

$$\hat{c}_{n+1} = \frac{g_1 + h_1 e^{-ik_m\Delta x} + j_1 e^{ik_m\Delta x}}{f_1 - h_1 e^{-ik_m\Delta x} - j_1 e^{ik_m\Delta x}}\hat{c}_n$$

Applying a norm on both sides,

$$|\hat{c}_{n+1}| < \frac{|g_1| + \left|h_1 e^{-ik_m\Delta x}\right| + \left|j_1 e^{ik_m\Delta x}\right|}{|f_1| + |-h_1 e^{-ik_m\Delta x}| + |-j_1 e^{ik_m\Delta x}|}|\hat{c}_n|$$

Remembering $|e^n| = 1$, the condition becomes

$$|\hat{c}_{n+1}| < \frac{|g_1| + |h_1| + |j_1|}{|f_1| + |h_1| + |j_1|}|\hat{c}_n|$$

Remembering that it has been proven that for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Thus,

$$|\hat{c}_{n+1}| < \frac{|g_1| + |h_1| + |j_1|}{|f_1| + |h_1| + |j_1|}|\hat{c}_n| < \frac{|g_1| + |h_1| + |j_1|}{|f_1| + |h_1| + |j_1|}|\hat{c}_o|$$

and, it can be inferred that

$$|\hat{c}_{n+1}| < \frac{|g_1| + |h_1| + |j_1|}{|f_1| + |h_1| + |j_1|}|\hat{c}_o|$$

Thus, the solution will be stable when,

$$\frac{|g_1| + |h_1| + |j_1|}{|f_1| + |h_1| + |j_1|} < 1$$

The term is expanded using the simplification terms associated with Equation (2-13),

$$\frac{\left|\frac{1}{\Delta t} - 0.5\frac{v_x}{\Delta x} - \frac{D_L}{(\Delta x)^2} + 0.5\left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + 0.5\frac{D_L}{(\Delta x)^2}\right|}{\left|\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + 0.5\left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + 0.5\frac{D_L}{(\Delta x)^2}\right|} < 1$$

Simplifying,

$$\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} > 0 \tag{2-37}$$

Equation (2-37) is similar to Equation (2-36), and thus by following a similar procedure the condition for $|\hat{c}_{n+1}| < |\hat{c}_o|$ is, unconditionally stable for both perspectives.

### 2.3.4 Upwind advection Crank-Nicolson scheme

Remembering that the advection-dominated system is the main culprit for the numerical instabilities, the Crank-Nicolson scheme is applied to the advection term only for the first-order. The upwind advection Crank-Nicolson scheme is determined to be (Equation (2-15)), and now substituting induction method terms,

$$k_1\hat{c}_{n+1}e^{ik_mx} = l_1\hat{c}_ne^{ik_mx} + m_1\hat{c}_ne^{ik_m(x-\Delta x)} + d_1\hat{c}_ne^{ik_m(x+\Delta x)} + o_1\hat{c}_{n+1}e^{i(x-\Delta x)k_m}$$

Multiple out,

$$k_1\hat{c}_{n+1}e^{ik_mx} = l_1\hat{c}_ne^{ik_mx} + m_1\hat{c}_ne^{ik_mx}e^{-ik_m\Delta x} + d_1\hat{c}_ne^{ik_mx}e^{ik_m\Delta x} + o_1\hat{c}_{n+1}e^{ik_mx}e^{ik_m\Delta x}$$

Divide by $e^{ik_mx}$,

$$k_1\hat{c}_{n+1} = l_1\hat{c}_n + m_1\hat{c}_ne^{-ik_m\Delta x} + d_1\hat{c}_ne^{ik_m\Delta x} + o_1\hat{c}_{n+1}e^{ik_m\Delta x} \tag{2-38}$$

The induction numerical stability analysis is performed in two parts, firstly it is proved for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 0$, then

$$k_1\hat{c}_1 = l_1\hat{c}_0 + m_1\hat{c}_0e^{-ik_m\Delta x} + d_1\hat{c}_0e^{ik_m\Delta x} + o_1\hat{c}_1e^{ik_m\Delta x}$$

Rearrange,

$$k_1\hat{c}_1 - o_1\hat{c}_1e^{ik_m\Delta x} = l_1\hat{c}_0 + m_1\hat{c}_0e^{-ik_m\Delta x} + d_1\hat{c}_0e^{ik_m\Delta x}$$

Simplifying,

$$\hat{c}_1\left(k_1 - o_1e^{ik_m\Delta x}\right) = \hat{c}_0\left(l_1 + m_1e^{-ik_m\Delta x} + d_1e^{ik_m\Delta x}\right)$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{l_1 + m_1 e^{-ik_m \Delta x} + d_1 e^{ik_m \Delta x}}{k_1 - o_1 e^{ik_m \Delta x}}$$

The norm is taken on both sides,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < \frac{|l_1| + \left|m_1 e^{-ik_m \Delta x}\right| + \left|d_1 e^{ik_m \Delta x}\right|}{|k_1| + \left|-o_1 e^{ik_m \Delta x}\right|}$$

The stability condition required $|\hat{c}_n| < |\hat{c}_o|$, develops to,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, the condition becomes

$$\frac{|l_1| + |m_1| + |d_1|}{|k_1| + |o_1|} < 1$$

The term is expanded using the simplification terms associated with Equation (2-15)

$$\frac{\left|\frac{1}{\Delta t} - 0.5\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|}{\left|\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x}\right| + \left|0.5\frac{v_x}{\Delta x}\right|} < 1 \tag{2-39}$$

If the assumption is made, where

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} > 0.5\frac{v_x}{\Delta x}$$

Then,

$$\frac{\frac{1}{\Delta t} - 0.5\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} + 0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}}{\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x} + 0.5\frac{v_x}{\Delta x}} < 1$$

Simplifying,

$$\frac{4D_L}{(\Delta x)^2} < \frac{v_x}{\Delta x} \tag{2-40}$$

Under this assumption, the upwind advection Crank-Nicolson scheme for the advection-dispersion equation is conditionally stable.

However, if the complementary assumption is made, where

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} < 0.5\frac{v_x}{\Delta x}$$

Then,

$$\frac{-\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2} + 0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}}{\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x} + 0.5\frac{v_x}{\Delta x}} < 1$$

Simplifying,

$$\frac{2}{\Delta t} > 0 \tag{2-41}$$

Under this assumption, the upwind advection Crank-Nicolson scheme for the advection-dispersion equation is unconditionally stable.

Secondly, making the assumption that $|\hat{c}_n| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_{n+1}| < |\hat{c}_o|$$

Rearranging Equation (2-38),

$$k_1 \hat{c}_{n+1} - o_1 \hat{c}_{n+1} e^{ik_m \Delta x} = l_1 \hat{c}_n + m_1 \hat{c}_n e^{-ik_m \Delta x} + d_1 \hat{c}_n e^{ik_m \Delta x}$$

Simplifying,

$$\hat{c}_{n+1} = \frac{l_1 + m_1 e^{-ik_m \Delta x} + d_1 e^{ik_m \Delta x}}{k_1 - o_1 e^{ik_m \Delta x}} \hat{c}_n$$

A norm is applied to,

$$|\hat{c}_{n+1}| < \frac{|l_1| + \left|m_1 e^{-ik_m \Delta x}\right| + \left|d_1 e^{ik_m \Delta x}\right|}{|k_1| + \left|-o_1 e^{ik_m \Delta x}\right|} |\hat{c}_n|$$

Remembering $|e^n| = 1$, the condition becomes

$$|\hat{c}_{n+1}| < \frac{|l_1| + |m_1| + |d_1|}{|k_1| + |o_1|} |\hat{c}_n|$$

Remembering that it has been proven that for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Thus,

$$|\hat{c}_{n+1}| < \frac{|l_1| + |m_1| + |d_1|}{|k_1| + |o_1|} |\hat{c}_n| < \frac{|l_1| + |m_1| + |d_1|}{|k_1| + |o_1|} |\hat{c}_o|$$

and, it can be inferred that

$$|\hat{c}_{n+1}| < \frac{|l_1| + |m_1| + |d_1|}{|k_1| + |o_1|} |\hat{c}_o|$$

Thus, the solution will be stable when,

$$\frac{|l_1| + |m_1| + |d_1|}{|k_1| + |o_1|} < 1$$

The term is expanded using the simplification terms associated with Equation (2-15)

$$\frac{\left|\frac{1}{\Delta t} - 0.5\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|}{\left|\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x}\right| + \left|0.5\frac{v_x}{\Delta x}\right|} < 1 \tag{2-42}$$

Equation (2-42) is similar to Equation (2-39), and thus by following a similar procedure the condition for $|\hat{c}_{n+1}| < |\hat{c}_o|$ becomes,

$$\frac{4D_L}{(\Delta x)^2} < \frac{v_x}{\Delta x}$$

under the assumption

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} > 0.5\frac{v_x}{\Delta x}.$$

And, if the opposite assumption applies

$$\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} < 0.5\frac{v_x}{\Delta x}$$

then, the first-order upwind advection Crank-Nicolson scheme for the advection-dispersion equation is unconditionally stable.

In summary, the first-order upwind advection Crank-Nicolson finite difference approximation of the one-dimensional advection-dispersion equation has the following stability criterion,

$$\frac{4D_L}{(\Delta x)^2} < \frac{v_x}{\Delta x}$$

Under these conditions, the error of the approximation is not proliferated throughout the solution.

### 2.3.5 Explicit upwind-downwind weighted scheme

The explicit first-order upwind-downwind weighted finite difference approximation of the one-dimensional advection-dispersion equation was determined to be (Equation (2-17)). Substituting induction stability analysis method terms,

$$a_1\hat{c}_{n+1}e^{ik_m x} = p_1\hat{c}_n e^{ik_m x} + q_1\hat{c}_n e^{ik_m(x-\Delta x)} + r_1\hat{c}_n e^{ik_m(x+\Delta x)}$$

Multiple out,

$$a_1\hat{c}_{n+1}e^{ik_m x} = p_1\hat{c}_n e^{ik_m x} + q_1\hat{c}_n e^{ik_m x}e^{-ik_m\Delta x} + r_1\hat{c}_n e^{ik_m x}e^{ik_m\Delta x}$$

Divide by $e^{ik_m x}$,

$$a_1\hat{c}_{n+1} = p_1\hat{c}_n + q_1\hat{c}_n e^{-ik_m\Delta x} + r_1\hat{c}_n e^{ik_m\Delta x} \tag{2-43}$$

The induction numerical stability analysis is performed in two parts, firstly it is proved for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 0$, then

$$a_1\hat{c}_1 = p_1\hat{c}_0 + q_1\hat{c}_0 e^{-ik_m\Delta x} + r_1\hat{c}_0 e^{ik_m\Delta x}$$

Rearrange,

$$a_1\hat{c}_1 = p_1\hat{c}_0 + q_1\hat{c}_0 e^{-ik_m\Delta x} + r_1\hat{c}_0 e^{ik_m\Delta x}$$

Simplifying,

$$a_1\hat{c}_1 = \hat{c}_0\left(p_1 + q_1 e^{-ik_m\Delta x} + r_1 e^{ik_m\Delta x}\right)$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{p_1 + q_1 e^{-ik_m\Delta x} + r_1 e^{ik_m\Delta x}}{a_1}$$

Applying the norm on both sides,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < \frac{|p_1| + \left|q_1 e^{-ik_m\Delta x}\right| + \left|r_1 e^{ik_m\Delta x}\right|}{|a_1|}$$

The condition required can be expressed as,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$ and $a_1 = \frac{1}{\Delta t}$, the condition becomes

$$\Delta t(|p_1| + |q_1| + |r_1|) < 1$$

The term is expanded using the simplification terms associated with Equation (2-17)

$$\Delta t\left(\left|\frac{1}{\Delta t} - \theta\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}\right| + \left|\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}\right|\right) < 1 \qquad \text{(2-44)}$$

If the assumption is made, where

$$\frac{1}{\Delta t} + (1-\theta)\frac{v_x}{\Delta x} > \theta\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2},$$

and

$$\frac{D_L}{(\Delta x)^2} > (1-\theta)\frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(\left(\frac{1}{\Delta t} - \theta\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}\right) + \left(\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + \left(\frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}\right)\right) < 1$$

Simplifying,

$$\Delta t\left(\frac{1}{\Delta t} - \theta\frac{v_x}{\Delta x} + \theta\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} - (1-\theta)\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}\right) < 1 \qquad \text{(2-45)}$$

Under these assumptions, the first-order explicit upwind-downwind weighted scheme for the one-dimensional advection-dispersion equation is highly unstable. Conversely, if the assumptions are made, where

$$\frac{1}{\Delta t} + (1-\theta)\frac{v_x}{\Delta x} < \theta\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2},$$

and

$$\frac{D_L}{(\Delta x)^2} < (1-\theta)\frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(\left(-\frac{1}{\Delta t} + \theta\frac{v_x}{\Delta x} - (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right) + \left(\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + \left(-\frac{D_L}{(\Delta x)^2} + (1-\theta)\frac{v_x}{\Delta x}\right)\right) < 1$$

Simplifying,

$$\Delta t\left(-\frac{1}{\Delta t} + \theta\frac{v_x}{\Delta x} + \theta\frac{v_x}{\Delta x} - (1-\theta)\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} - \frac{D_L}{(\Delta x)^2}\right) < 1$$

$$\Delta t\left(\theta\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right) < 1 \qquad (2\text{-}46)$$

Under these assumptions, the first-order explicit upwind-downwind weighted scheme for the one-dimensional advection-dispersion equation is conditionally stable, when $\theta < 1$. Thus, under these assumptions, the weighted explicit upwind-downwind scheme ($0 < \theta < 1$) and the full downwind scheme ($\theta = 0$) are stable. Yet, the full upwind scheme ($\theta = 1$) is invalid under these assumptions.

Secondly, making the assumption that $|\hat{c}_n| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_{n+1}| < |\hat{c}_o|$$

Remembering Equation (2-43), and simplifying,

$$a_1\hat{c}_{n+1} = \hat{c}_n(p_1 + q_1 e^{-ik_m\Delta x} + r_1 e^{ik_m\Delta x})$$

$$\hat{c}_{n+1} = \frac{p_1 + q_1 e^{-ik_m\Delta x} + r_1 e^{ik_m\Delta x}}{a_1}\hat{c}_n$$

Applying a norm,

$$|\hat{c}_{n+1}| < \frac{|p_1| + |q_1 e^{-ik_m\Delta x}| + |r_1 e^{ik_m\Delta x}|}{|a_1|}|\hat{c}_n|$$

Remembering $|e^n| = 1$ and $a_1 = \frac{1}{\Delta t}$, the condition becomes

$$|\hat{c}_{n+1}| < \Delta t(|p_1| + |q_1| + |r_1|)|\hat{c}_n|$$

Remembering that it has been proven that for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Thus,

$$|\hat{c}_{n+1}| < \Delta t(|p_1| + |q_1| + |r_1|)|\hat{c}_n| < \Delta t(|p_1| + |q_1| + |r_1|)|\hat{c}_o|$$

and, it can be inferred that

$$|\hat{c}_{n+1}| < \Delta t\left(|p_1| + |q_1| + |r_1|\right)|\hat{c}_o|$$

Thus, the solution will be stable when,

$$\Delta t(|p_1| + |q_1| + |r_1|) < 1$$

The term is expanded using the simplification terms associated with Equation (2-17)

$$\Delta t\left(\left|\frac{1}{\Delta t} - \theta\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}\right| + \left|\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}\right|\right) < 1 \qquad (2\text{-}47)$$

Equation (2-47) is similar to Equation (2-44), and thus by following a similar procedure the explicit weighted upwind-downwind numerical scheme is unstable under the assumptions,

$$\frac{1}{\Delta t} + (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} > \theta\frac{v_x}{\Delta x},$$

and

$$\frac{D_L}{(\Delta x)^2} > (1-\theta)\frac{v_x}{\Delta x}$$

Yet, is conditionally stable, when $\theta < 1$, under the assumptions

$$\frac{1}{\Delta t} + (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} < \theta\frac{v_x}{\Delta x},$$

and

$$\frac{D_L}{(\Delta x)^2} < (1-\theta)\frac{v_x}{\Delta x}$$

In summary, the weighted explicit upwind-downwind numerical scheme for the advection-dispersion equation for $0 < \theta < 1$ is conditionally stable. Yet, under certain assumptions the extreme cases of the full upwind scheme ($\theta = 0$) are invalid.

### 2.3.6 Implicit upwind-downwind weighted scheme

The first-order upwind-downwind (implicit) weighted finite difference approximation of the one-dimensional advection-dispersion equation was determined to be (Equation (2-19)). Now, substituting induction method terms to assess the stability of the scheme,

$$v_1\hat{c}_{n+1}e^{ik_mx} = a_1\hat{c}_ne^{ik_mx} + q_1\hat{c}_{n+1}e^{ik_m(x-\Delta x)} + r_1\hat{c}_{n+1}e^{ik_m(x+\Delta x)}$$

Multiple out,

$$v_1\hat{c}_{n+1}e^{ik_mx} = a_1\hat{c}_ne^{ik_mx} + q_1\hat{c}_{n+1}e^{ik_mx}e^{-ik_m\Delta x} + r_1\hat{c}_{n+1}e^{ik_mx}e^{ik_m\Delta x}$$

Divide by $e^{ik_mx}$,

$$v_1\hat{c}_{n+1} = a_1\hat{c}_n + q_1\hat{c}_{n+1}e^{-ik_m\Delta x} + r_1\hat{c}_{n+1}e^{ik_m\Delta x} \qquad (2\text{-}48)$$

The induction numerical stability analysis is performed in two parts, firstly it is proved for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 0$, then

$$v_1\hat{c}_1 = a_1\hat{c}_0 + q_1\hat{c}_1 e^{-ik_m\Delta x} + r_1\hat{c}_1 e^{ik_m\Delta x}$$

Rearrange,

$$v_1\hat{c}_1 - q_1\hat{c}_1 e^{-ik_m\Delta x} - r_1\hat{c}_1 e^{ik_m\Delta x} = a_1\hat{c}_0$$

Simplifying,

$$\hat{c}_1\left(v_1 - q_1 e^{-ik_m\Delta x} - r_1 e^{ik_m\Delta x}\right) = \hat{c}_0(a_1)$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{a_1}{v_1 - q_1 e^{-ik_m\Delta x} - r_1 e^{ik_m\Delta x}}$$

Applying a norm,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < \frac{|a_1|}{|v_1| + |-q_1 e^{-ik_m\Delta x}| + |-r_1 e^{ik_m\Delta x}|}$$

The stability condition necessary $|\hat{c}_n| < |\hat{c}_o|$, becomes:

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$ and $a_1 = \frac{1}{\Delta t}$, the condition becomes

$$\frac{1}{\Delta t(|v_1| + |q_1| + |r_1|)} < 1$$

It can be concluded that $|\hat{c}_1| < |\hat{c}_o|$, when

$$\Delta t(|v_1| + |q_1| + |r_1|) > 1$$

The term is expanded using the simplification terms associated with Equation (2-19)

$$\Delta t\left(\left|\frac{1}{\Delta t} + \theta\frac{v_x}{\Delta x} - (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}\right|\right) > 1 \qquad (2\text{-}49)$$

If the assumption is made, where

$$\frac{1}{\Delta t} + \theta\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} > (1-\theta)\frac{v_x}{\Delta x},$$

and

$$\frac{D_L}{(\Delta x)^2} > (1-\theta)\frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(\left(\frac{1}{\Delta t} + \theta\frac{v_x}{\Delta x} - (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right) + \left(\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + \left(\frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}\right)\right) > 1$$

Simplifying,

$$\frac{v_x}{\Delta x}(2\theta - 1) + \frac{2D_L}{(\Delta x)^2} > 1 \qquad (2\text{-}50)$$

Under these assumptions, the first-order implicit upwind-downwind weighted scheme for the one-dimensional advection-dispersion equation is conditionally stable, where $\theta > 0$. When $\theta > 0$, the solution becomes the weighted upwind-downwind solution, while when $\theta = 1$, the solution becomes the upwind formation. When $\theta = 0$, the solution becomes the downward formulation of the advection, and this is shown to be numerically unstable under these assumptions.

On the other hand, if the assumptions are made, where

$$\frac{1}{\Delta t} + \theta \frac{v_x}{\Delta x} < (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2},$$

and

$$\frac{D_L}{(\Delta x)^2} < (1-\theta)\frac{v_x}{\Delta x}$$

Then,

$$\Delta t\left(\left(-\frac{1}{\Delta t} - \theta\frac{v_x}{\Delta x} + (1-\theta)\frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}\right) + \left(\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) + \left(-\frac{D_L}{(\Delta x)^2} + (1-\theta)\frac{v_x}{\Delta x}\right)\right) > 1$$

Simplifying,

$$(1-\theta)\frac{v_x \Delta t}{\Delta x} > 1 \tag{2-51}$$

Under these assumptions, the first-order implicit upwind-downwind weighted scheme for the one-dimensional advection-dispersion equation is conditionally stable, where $\theta < 1$. When $\theta = 0$, the solution becomes the downward formulation of the advection, while when $0 < \theta < 1$, the solution becomes the weighted upwind-downwind solution. When $\theta = 1$, the solution becomes the upwind formation and is numerically unstable under these assumptions.

Secondly, making the assumption that $|\hat{c}_n| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_{n+1}| < |\hat{c}_o|$$

Remembering Equation (2-48),

$$v_1\hat{c}_{n+1} = a_1\hat{c}_n + q_1\hat{c}_{n+1}e^{-ik_m\Delta x} + r_1\hat{c}_{n+1}e^{ik_m\Delta x}$$

Simplifying,

$$\hat{c}_{n+1}\left(v_1 - q_1e^{-ik_m\Delta x} - r_1e^{ik_m\Delta x}\right) = a_1\hat{c}_n$$

$$\hat{c}_{n+1} = \frac{a_1}{v_1 - q_1e^{-ik_m\Delta x} - r_1e^{ik_m\Delta x}}\hat{c}_n$$

Taking the norm on both sides,

$$|\hat{c}_{n+1}| < \frac{|a_1|}{|v_1| + |-q_1e^{-ik_m\Delta x}| + |-r_1e^{ik_m\Delta x}|}|\hat{c}_n|$$

Remembering $|e^n| = 1$ and $a_1 = \frac{1}{\Delta t}$, the condition becomes

$$|\hat{c}_{n+1}| < \frac{1}{\Delta t(|v_1| + |q_1| + |r_1|)} |\hat{c}_n|$$

Remembering that it has been proven that for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Thus,

$$|\hat{c}_{n+1}| < \frac{1}{\Delta t(|v_1| + |q_1| + |r_1|)} |\hat{c}_n| < \frac{1}{\Delta t(|v_1| + |q_1| + |r_1|)} |\hat{c}_o|$$

and, it can be inferred that

$$|\hat{c}_{n+1}| < \frac{1}{\Delta t(|v_1| + |q_1| + |r_1|)} |\hat{c}_o|$$

Thus, the solution will be stable when,

$$\frac{1}{\Delta t(|v_1| + |q_1| + |r_1|)} < 1$$

It can be concluded that $|\hat{c}_{n+1}| < |\hat{c}_o|$, when

$$\Delta t(|v_1| + |q_1| + |r_1|) > 1$$

The term is expanded using the simplification terms associated with Equation (2-19)

$$\Delta t\left(\left|\frac{1}{\Delta t} + \theta\frac{v_x}{\Delta x} - (1-\theta)\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right| + \left|\theta\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2} - (1-\theta)\frac{v_x}{\Delta x}\right|\right) > 1 \qquad (2\text{-}52)$$

Equation (2-52) is similar to Equation (2-49), and thus by following a similar procedure the condition for $|\hat{c}_{n+1}| < |\hat{c}_o|$ becomes,

$$\frac{v_x}{\Delta x}(2\theta - 1) + \frac{2D_L}{(\Delta x)^2} > 1$$

when the first assumptions are made.

And, similarly, the condition for $|\hat{c}_{n+1}| < |\hat{c}_o|$ becomes,

$$(1-\theta)\frac{v_x \Delta t}{\Delta x} > 1$$

when the second set of assumptions are made.

In summary, the weighted implicit upwind-downwind numerical scheme for the advection-dispersion equation for $0 < \theta < 1$ is conditionally stable. Yet, under certain assumptions, the extreme cases of the full upwind scheme ($\theta = 0$) and full downwind ($\theta = 1$) are unstable under certain assumptions.

## 2.4 Comparison of numerical schemes stability conditions

Traditional upwind numerical schemes for the one-dimensional advection-dispersion equation, as well as new upwind numerical schemes, are developed and subjected to numerical stability analysis using the recursive method. The stability conditions and related assumptions are tabulated for the traditional approaches in Table 2-1, and for the new schemes in Table 2-2.

The first-order explicit upwind finite difference scheme is found to be unstable for the first assumption made, and conditionally stable for the second assumption, where the condition found is the Courant condition traditionally applied for explicit finite difference schemes (Table 2-1). The correspondence to the Courant condition for this scheme validates the stability analysis method used.

The first-order upwind implicit finite difference scheme is unconditionally stable for all conditions. The first-order upwind implicit scheme is more stable than the explicit formulation, which is typically the case when comparing explicit and implicit formulations. However, implicit schemes tend to compromise on accuracy to achieve the improved stability.

The first-order upwind Crank-Nicolson finite difference scheme is found to be unconditionally stable, and thus the combination of the first-order upwind numerical scheme with the Crank-Nicolson numerical scheme applied to the entire advection-dispersion equation is appropriate. This leads on to the next numerical scheme to be analysed, where now the Crank-Nicolson scheme is only considered for the advection term of the advection-dispersion equation (Table 2-1).

The newly proposed upwind advection Crank-Nicolson finite difference scheme is conditionally stable for the first assumption made, and unconditionally stable for the second assumption (Table 2-2). Thus, it can be concluded that an upwind and advection Crank-Nicolson scheme only applied to the advection term of the advection-dispersion equation is appropriate under certain conditions.

Furthermore, a weighted upwind-downwind finite difference numerical scheme is proposed for the one-dimensional advection-dispersion equation. The explicit weighted upwind-downwind scheme is found to be unstable for the first assumption made, yet unconditionally stable for the second assumption (Table 2-2).

The weighted explicit upwind-downwind numerical scheme for the advection-dispersion equation for $0 < \theta < 1$ is conditionally stable. Yet, under certain assumptions the extreme cases of the full upwind scheme ($\theta = 0$) are unstable. The weighted implicit upwind-downwind numerical scheme for the advection-dispersion equation for $0 < \theta < 1$ is conditionally stable. Yet, under certain assumptions, the extreme cases of the full upwind scheme ($\theta = 0$) and full downwind ($\theta = 1$) are unstable under certain assumptions (Table 2-2).

When comparing the explicit first-order upwind scheme with the explicit weighted first-order upwind-downwind scheme, both solutions have an instability under one assumption, However, the explicit weighted first-order upwind-downwind scheme is unconditionally stable for the second assumption for certain weighting, while the explicit first-order upwind scheme is conditionally stable. From a comparison on stability, the new explicit weighted first-order upwind-downwind scheme is an improvement on the explicit first-order upwind scheme for the finite difference method of numerical approximation. Considering that generally explicit formulations are less stable, the weighted approach could improve the stability of the scheme while retaining the accuracy advantages of the explicit formulation.

**Table 2-1 Traditional upwind numerical schemes for the one dimensional advection-dispersion equation with associated assumptions in the numerical stability analysis and the resulting stability conditions**

| Scheme | Numerical approximation | Assumptions | Stability condition |
|---|---|---|---|
| **Explicit Upwind** | $\left(\frac{1}{\Delta t}\right) c_i^{n+1} = \left(\frac{1}{\Delta t} - \frac{v_x}{\Delta x} - \frac{2D_L}{(\Delta x)^2}\right) c_i^n + \left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) c_{i-1}^n + \left(\frac{D_L}{(\Delta x)^2}\right) c_{i+1}^n$ | $\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} > \frac{v_x}{\Delta x}$ | Unstable |
| | | $\frac{1}{\Delta t} + \frac{2D_L}{(\Delta x)^2} < \frac{v_x}{\Delta x}$ | $v_x \frac{\Delta t}{\Delta x} < 1$ Conditionally stable |
| **Implicit Upwind** | $\left(\frac{1}{\Delta t} + \frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2}\right) c_i^{n+1} = \left(\frac{1}{\Delta t}\right) c_i^n + \left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) c_{i-1}^{n+1} + \left(\frac{D_L}{(\Delta x)^2}\right) c_{i+1}^{n+1}$ | No assumptions required | $\frac{2v_x}{\Delta x} + \frac{4D_L}{(\Delta x)^2} > 0$ Unconditionally stable |
| **Upwind Crank-Nicolson** | $\left(\frac{1}{\Delta t} + 0.5\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) c_i^{n+1} = \left(\frac{1}{\Delta t} - 0.5\frac{v_x}{\Delta x} - \frac{D_L}{(\Delta x)^2}\right) c_i^n + 0.5\left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) c_{i-1}^n + 0.5\left(\frac{v_x}{\Delta x} + \frac{D_L}{(\Delta x)^2}\right) c_{i-1}^{n+1} + 0.5\left(\frac{D_L}{(\Delta x)^2}\right) c_{i+1}^n + 0.5\left(\frac{D_L}{(\Delta x)^2}\right) c_{i+1}^{n+1}$ | No assumptions required | $\frac{v_x}{\Delta x} + \frac{2D_L}{(\Delta x)^2} > 0$ Unconditionally stable |

Interestingly, the implicit weighted first-order upwind-downwind scheme is not more stable than the implicit first-order upwind scheme. This is contrasting to the usual trend where implicit formulations are more stable than explicit formulations. It would thus appear that the explicit weighted first-order upwind-downwind scheme is dependent on dispersivity, cell size and time step; while the implicit weighted first-order upwind-downwind scheme is dependent on chosen weighting factor ($\theta$). However, if an appropriate weighting factor is selected the scheme is stable under all assumptions.

In summary, based on the stability analysis solely, an upwind and Crank-Nicolson scheme is appropriate when the Crank-Nicolson scheme is applied to the advection term of the advection-dispersion equation. Furthermore, the proposed explicit weighted first-order upwind-downwind finite difference numerical scheme is an improvement on the traditional explicit first-order upwind scheme, while the implicit weighted first-order upwind-downwind finite difference numerical scheme is stable under all assumption when the appropriate weighting factor ($\theta$) is assigned.

**Table 2-2 New upwind schemes for the one dimensional advection-dispersion equation with associated assumptions in the numerical stability analysis and the resulting stability conditions**

| Scheme | Numerical approximation | Assumptions | Stability condition |
|---|---|---|---|
| **Upwind advection Crank-Nicolson** | $\left(\frac{1}{\Delta t}+0.5\frac{v_x}{\Delta x}\right)c_i^{n+1}=\left(\frac{1}{\Delta t}-0.5\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}\right)c_i^n+\left(0.5\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_{i-1}^n+\left(\frac{D_L}{(\Delta x)^2}\right)c_{i+1}^n+\left(0.5\frac{v_x}{\Delta x}\right)c_{i-1}^{n+1}$ | $\frac{1}{\Delta t}+\frac{2D_L}{(\Delta x)^2}>0.5\frac{v_x}{\Delta x}$ | $\frac{4D_L}{\Delta x}<v_x$ Conditionally stable |
| | | $\frac{1}{\Delta t}+\frac{2D_L}{(\Delta x)^2}<0.5\frac{v_x}{\Delta x}$ | $\frac{2}{\Delta t}>0$ Unconditionally stable |
| **Explicit upwind-downwind weighted scheme** | $\left(\frac{1}{\Delta t}\right)c_i^{n+1}=\left(\frac{1}{\Delta t}-\theta\frac{v_x}{\Delta x}+(1-\theta)\frac{v_x}{\Delta x}-\frac{2D_L}{(\Delta x)^2}\right)c_i^n+\left(\theta\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_{i-1}^n+\left(\frac{D_L}{(\Delta x)^2}-(1-\theta)\frac{v_x}{\Delta x}\right)c_{i+1}^n$ | $\frac{1}{\Delta t}+(1-\theta)\frac{v_x}{\Delta x}>\theta\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}$ $\frac{D_L}{(\Delta x)^2}>(1-\theta)\frac{v_x}{\Delta x}$ | Unstable |
| | | $\frac{1}{\Delta t}+(1-\theta)\frac{v_x}{\Delta x}<\theta\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}$ $\frac{D_L}{(\Delta x)^2}<(1-\theta)\frac{v_x}{\Delta x}$ | $\Delta t\left(\theta\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}\right)<1$ Conditionally stable |
| **Implicit upwind-downwind weighted scheme** | $\left(\frac{1}{\Delta t}+\theta\frac{v_x}{\Delta x}-(1-\theta)\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}\right)c_i^{n+1}=\left(\frac{1}{\Delta t}\right)c_i^n+\left(\theta\frac{v_x}{\Delta x}+\frac{D_L}{(\Delta x)^2}\right)c_{i-1}^{n+1}+\left(\frac{D_L}{(\Delta x)^2}-(1-\theta)\frac{v_x}{\Delta x}\right)c_{i+1}^{n+1}$ | $\frac{1}{\Delta t}+\theta\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}>(1-\theta)\frac{v_x}{\Delta x}$, $\frac{D_L}{(\Delta x)^2}>(1-\theta)\frac{v_x}{\Delta x}$ | $\frac{v_x}{\Delta x}(2\theta-1)+\frac{2D_L}{(\Delta x)^2}>1$ Conditionally stable |
| | | $\frac{1}{\Delta t}+\theta\frac{v_x}{\Delta x}<(1-\theta)\frac{v_x}{\Delta x}+\frac{2D_L}{(\Delta x)^2}$, $\frac{D_L}{(\Delta x)^2}<(1-\theta)\frac{v_x}{\Delta x}$ | $(1-\theta)\frac{v_x\Delta t}{\Delta x}>1$ Conditionally stable |

## 2.5 Numerical simulation

The developed numerical schemes have been assessed based on the stability analysis performed. To supplement the analysis a simulation using these schemes is performed to additionally assess the computational times and practicality. A generic one-dimensional transport problem is made use of for the simulation (Figure 2-1). The velocity within the aquifer is constant at 0.5 m/d, the hydrodynamic dispersivity in the x-direction is 0.3 $m^2/d$, and the initial contaminant concentration is 10 mg/l. The initial condition and boundary conditions for the defined problem are:

$$
\left.\begin{array}{ll}
c(x,0) = 0\, mg/l & \\
c(0,t) = 10\, mg/l & \\
c(L,t) = 0\, mg/l &
\end{array}\right]
\begin{array}{l}
x \geq 0 \\
t \geq 0 \\
t \geq 0
\end{array}
$$

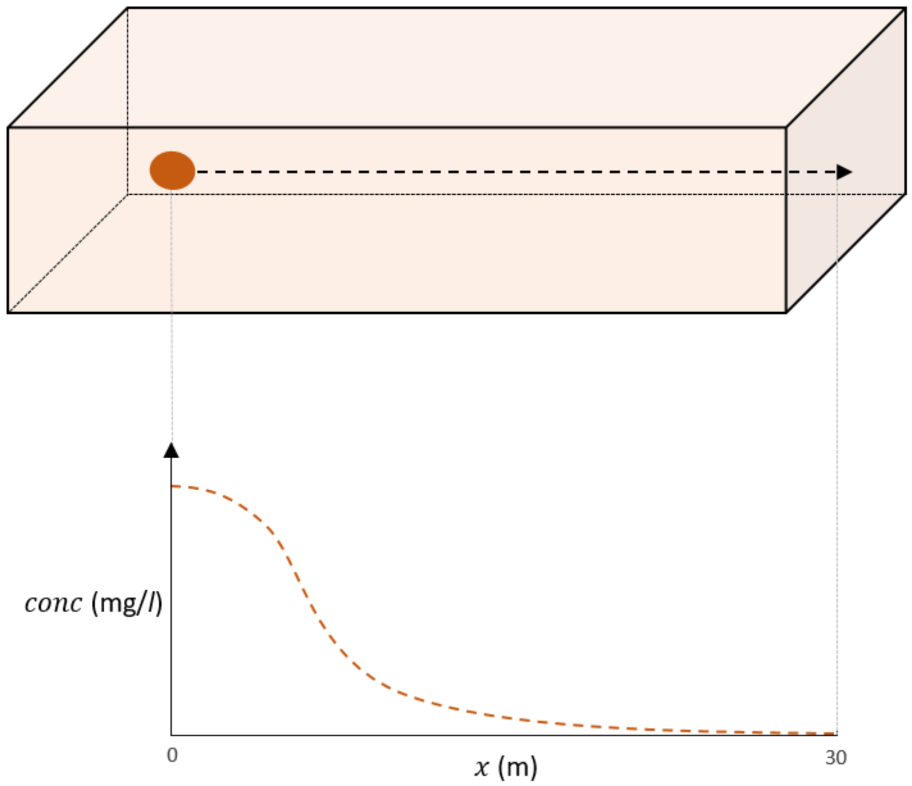


**Figure 2-1 Generic one-dimensional transport problem, where an initial contaminant concentration in an aquifer is simulated along a single line in the x-direction.**

The numerical schemes described in Section 2.2 are applied to this problem, and coding the numerical approximations in the software program *Scilab*, the resulting breakthrough curves are displayed for in Figure 2-2 to Figure 2-8. The codes for each numerical scheme are provided in Appendix A. The traditional first-order upwind (implicit and explicit) schemes are included as a base with which to compare the newly developed schemes. The traditional upwind explicit formulation is unstable at early times (Figure 2-2), and corresponds to the stability analysis where no unconditionally stable condition was found (Section 2.3.1). The traditional upwind implicit formulation is stable (Figure 2-3), and confirms the stability analysis where the scheme is found to be unconditionally stable under certain assumptions (2.3.2).

A combination of the traditional upwind and Crank-Nicolson schemes are considered as a foundation with which to compare the newly developed upwind advection Crank-Nicolson schemes (explicit and implicit). The combination of the traditional upwind and Crank-Nicolson scheme is found to produce the expected breakthrough curve, but with instabilities at early times (Figure 2-4). However, the stability analysis did not indicate instabilities for this formulation (Section 2.3.3 and 2.4). The explicit formulation of the advection-specific upwind Crank-Nicolson combination is also found to be unstable (Figure 2-5), yet the implicit formulation improves the instabilities where the instabilities smooth out quicker (Figure 2-6).

The developed weighted upwind-downwind formulation is simulated for this generic transport problem in Figure 2-7 (explicit) and Figure 2-8 (implicit). The weighting factor ($\theta$) provides a means to adapt the scheme, and the simulated breakthrough curve for variable weightings is displayed. Incorporating the weighted component of the downward scheme for the explicit formulation creates instabilities in the solution where increasing the weighting artificially reduces the plume extent (Figure 2-7). Thus, for this specific transport problem, the weighted explicit formulation is not an improvement on the traditional explicit upwind formulation. However, the stability analysis found that for some cases/assumptions the weighted upwind-downwind formulation could improve the stability of the scheme while retaining the accuracy advantages of the explicit formulation. The weighted upwind-downwind implicit formulation is stable for all theta values (Figure 2-8), yet the solution has some variability with the theta value. Thus, this formulation could provide a more flexible solution to calibrate and match the simulated break-through curve with the measured concentrations.

The computational times for each of these schemes is considered for this simple 1D transport problem. The computational times recorded in *Scilab* for each scheme are reported in Table 2-3. For all the schemes, the implicit formulations had a slightly higher computational time, which can be expected due to the additional inverse simulation required for implicit formulations. The advection Crank-Nicolson schemes had the highest computational times, and the weighted implicit is slightly quicker than the traditional upwind implicit scheme. The difference in computational times on this scale are small, but for a larger complex 3D system, these differences could become substantial.

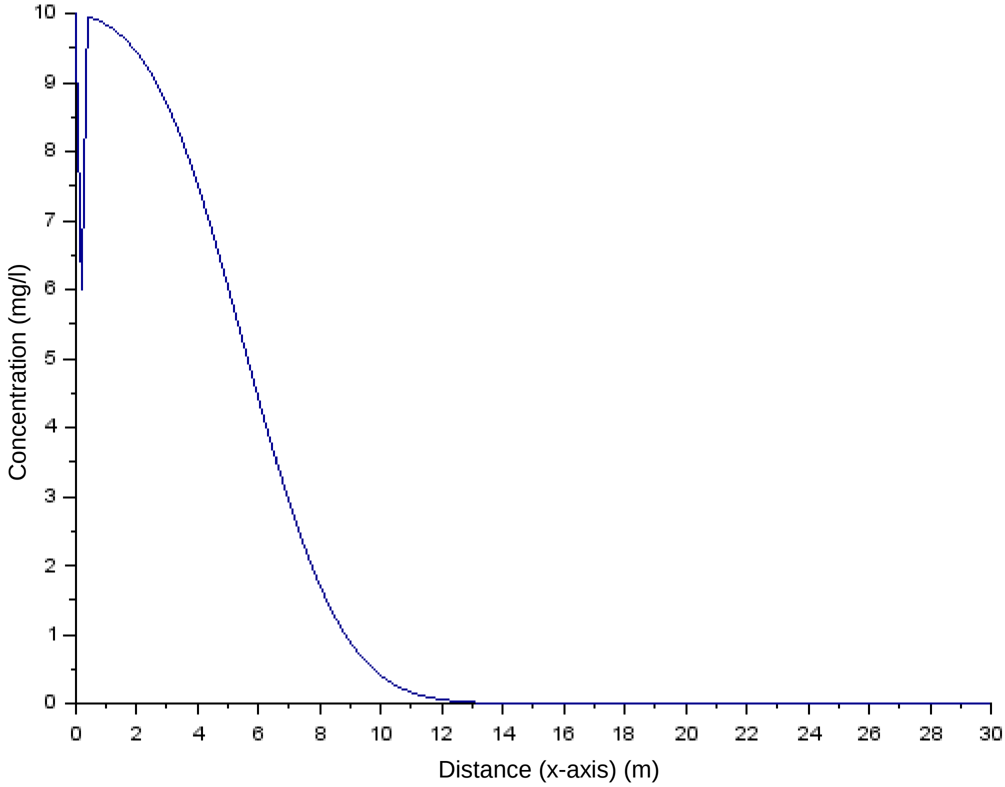


**Figure 2-2 Simulated breakthrough curve of concentration (concentration against distance) for the First-order upwind explicit numerical scheme**

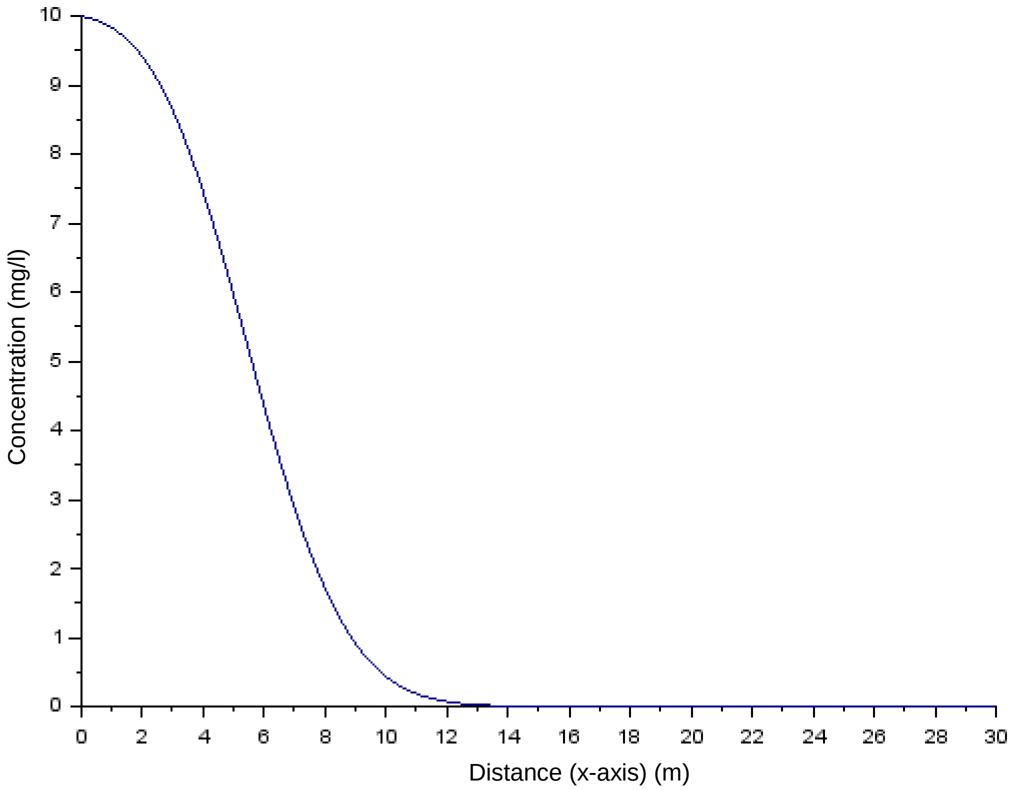


**Figure 2-3 Simulated breakthrough curve of concentration (concentration against distance) for the First-order upwind implicit numerical scheme**

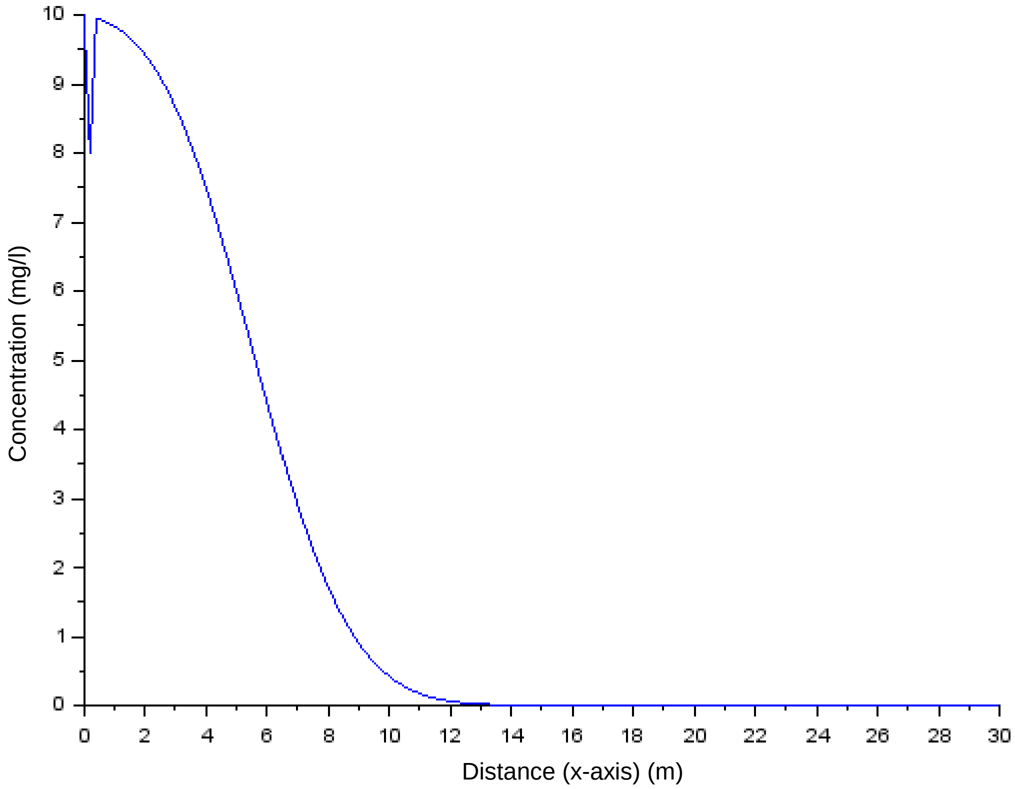


**Figure 2-4 Simulated breakthrough curve of concentration (concentration against distance) for the First-order upwind Crank-Nicolson numerical scheme**

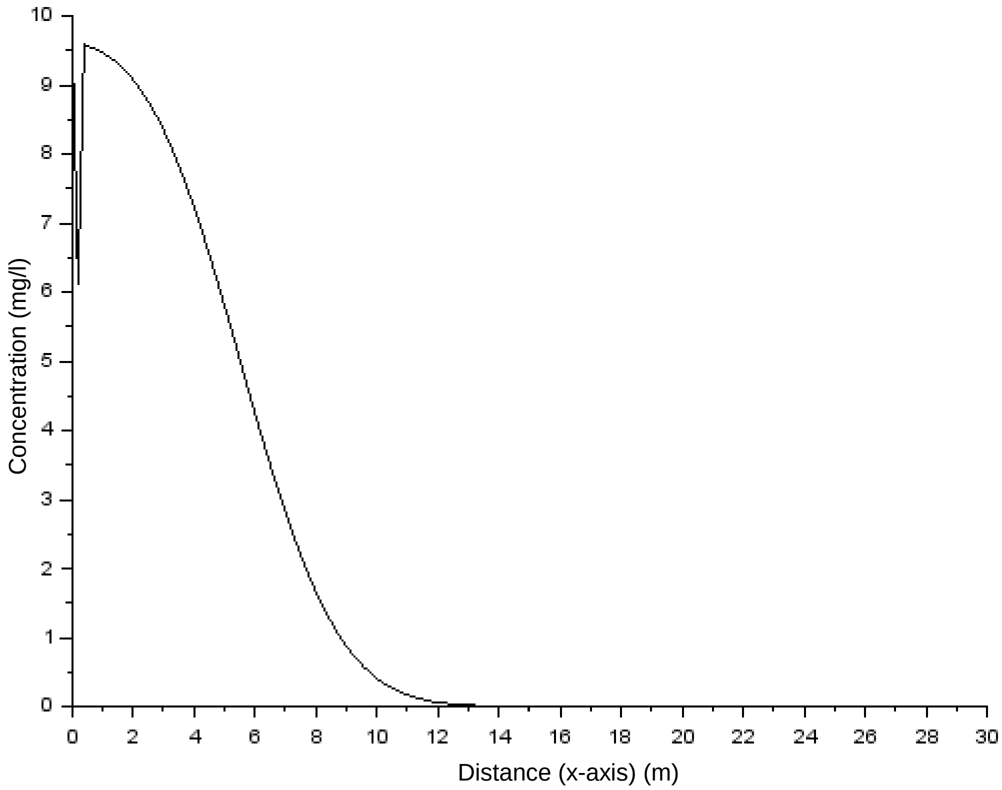


**Figure 2-5 Simulated breakthrough curve of concentration (concentration against distance) for the First-order upwind advection Crank-Nicolson (explicit) numerical scheme**

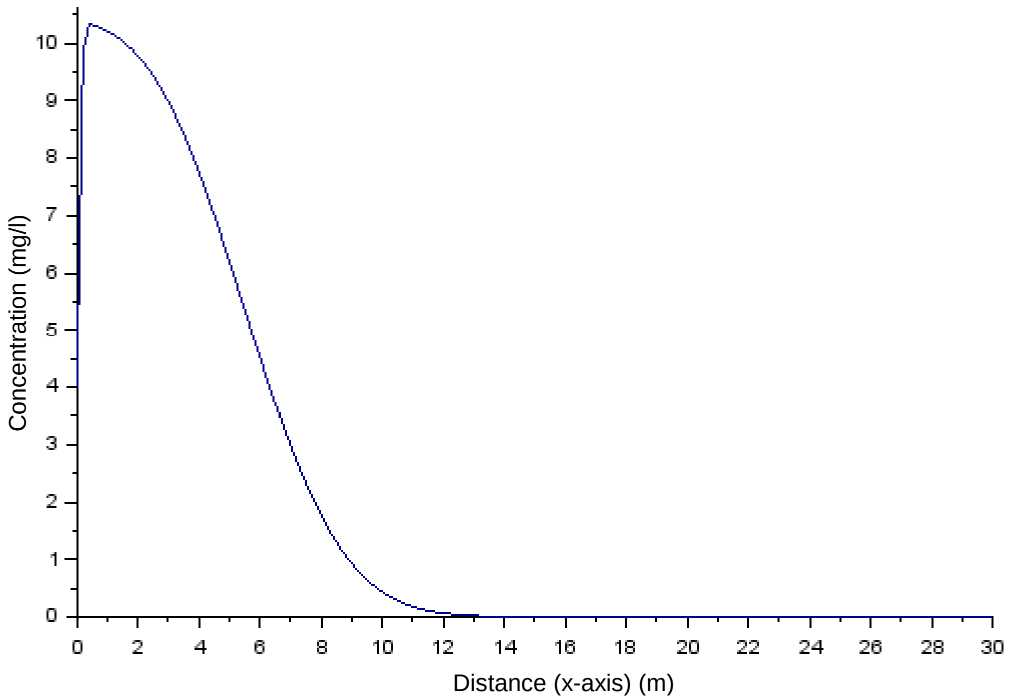


**Figure 2-6 Simulated breakthrough curve of concentration (concentration against distance) for the First-order upwind advection Crank-Nicolson (implicit) numerical scheme**

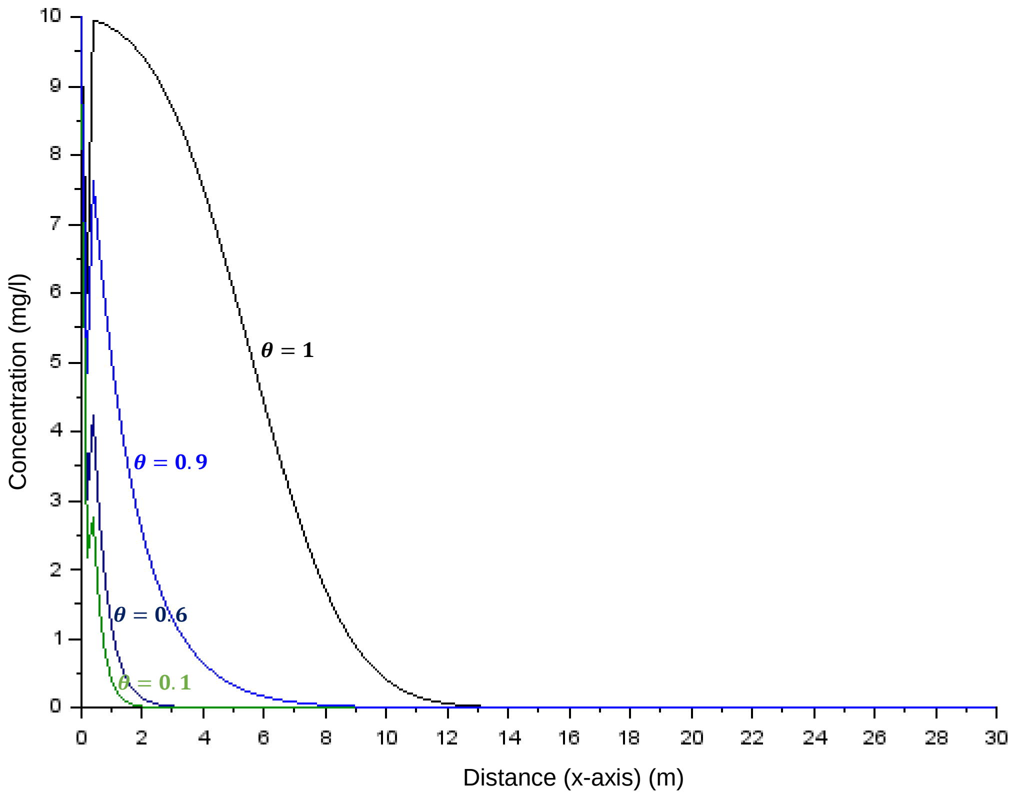


**Figure 2-7 Simulated breakthrough curve of concentration (concentration against distance) for the First-order upwind-downwind weighted (explicit) numerical scheme with variable theta ($\theta$) values from 1 (black), 0.9 (blue), 0.6 (dark blue), and 0.1 (green)**

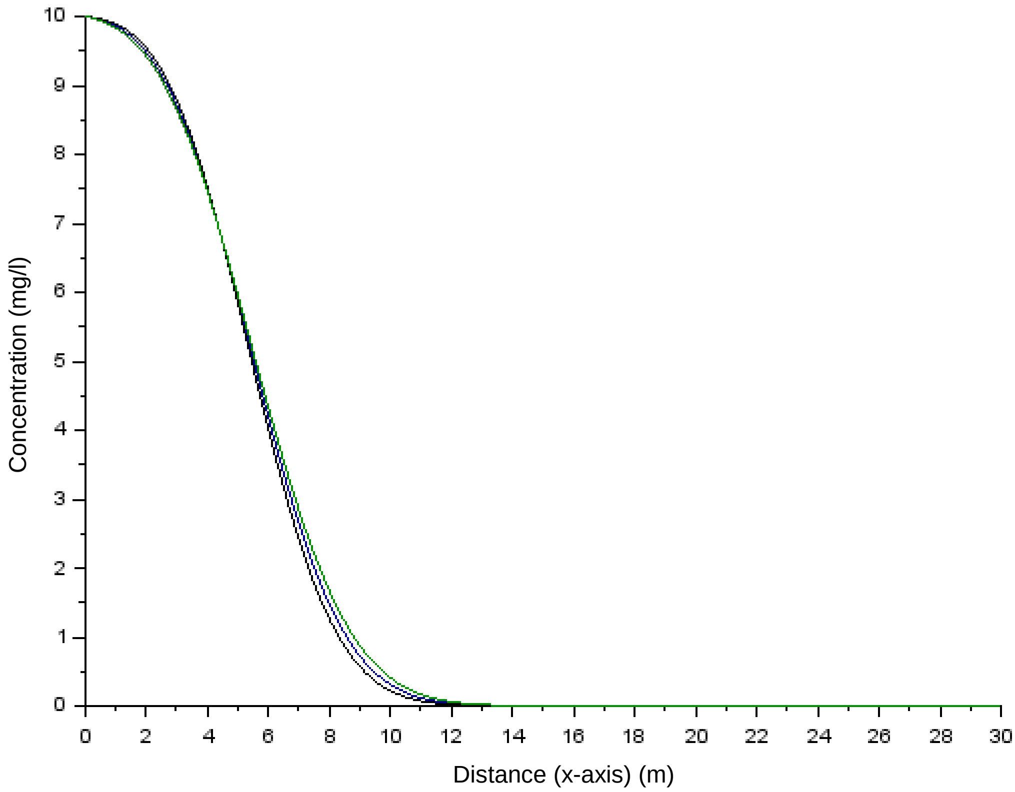


**Figure 2-8 Simulated breakthrough curve of concentration (concentration against distance) for the First-order upwind-downwind weighted (implicit) numerical scheme with variable theta ($\theta$) values from 1 (green), 0.5 (dark blue), and 0.1 (black)**

**Table 2-3 Computational times (in nanoseconds) for each numerical scheme investigated**

| **Numerical approximation scheme** | **Computational time** (*ns* – *Nano* seconds) | | | |
|---|---|---|---|---|
| | **1** | **2** | **3** | **Average** |
| Upwind (explicit) | 1.093 | 1.015 | 1.328 | 1.15 |
| Upwind (implicit) | 1.531 | 1.578 | 1.421 | 1.51 |
| Upwind-Crank-Nicolson (full) | 1.531 | 1.390 | 1.406 | 1.44 |
| Upwind-Crank-Nicolson (advection-explicit) | 2.250 | 1.656 | 1.328 | 1.74 |
| Upwind-Crank-Nicolson (advection-implicit) | 2.265 | 1.859 | 1.703 | 1.94 |
| Weighted upwind-downwind (explicit) | 1.375 | 1.453 | 1.390 | 1.41 |
| Weighted upwind-downwind (implicit) | 1.421 | 1.437 | 1.593 | 1.48 |

In general, the implicit formulations are more numerically stable, yet have slightly higher computational times. The first-order upwind advection Crank-Nicolson (implicit) scheme is an improvement on the combination of the traditional upwind and Crank-Nicolson schemes, yet runs slightly longer. The weighted implicit upwind-downwind scheme is an improvement on the traditional upwind scheme for the considered system as theta provides a more flexible solution and the computational times are slightly faster.

## 2.6 Chapter summary

In this chapter, the limitations identified with the advection-dispersion equation, especially with respect to fractured systems, are improved within the local or traditional space by applying augmented upwind numerical approximation schemes that are better suited for advection-dominated fractured systems. A numerical scheme combining the traditional upwind and Crank-Nicolson schemes is developed, along with new schemes including the advection-specific upwind Crank-Nicolson combination, and weighted upwind-downwind schemes. The developed numerical schemes, along with the traditional approaches for comparison, are analysed for stability using the recursive stability analysis method, applied to a simple one-dimensional transport problem, and computational time assessment. From these analyses, the implicit formulations are found to be more stable and practically viable, and the new advection Crank-Nicolson and weighted upwind-downwind schemes are found to be improvements from the traditional methods. Thus, the augmented upwind schemes have the potential to improve the simulation of the local advection-dispersion equation for fractured systems. However, these improves do not address the problem of anomalous diffusion and therefore in the following chapters the reformulation of the advection-dispersion equation will be investigated.

# 3 FRACTAL ADVECTION-DISPERSION EQUATION

The typical application of a Fickian advection-dispersion transport equation to model groundwater transport depends on the availability of information to characterise the physical system in its entirety. Yet, where preferential flow pathways (fractures, faults or dykes) are present there is often inadequate data to accurately characterise the heterogeneity of these systems. Thus, when there is an incomplete characterisation of heterogeneity, the classical Fickian advection-dispersion transport equation is unable to simulate the observed plume movement accurately. The dissimilarity between the modelled and measured plume is commonly referred to as anomalous diffusion, because the plume diverges from the Fickian model of groundwater transport (Zheng and Bennett, 2002; Pickens and Grisak, 1981).

Describing the heterogeneity of a system is complicated by dispersivity increasing with the scale of measurement (Freeze and Cherry, 1979; Pickens and Grisak, 1981; Molz et al., 1983; Neuman, 1990; Zheng and Bennett, 2002). Solutions to the dispersivity scale-dependency problem include establishing scaling relationships (Pickens and Grisak, 1981), or models incorporating fractures (or preferential flow pathways). Modelling methods to physically include preferential pathways include the dual porosity model; random array of fractures; multiple continuum; and others (Acuna and Yortsos, 1995; Cello et al., 2009). Yet, these models cannot account for the fractal nature of fractured systems. Fractal geometry and fractured systems were originally associated in 1985 for a nuclear waste disposal site investigation (Barton and Hsieh, 1989), and since several authors have validated the relationship (Cello et al., 2009; Rodrigues and Pandolfelli, 1998; Roy et al., 2007; Borodich, 1999).

An alternative approach to overcome the difficulty of defining dispersion is to reformulate the traditional advection-dispersion equation into fractional advection-dispersion equations, where fractional-order derivatives are used rather than integer-order derivatives (Benson, 1998). Formulating the transport equation in terms of fractional derivatives can account for non-Fickian long-tailed breakthrough curves and improves the simulation of anomalous diffusion (Chen et al., 2010), yet has also proven to be susceptible to scale-dependency problems in three-dimensional natural porous media applications (Lu et al., 2002).

Considering the current limitations of transport modelling, especially in fractured groundwater systems, a fractal groundwater advection-dispersion transport equation is developed to provide a tool to simulate anomalous diffusion in these systems.

Fractal differentiation is discussed in terms of the fractal derivative and the fractal integral. The fractal derivative is commonly used and known, yet the fractal integral is developed in this paper along with the appropriate theorem and proof. The numerical approximation of the fractal derivative and integral are given, where Simpson's 3/8 *Rule* and *Boole's Rule* for numerical integration are applied for the fractal integral. Upon the given foundation, the fractal advection-dispersion transport equation is formulated to develop a new groundwater transport model. The qualitative properties of the new groundwater transport model are investigated to determine boundedness, existence and uniqueness of the solution. To validate the developed fractal advection-dispersion equation, a numerical simulation is performed with different fractal dimensions to demonstrate the applicability of the model to fractal groundwater systems.

## 3.1 Fractal differentiation

### 3.1.1 Fractal derivative

A fractal derivative and conventional integer-order derivative are different in that the integer-order derivative represents the change of a function (dependent variable) with the change of another quantity (independent variable) in ordinary space, while the fractal derivative represents the ratio of change of two quantities in a fractal space. The fractal derivative can be defined by transforming standard integer dimensional space-time $(u, t)$ into fractal time $(u, t^{\alpha})$ (Chen et al., 2010a; Chen et al., 2010b; Cheng, 2016):

$$\frac{\partial u}{\partial t^{\alpha}} = \lim_{t \to t_1} \frac{u(t) - u(t_1)}{t^{\alpha} - t_1^{\alpha}} \qquad \alpha > 0 \tag{3-1}$$

where,

$\alpha$ denotes fractal dimension of time.

Furthermore, the fractal derivative can be defined by transforming the standard dimensional space-time $(u, t)$ into fractal space-time $(u^{\beta}, t^{\alpha})$ (Chen et al., 2010a):

$$\frac{\partial u^{\beta}}{\partial t^{\alpha}} = \lim_{t \to t_1} \frac{u^{\beta}(t) - u^{\beta}(t_1)}{t^{\alpha} - t_1^{\alpha}} \qquad \alpha > 0, \beta > 0 \tag{3-2}$$

where,

$\beta$ denotes fractal dimension of space.

### 3.1.2 Fractal integral

The fractal integral or antiderivative can be determined by considering the fractal time derivative of a function, and assuming that the derivative is known and denoted by a function $u(t)$:

$$\frac{d}{dt^{\alpha}} f(t) = u(t) \tag{3-3}$$

Expanding and approximating the fractal derivative contributes,

$$\frac{f(t) - f(t_1)}{t^{\alpha} - {t_1}^{\alpha}} = u(t) \tag{3-4}$$

Multiply the fractal derivative by a unity,

$$\frac{f(t) - f(t_1)}{t^{\alpha} - {t_1}^{\alpha}} \times \left(\frac{t - t_1}{t - t_1}\right) = u(t) \tag{3-5}$$

Rearrange,

$$\frac{f(t) - f(t_1)}{t - t_1} \times \left(\frac{t - t_1}{t^{\alpha} - {t_1}^{\alpha}}\right) = u(t) \tag{3-6}$$

Recognising the left component is the integer-order derivative ($f'(t)$), and taking the inverse of the inverse,

$$f'(t) \times \left(\frac{1}{\frac{t^{\alpha} - {t_1}^{\alpha}}{t - t_1}}\right) = u(t) \tag{3-7}$$

Simplifying,

$$f'(t) \times \left(\frac{1}{\alpha t^{\alpha - 1}}\right) = u(t) \tag{3-8}$$

Rearranging,

$$f'(t) = \alpha t^{\alpha - 1}\, u(t) \tag{3-9}$$

To further solve Equation (3-9) the Laplace transform ($\mathcal{L}$) is applied,

$$\mathcal{L}\{f'(t)\} = \mathcal{L}\{\alpha t^{\alpha - 1}\, u(t)\} \tag{3-10}$$

Remembering the Laplace transform of an integer-order derivative:

$$s\mathcal{L}\{f(t)\} - f(0) = \mathcal{L}\{\alpha t^{\alpha-1}\, u(t)\} \tag{3-11}$$

Rearranging, simplifying and dividing by the Laplace space ($s$):

$$\mathcal{L}\{f(t)\} = \frac{\alpha}{s}\mathcal{L}\{t^{\alpha-1}\, u(t)\} + \frac{f(0)}{s} \tag{3-12}$$

The inverse Laplace transform is applied to convert back from the Laplace domain:

$$\mathcal{L}^{-1}[\mathcal{L}\{f(t)\}] = \mathcal{L}^{-1}\left[\frac{\alpha}{s}\mathcal{L}\{t^{\alpha-1}\, u(t)\} + \frac{f(0)}{s}\right] \tag{3-13}$$

The convolution theorem provides the inverse transform of the product of two transforms. Considering two functions $f$ and $g$, which are piecewise continuous on $t \geq 0$, the Laplace transform is (Logan, 2006):

$$\mathcal{L}(f * g)(s) = F(s)G(s) \tag{3-14}$$

The convolution of $f$ and $g$ is:

$$(f * g)(t) \equiv \int_0^t f(\tau)\, g(t-\tau)\, d\tau \tag{3-15}$$

and, the inverse Laplace transform is thus:

$$\mathcal{L}^{-1}(FG)(s) = (f * g)(t) \tag{3-16}$$

The Laplace transform is additive, but not multiplicative. This means that the Laplace transform of a product is not the product of the Laplace transforms. The convolution theorem gives the transform required to get a product of Laplace transforms, i.e. the convolution (Logan, 2006). Applying the convolution theorem to Equation (3-13):

$$f(t) = \alpha \int_0^t \tau^{\alpha-1}\, f(\tau)\, d\tau \; + \; f(0) \tag{3-17}$$

Thus, the fractal integral can be defined as:

$$ {}_0^F I_t^\alpha\, f(t) = \alpha \int_0^t \tau^{\alpha-1}\, f(\tau)\, d\tau \tag{3-18}$$

**Theorem:** Let the function $(f)$ be differentiable in an open interval $I$. Then the fractal integral of the function $(f)$ is given as:

$$ {}_0^F I_t^\alpha\, f(t) = \alpha \int_0^t \tau^{\alpha-1}\, f(\tau)\, d\tau \tag{3-19}$$

**Proof:** ${}_0^F I_t^\alpha \left(\frac{d}{dt^\alpha} f(t)\right) = f(t) - f(0)$

Consider the definition of the fractal integral (Equation (3-19) for a fractal-order derivative function:

$$ {}_{0}^{F}I_{t}^{\alpha}\left(\frac{d}{dt^{\alpha}}f(t)\right) = \alpha\int_{0}^{t}\tau^{\alpha-1}\,\frac{d}{d\tau^{\alpha}}f(\tau)\,d\tau \tag{3-20}$$

Remembering that the fractal derivative can be expressed as $\frac{d}{dt^{\alpha}}f(t) = f'(t)\left(\frac{1}{\alpha t^{\alpha-1}}\right)$ (Equations ((3-4) to (3-8)):

$$ {}_{0}^{F}I_{t}^{\alpha}\left(\frac{d}{dt^{\alpha}}f(t)\right) = \alpha\int_{0}^{t}\tau^{\alpha-1}f^{'}(\tau)\left(\frac{1}{\alpha\tau^{\alpha-1}}\right)\,d\tau \tag{3-21}$$

Simplifying,

$$ {}_{0}^{F}I_{t}^{\alpha}\left(\frac{d}{dt^{\alpha}}f(t)\right) = \int_{0}^{t}f^{'}(\tau)\,d\tau \tag{3-22}$$

Applying the integral from $t$ to 0:

$$ {}_{0}^{F}I_{t}^{\alpha}\left(\frac{d}{dt^{\alpha}}f(t)\right) = f(t) - f(0) \tag{3-23}$$

Secondly, the following is considered for the proof $\frac{d}{dt^{\alpha}}\left({}_{0}^{F}I_{t}^{\alpha}f(t)\right) = f(t)$

Let the new function $F$ be defined as $F(t) = {}_{0}^{F}I_{t}^{\alpha}f(t)$:

$$\frac{d}{dt^{\alpha}}\,{}_{0}^{F}I_{t}^{\alpha}\,f(t) = \frac{d}{dt^{\alpha}}F(t) \tag{3-24}$$

Applying the definition of a fractal derivative (Equation (3-1)):

$$\frac{d}{dt^{\alpha}}F(t) = \lim_{t\to t_1}\frac{F(t) - F(t_1)}{t^{\alpha} - t_1^{\alpha}} \tag{3-25}$$

Remembering that the fractal derivative can be expressed as $\frac{d}{dt^{\alpha}}f(t) = f'(t)\left(\frac{1}{\alpha t^{\alpha-1}}\right)$ (Equations (3-4) to (3-8)):

$$\frac{d}{dt^{\alpha}}F(t) = F^{'}(t)\left(\frac{1}{\alpha t^{\alpha-1}}\right) \tag{3-26}$$

Substituting back the new function $F$, where $F(t) = {}_{0}^{F}I_{t}^{\alpha}f(t)$, and and $F' = \frac{d}{dt}$

$$\frac{d}{dt^{\alpha}}F(t) = \frac{d}{dt}\left({}_{0}^{F}I_{t}^{\alpha}f(t)\right)\left(\frac{1}{\alpha t^{\alpha-1}}\right) \tag{3-27}$$

Consider the definition of the fractal integral (Equation (3-19)):

$$\frac{d}{dt^{\alpha}}\,{}_{0}^{F}I_{t}^{\alpha}\,f(t) = \frac{d}{dt}\left(\alpha\int_{0}^{t}\tau^{\alpha-1}\,f(\tau)\,d\tau\right)\left(\frac{1}{\alpha t^{\alpha-1}}\right) \tag{3-28}$$

Simplifying using the fact that $\frac{d}{dt}\left(\int_0^t f(\tau)\, d\tau\right) = f(t)$:

$$\frac{d}{dt^{\alpha}}\, {}_0^F I_t^{\alpha}\, f(t) = \alpha t^{\alpha-1}\, f(t) \left(\frac{1}{\alpha t^{\alpha-1}}\right) \tag{3-29}$$
$$= f(t)$$

This completes the proof.

## 3.2 New groundwater transport model in a fractured aquifer with self-similarities

Groundwater transport within a fractured aquifer with a fractal nature exhibiting self-similarity cannot be accurately simulated by the classical Fickian advection-dispersion transport equation due to: 1) lack of a detailed characterisation of the fracture network and heterogeneity of the system, and 2) the occurrence of subdiffusion and superdiffusion (limitation of the mathematical formulation). Because the information to characterise such a system to an appropriate level of detail is often not available, and the advection-dispersion equation cannot account for anomalous diffusion, most applications fail to accurately simulate the observed contaminant transport.

The limitations of the classical advection-dispersion equation have motivated alternative *non-local* conceptualisations of flow and transport, and various methods for addressing scale and space-time dependencies. Unconventional methods include stochastic averaging of the classical advection-dispersion equation, multiple-rate mass transfer method, continuous time random walk method, time fractional advection-dispersion equation method, space fractional advection-dispersion equation method, and others (Zhang et al., 2009). In these alternative methods, the dispersive state is allowed to vary between superdiffusion, subdiffusion and normal diffusion, termed *transient dispersion* (Sun et al., 2014). Yet, each method is formulated for a specific transition and thus might not be appropriate for all types of *transient dispersion*. The fractional advection-dispersion equation formulations have proven successful in describing non-Fickian transport, but three-dimensional applications have been found to also show scale-dependent dispersivity problems (Lu et al., 2002; Huang et al., 2006).

Anomalous behaviour has been recorded in unsaturated flow systems, defined by Richard's equation, in heterogeneous systems of preferential pathways in soil, where the development of a horizontal wetting front deviates from the Boltzmann scaling (anomalous Boltzmann scaling) in a similar manner to how groundwater transport deviates from the Fickian model for diffusion (anomalous diffusion) (Gerolymatou et al., 2006; Hall, 2007). Sun et al. (2013) developed a fractal Richard's equation to model unsaturated flow in heterogeneous soils that exhibit anomalous Boltzmann scaling. The fractal Richard's equation was able to model the full range of observed non-Boltzmann behaviour, from subdiffusion to superdiffusion, which is related to the well-established fractal model for soils (Rieu and Sposito, 1991; Tyler and Wheatcraft, 1990).

In response to the current limitations of groundwater transport modelling in fractured systems and the success of the fractal Richard's equation, a fractal groundwater advection-dispersion transport equation is deemed a suitable and meaningful investigation. A fractal advection-dispersion equation has the potential to provide the same advantages as the proven fractal Richard's equation, where a fractal model could simulate the full range of observed non-Fickian behaviour, from subdiffusion to superdiffusion, which is related to the well-established fractal model for fractured systems without the detailed characterisation of the heterogeneity of the system. This formulation of a fractal advection-dispersion equation has not been developed previously because there was no definition of a fractal integral. Now however, with the developed definition of the fractal integral (proven with a theorem and proofs in Section 3.1.2, it is possible and described in detail in the following section.

### 3.2.1 Fractal formulation of the advection-dispersion transport equation

The effects of self-similarity inherent in groundwater transport with preferential pathways formed by fractures are included by incorporating a fractal space component into the mathematical formulation of the one dimensional advection-dispersion equation:

$$\frac{\partial}{\partial t}c(x,t) = -v_x\frac{\partial}{\partial x^\alpha}c(x,t) + D_L\frac{\partial}{\partial x^\alpha}\left[\frac{\partial}{\partial x^\alpha}c(x,t)\right] \tag{3-30}$$

To express the fractal ADE in terms of integer-order dimensions, the defined property of the fractal derivative $\frac{d}{dt^\alpha}f(t) = f'(t)\left(\frac{1}{\alpha t^{\alpha-1}}\right)$ (Equations (3-4) to (3-8)) is considered:

$$\frac{\partial}{\partial x^\alpha}c(x,t) = \frac{\partial}{\partial x}c(x,t)\cdot\left(\frac{1}{\alpha x^{\alpha-1}}\right) \tag{3-31}$$

Rearranging,

$$\frac{\partial}{\partial x^\alpha}c(x,t) = \frac{\partial}{\partial x}c(x,t)\cdot\left(\frac{x^{1-\alpha}}{\alpha}\right) \tag{3-32}$$

Without the loss of generality, the advection transport term of the fractal advection-dispersion (Equation (3-30)) is considered:

$$-v_x\frac{\partial}{\partial x^\alpha}c(x,t) = -v_x\frac{\partial}{\partial x}c(x,t)\cdot\left(\frac{x^{1-\alpha}}{\alpha}\right) \tag{3-33}$$

Now, the dispersion transport term of the fractal advection-dispersion (Equation (3-30)) is considered, and the defined property of the fractal derivative $\frac{d}{dt^\alpha}f(t) = f'(t)\left(\frac{1}{\alpha t^{\alpha-1}}\right)$ (Equations (3-4) to (3-8) is applied:

$$D_L\frac{\partial}{\partial x^\alpha}\left[\frac{\partial}{\partial x^\alpha}c(x,t)\right] = D_L\frac{\partial}{\partial x^\alpha}\left[\frac{\partial}{\partial x}c(x,t)\left(\frac{1}{\alpha x^{\alpha-1}}\right)\right] \tag{3-34}$$

Let $\left[\frac{\partial}{\partial x}c(x,t)\left(\frac{1}{\alpha t^{\alpha-1}}\right)\right]$ be equal to a function $F(x)$:

$$D_L \frac{\partial}{\partial x^\alpha}\left[\frac{\partial}{\partial x^\alpha} c(x,t)\right] = D_L \frac{\partial}{\partial x^\alpha}[F(x)] \tag{3-35}$$

Applying the defined property of the fractal derivative $\frac{d}{dt^\alpha} f(t) = f'(t)\left(\frac{1}{\alpha t^{\alpha-1}}\right)$ (Equations (3-4) to (3-8)) again to remove the second fractal derivative,

$$D_L \frac{\partial}{\partial x^\alpha}\left[\frac{\partial}{\partial x^\alpha} c(x,t)\right] = D_L\, F'(x)\left(\frac{1}{\alpha x^{\alpha-1}}\right) \tag{3-36}$$

Applying the product rule $(h(x) = f(x)g(x); then\ h'(x) = f'(x)g(x) + f(x)g'(x))$ to determine $\frac{\partial}{\partial x} F(x)$:

$$\begin{aligned} F'(x) &= \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} c(x,t)\right)\left(\frac{1}{\alpha x^{\alpha-1}}\right) + \frac{\partial}{\partial x} c(x,t)\left(\frac{\partial}{\partial x}\left(\frac{1}{\alpha x^{\alpha-1}}\right)\right) \\ &= \frac{\partial^2}{\partial x^2} c(x,t)\left(\frac{x^{1-\alpha}}{\alpha}\right) + \frac{\partial}{\partial x} c(x,t)\left(\frac{1-\alpha}{\alpha} x^{-\alpha}\right) \end{aligned} \tag{3-37}$$

Substituting back into the function $F(x)$ (Equation (3-36)):

$$\begin{aligned} D_L \frac{\partial}{\partial x^\alpha}\left[\frac{\partial}{\partial x^\alpha} c(x,t)\right] &= D_L \left(\frac{\partial^2}{\partial x^2} c(x,t)\left(\frac{x^{1-\alpha}}{\alpha}\right) + \frac{\partial}{\partial x} c(x,t)\left(\frac{1-\alpha}{\alpha} x^{-\alpha}\right)\right)\left(\frac{x^{1-\alpha}}{\alpha}\right) \\ &= D_L \left(\frac{\partial^2}{\partial x^2} c(x,t) \cdot \frac{x^{2-2\alpha}}{\alpha^2} + \frac{(1-\alpha)}{\alpha} x^{1-2\alpha} \cdot \frac{\partial}{\partial x} c(x,t)\right) \end{aligned} \tag{3-38}$$

Substituting the advection (Equation (3-32)) and dispersion (Equation (3-38)) terms back into the one-dimensional fractal (space) advection-dispersion equation (Equation (3-30)):

$$\frac{\partial}{\partial t} c(x,t) = -v_x \frac{\partial}{\partial x} c(x,t) \cdot \left(\frac{x^{1-\alpha}}{\alpha}\right) + D_L \frac{\partial^2}{\partial x^2} c(x,t) \cdot \frac{x^{2-2\alpha}}{\alpha^2} + D_L \frac{(1-\alpha)}{\alpha} x^{1-2\alpha} \cdot \frac{\partial}{\partial x} c(x,t) \tag{3-39}$$

Factorising,

$$\frac{\partial}{\partial t} c(x,t) = \left(-v_x \cdot \left(\frac{x^{1-\alpha}}{\alpha}\right) + D_L \frac{(1-\alpha)}{\alpha} x^{1-2\alpha}\right)\frac{\partial}{\partial x} c(x,t) + \left(D_L \cdot \frac{x^{2-2\alpha}}{\alpha^2}\right)\frac{\partial^2}{\partial x^2} c(x,t) \tag{3-40}$$

Let a function $V_F^\alpha(x) = -v_x \cdot \left(\frac{x^{1-\alpha}}{\alpha}\right) + D_L \frac{(1-\alpha)}{\alpha} x^{1-2\alpha}$, and function $D_F^\alpha(x) = D_L \cdot \frac{x^{2-2\alpha}}{\alpha^2}$:

$$\frac{\partial}{\partial t} c(x,t) = V_F^\alpha(x) \frac{\partial}{\partial x} c(x,t) + D_F^\alpha(x) \frac{\partial^2}{\partial x^2} c(x,t) \tag{3-41}$$

where,

$V_F^\alpha(x)$ is the velocity with fractal dimension with respect to $x$, and
$D_F^\alpha(x)$ is the dispersion coefficient with fractal dimension with respect to $x$.

Equation (3-41) is the developed new transport model called the fractal (space) advection dispersion equation (FADE). The FADE equation resembles the traditional advection-dispersion equation, yet the newly defined velocity and dispersion coefficients ($V_F^\alpha(x)$ and $D_F^\alpha(x)$) have fractal dimensions with respect to $x$.

**Remark:** The fractal advection-dispersion equation should return to the classical formulation of the advection-dispersion equation when $\alpha = 1$, to be valid.

Considering the fractal dimension velocity term ($\alpha = 1$):

$$\begin{aligned} V_F^\alpha(x) &= D_L \frac{(1-\alpha)}{\alpha^2} x^{2-\alpha} - v_x \cdot \left(\frac{x^{1-\alpha}}{\alpha}\right) \\ &= -v_x \end{aligned} \tag{3-42}$$

Considering the fractal dimension dispersion term ($\alpha = 1$):

$$\begin{aligned} D_F^\alpha(x) &= D_L \cdot \frac{x^{1-\alpha}}{\alpha^2} \\ &= D_L \end{aligned} \tag{3-43}$$

When $\alpha = 1$, the fractal advection-dispersion equation reverts to the classical formulation of the advection-dispersion equation, and thus can be considered valid. To further validate the developed fractal advection-dispersion equation, the qualitative properties of the formulation are investigated in the following section.4

### 3.2.2 Qualitative properties

The qualitative properties of boundedness, existence and uniqueness for the developed fractal advection-dispersion equation are presented, using the Picard-Lindelöf theorem.

**Lipschitz condition boundedness for partial differential**

The Lipschitz condition is used for a bound on the modulus of continuity for a function. A function $f$ satisfies a Lipschitz condition on a set $B$, if there is a constant $M \geq 0$, such that:

$$\|f(t,u) - f(t,v)\| \leq M\|u - v\| \tag{3-44}$$

for all $(t,u),(t,v) \in B$.

A function that has a bounded first derivative is considered Lipschitz, and this has been assumed true for partial differential operators. A theorem and proof are proposed here for the partial differential equations.

**Theorem**: Let $B$ be a set of non-zero differentiable functions, such that $f, g \in B$ and $\left\|\frac{\partial}{\partial x} g\right\| < M < \infty$. For $f, g \in B$:

$$\left\|\frac{\partial}{\partial x}f - \frac{\partial}{\partial x}g\right\| \leq k\|f-g\| \tag{3-45}$$

**Proof**: Let $f, g \in B$, such that that $f \neq g$, then

$$\left\|\frac{\partial}{\partial x}f - \frac{\partial}{\partial x}g\right\| = \left\|\frac{\partial}{\partial x}(f-g)\right\| \tag{3-46}$$

Since $f, g \in B$, and similarly $f - g \in B$, then by assumption a positive constant $M$ can be found, such that

$$\left\|\frac{\partial}{\partial x}(f-g)\right\| < M \tag{3-47}$$

And, multiplying by $\frac{\|f-g\|}{\|f-g\|}$

$$\left\|\frac{\partial}{\partial x}(f-g)\right\| < M\frac{\|f-g\|}{\|f-g\|}$$
$$\left\|\frac{\partial}{\partial x}(f-g)\right\| < \frac{M}{\|f-g\|}\cdot\|f-g\| \tag{3-48}$$

Let $\frac{M}{\|f-g\|} = k$,

$$\left\|\frac{\partial}{\partial x}(f-g)\right\| < k\|f-g\| \tag{3-49}$$

This completes the proof.

**Fixed-point theorem for existence and uniqueness**

An integral is applied to both sides of the fractal transport equation (Equation (3-41)), to obtain:

$$c(x,t) - c(x,0) = \int_0^t \left\{V_F^\alpha(x)\frac{\partial}{\partial x}c(x,\tau) + D_F^\alpha(x)\frac{\partial^2}{\partial x^2}c(x,\tau)\right\}d\tau \tag{3-50}$$

Let a new function $FC(x,t)$ be expressed as:

$$FC(x,t) = \int_0^t \left\{V_F^\alpha(x)\frac{\partial}{\partial x}c(x,\tau) + D_F^\alpha(x)\frac{\partial^2}{\partial x^2}c(x,\tau)\right\}d\tau \tag{3-51}$$

and, state the Lipschitz condition (Equation (3-44)):

$$\|FC_1(x,t) - FC_2(x,t)\| < k\|c_1(x,t) - c_2(x,t)\| \tag{3-52}$$

Without the loss of generality, consider the term left of the inequality sign, and substitute the function $FC(x,t)$:

$$\|FC_1(x,t) - FC_2(x,t)\| = \left\| \begin{array}{l} \int_0^t \left\{ V_F^\alpha(x) \frac{\partial}{\partial x} c_1(x,\tau) + \ D_F^\alpha(x) \frac{\partial^2}{\partial x^2} c_1(x,\tau) \right\} d\tau \\ - \int_0^t \left\{ V_F^\alpha(x) \frac{\partial}{\partial x} c_2(x,\tau) + \ D_F^\alpha(x) \frac{\partial^2}{\partial x^2} c_2(x,\tau) \right\} d\tau \end{array} \right\| \tag{3-53}$$

Simplifying and factorising,

$$\|FC_1(x,t) - FC_2(x,t)\| = \left\| \begin{array}{l} \int_0^t \left\{ V_F^\alpha(x) \frac{\partial}{\partial x} (c_1(x,\tau) - c_2(x,\tau) \right\} d\tau \\ + \int_0^t \left\{ D_F^\alpha(x) \frac{\partial^2}{\partial x^2} (c_1(x,\tau) - c_2(x,\tau) \right\} d\tau \end{array} \right\| \tag{3-54}$$

Applying the triangular inequality,

$$\begin{aligned} \|FC_1(x,t) - FC_2(x,t)\| \leq & \left\| \int_0^t \left\{ V_F^\alpha(x) \frac{\partial}{\partial x} (c_1(x,\tau) - c_2(x,\tau) \right\} d\tau \right\| \\ & + \left\| \int_0^t \left\{ D_F^\alpha(x) \frac{\partial^2}{\partial x^2} (c_1(x,\tau) - c_2(x,\tau) \right\} d\tau \right\| \end{aligned} \tag{3-55}$$

And, remembering $\left\| \int_0^t f(x) \right\| \leq \int_0^t \|f(x)\| dx$,

$$\begin{aligned} \|FC_1(x,t) - FC_2(x,t)\| \leq & \int_0^t \|V_F^\alpha(x)\| \left\| \frac{\partial}{\partial x} (c_1(x,\tau) - c_2(x,\tau) \right\| d\tau \\ & + \int_0^t \|D_F^\alpha(x)\| \left\| \frac{\partial^2}{\partial x^2} (c_1(x,\tau) - c_2(x,\tau) \right\| d\tau \end{aligned} \tag{3-56}$$

Applying the presented theorem for *Lipschitz condition boundedness for partial differential*,

$$\begin{aligned} \|FC_1(x,t) - FC_2(x,t)\| \leq & \|V_F^\alpha(x)\| \, \theta_1 \|(c_1(x,\tau) - c_2(x,\tau)\| \int_0^t d\tau \\ & + \|D_F^\alpha(x)\| \, \theta_2^2 \|(c_1(x,\tau) - c_2(x,\tau)\| \int_0^t d\tau \\ \leq & \{\|V_F^\alpha(x)\| \, \theta_1 \, T_{max} + \|D_F^\alpha(x)\| \, \theta_2^2 \, T_{max}\} \, \|(c_1(x,\tau) - c_2(x,\tau)\| \end{aligned} \tag{3-57}$$

Let $\|V_F^\alpha(x)\| \, \theta_1 \, T_{max} + \|D_F^\alpha(x)\| \, \theta_2^2 \, T_{max} = K$,

$$\|FC_1(x,t) - FC_2(x,t)\| \leq K \|(c_1(x,\tau) - c_2(x,\tau)\| \tag{3-58}$$

Thus, the fractal transport equation does uphold the Lipschitz condition.

To facilitate the evaluation of the fractal transport equation, a new function is introduced

$$\mathcal{F}(x,t,c(x,t)) = V_F^\alpha(x) \frac{\partial}{\partial x} c(x,t) + \ D_F^\alpha(x) \frac{\partial^2}{\partial x^2} c(x,t) \tag{3-59}$$

such that,

$$\frac{\partial}{\partial t} c(x,t) = \mathcal{F}(x,t,c(x,t) \tag{3-60}$$

Integrating on both sides of Equation (3-60),

$$c(x,t) = c(x,0) + \int_0^t \mathcal{F}(x,\tau,c(x,\tau))\, d\tau \tag{3-61}$$

A set is created in which to evaluate the fractal transport equation,

$$A_{a,b} = \overline{T_a(t_0)} \times \overline{Y_b(c_0)} \tag{3-62}$$

where,

$\overline{T_a(t_0)} = (t_0 - a, t_0 + a)$, and

$\overline{Y_b(c_0)} = (c_0 - b, c_0 + b)$.

The Banach fixed-point theorem is applied by introducing the norm of the supremum (statistical limit of a set) for $c(Y_b(c_0), T_a(t_0))$ denoted as $\varphi$,

$$\|\varphi\|_\infty = \sup_{A_{a,b}} |\varphi(b)| \tag{3-63}$$

Let $A_{a,b}$ be a set where, $F: A_{a,b} \rightarrow A_{a,b}$, such that

$$F\varphi = c_0 + \int_0^t \mathcal{F}(x,\tau,c(x,\tau))\, d\tau \tag{3-64}$$

Remembering the physical meaning of the fractal advection dispersion equation and the nature of groundwater transport, the spatial component $(b)$ of an aquifer domain is such that the simulated plume when the initial concentration source is removed cannot be greater than the aquifer total extent:

$$\|F\varphi - c_0\| \leq b \tag{3-65}$$

Now that the domain of the equation is defined, let us consider the following sequence:

$$\begin{gathered} c_{n+1}(x,t) = Fc_n(x,t) \\ \|c_{n+1} - c_n\|_\infty = \|Fc_n(x,t) - Fc_{n-1}(x,t)\|_\infty \end{gathered} \tag{3-66}$$

Equation (3-50) to Equation (3-58) proves that

$$\|Fc_n(x,t) - Fc_{n-1}(x,t)\|_\infty \leq K\|(c_n(x,t) - c_{n-1}(x,t)\|_\infty \tag{3-67}$$

and it follows that

$$\begin{aligned} \|Fc_{n-1}(x,t) - Fc_{n-2}(x,t)\|_\infty &\leq K^2\|(c_{n-1}(x,t) - c_{n-2}(x,t)\|_\infty \\ &\leq K^3\|(c_{n-3}(x,t) - c_{n-4}(x,t)\|_\infty \\ &\;\;\dots \\ &\leq K^n\|(c_1(x,t) - c_0(x,t)\|_\infty \end{aligned} \tag{3-68}$$

with $K < 1$, then

$$\lim_{n\to\infty} \|c_{n+1} - c_n\|_\infty < \lim_{n\to\infty} K^n\|(c_1(x,t) - c_0(x,t)\|_\infty \tag{3-69}$$

Thus, $(c_{n+1})_{n\in\mathbb{N}}$ is Cauchy in complex space. Then $Fc_n$ has a fixed point using the Banach fixed point theorem and the fractal transport advection dispersion equation has a unique solution.

## 3.3 Numerical approximation methods (fractal derivative)

The formulation of the fractal advection-dispersion equation has been proven to be bounded, exist and unique. Accordingly, numerical approximation methods for the developed fractal (space) advection-dispersion equation are provided for the solution of the new model. The fractal derivative is a local operator that allows for the application of traditional finite difference approximation methods for time and space. The numerical approximation makes use of the traditional explicit forward finite difference method, as well as the Crank-Nicolson finite difference method for the fractal derivative formulation. The numerical stability of these numerical solutions are investigated. In the following section, the numerical approximation for the fractal integral formulation makes use of the Simpson's 3/8 and Boole's numerical integration rules.

### 3.3.1 Forward finite difference scheme

Explicit forward difference in time and space, and the second-order approximation are applied to Equation (3-41):

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = V_F^\alpha \frac{c_{i+1}^n - c_i^n}{\Delta x} + D_F^\alpha \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2} \tag{3-70}$$

where,

$i$ denotes one-dimensional grid-centered framework with conventional unit vector ($\boldsymbol{i}$),

$V_F^\alpha$ is the fractal dimension velocity term, and

$D_F^\alpha$ is the fractal dimension dispersion term.

Rearranging,

$$\frac{c_i^{n+1}}{\Delta t} = \left(\frac{1}{\Delta t} - \frac{V_F^\alpha}{\Delta x} - \frac{2D_F^\alpha}{(\Delta x)^2}\right) c_i^n + \left(\frac{V_F^\alpha}{\Delta x} + \frac{D_F^\alpha}{(\Delta x)^2}\right) c_{i+1}^n + \left(\frac{D_F^\alpha}{(\Delta x)^2}\right) c_{i-1}^n \tag{3-71}$$

Simplifying by using constants $a_2$, $b_2$, $c_2$, and $d_2$

$$a_2 c_i^{n+1} = b_2 c_i^n + c_2 c_{i+1}^n + d_2 c_{i-1}^n \tag{3-72}$$

where,

$$a_2 = \frac{1}{\Delta t}$$
$$b_2 = \frac{1}{\Delta t} - \frac{V_F^\alpha}{\Delta x} - \frac{2D_F^\alpha}{(\Delta x)^2}$$
$$c_2 = \frac{V_F^\alpha}{\Delta x} + \frac{D_F^\alpha}{(\Delta x)^2}$$
$$d_2 = \frac{D_F^\alpha}{(\Delta x)^2}$$

Equation (3-72) is the traditional explicit finite difference approximation of the fractal (space) advection-dispersion equation.

A finite difference scheme is considered stable if the errors incurred at a discrete time step are not propagated throughout the simulation. A *Von Neumann* stability analysis is performed to evaluate the stability of the finite difference schemes applied to the fractal advection-dispersion equation. The error incurred in the numerical approximation can be defined as:

$$\lambda_i^k = N_i^k - c_i^k \tag{3-73}$$

where,

$\lambda_i^k$ is the approximation or round-off error,
$N_i^k$ is the numerical solution, and
$c_i^k$ is the exact solution.

Considering Equation (3-72) in terms of the recurrence relation for the error:

$$a_2\lambda_i^{k+1} = b_2\lambda_i^k + c_2\lambda_{i+1}^k + d_2\lambda_{i-1}^k \tag{3-74}$$

The error for each discrete point in time and space has been determined as:

$$\lambda_i^{k+1} = e^{a(t+\Delta t)}e^{jkx} \tag{3-75}$$

$$\lambda_i^k = e^{at}e^{jkx} \tag{3-76}$$

$$\lambda_{i+1}^k = e^{at}e^{jk(x+\Delta x)} \tag{3-77}$$

$$\lambda_{i-1}^k = e^{at}e^{jk(x-\Delta x)} \tag{3-78}$$

Substituting back into Equation (3-74):

$$a_2e^{a(t+\Delta t)}e^{jkx} = b_2e^{at}e^{jkx} + c_2e^{at}e^{jk(x+\Delta x)} + d_2e^{at}e^{jk(x-\Delta x)} \tag{3-79}$$

Expanding,

$$a_2e^{at}e^{a\Delta t}e^{jkx} = b_2e^{at}e^{jkx} + c_2e^{at}e^{jkx}e^{jk\Delta x} + d_2e^{at}e^{jkx}e^{-jk\Delta x} \tag{3-80}$$

Simplifying and rearranging,

$$e^{a\Delta t} = \frac{b_2}{a_2} + \frac{c_2}{a_2}e^{jk\Delta x} + \frac{d_2}{a_2}e^{-jk\Delta x} \tag{3-81}$$

The amplification factor ($G$) can be defined as:

$$G = \frac{\lambda_i^{k+1}}{\lambda_i^k} = \frac{e^{a(t+\Delta t)}e^{jkx}}{e^{at}e^{jkx}} = e^{a\Delta t} \tag{3-82}$$

where, for the solution to remain bounded the condition $|G| \leq 1$.

Thus, Equation (3-81) expresses the stability criteria for the forward finite difference scheme applied to the fractal advection-dispersion equation, where $\left|e^{a\Delta t}\right| \leq 1$, and remembering that $a_2 = \frac{1}{\Delta t}$:

$$e^{a\Delta t} = \Delta t b_2 + \Delta t c_2 e^{jk\Delta x} + \Delta t d_2 e^{-jk\Delta x} \tag{3-83}$$

Applying known identities and the absolute value of a complex number:

$$\left|e^{a\Delta t}\right| = \sqrt{[\Delta t b_1 + \Delta t c_1\{\cos(k\Delta x) + j\sin(k\Delta x)\}]^2 + [\Delta t d_1\{\cos(k\Delta x) - j\sin(k\Delta x)\}]^2} \leq 1 \quad (3\text{-}84)$$

Equation (3-84) is an expression of the stability criteria for Equation (3-70).

### 3.3.2 Crank-Nicolson finite difference scheme

The Crank-Nicolson finite difference scheme is applied to Equation (3-30):

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = 0.5\left(V_F^\alpha \frac{c_{i+1}^n - c_i^n}{\Delta x} + D_F^\alpha \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2}\right) + 0.5\left(V_F^\alpha \frac{c_{i+1}^{k+1} - c_i^{k+1}}{\Delta x} + D_F^\alpha \frac{c_{i+1}^{k+1} - 2c_i^{k+1} + c_{i-1}^{k+1}}{(\Delta x)^2}\right) \quad (3\text{-}85)$$

Rearranging,

$$c_i^{n+1}\left(\frac{1}{\Delta t} - 0.5\left(-\frac{V_F^\alpha}{\Delta x} - \frac{2D_F^\alpha}{(\Delta x)^2}\right)\right) = 0.5\left(\frac{1}{\Delta t} - \frac{V_F^\alpha}{\Delta x} - \frac{2D_F^\alpha}{(\Delta x)^2}\right)c_i^n + 0.5\left(\frac{V_F^\alpha}{\Delta x} + \frac{D_F^\alpha}{(\Delta x)^2}\right)c_{i+1}^n + 0.5\left(\frac{D_F^\alpha}{(\Delta x)^2}\right)c_{i-1}^n + 0.5\left(\frac{V_F^\alpha}{\Delta x} + \frac{D_F^\alpha}{(\Delta x)^2}\right)c_{i+1}^{n+1} + 0.5\left(\frac{D_F^\alpha}{(\Delta x)^2}\right)c_{i-1}^{n+1} \quad (3\text{-}86)$$

Simplifying by using constants $e_2$, $b_2$, $c_2$, and $d_2$

$$e_2 c_i^{n+1} = b_2 c_i^n + c_2 c_{i+1}^n + d_2 c_{i-1}^n + c_2 c_{i+1}^{n+1} + d_2 c_{i-1}^{n+1} \quad (3\text{-}87)$$

where,

$$e_2 = \frac{1}{\Delta t} - 0.5\left(-\frac{V_F^\alpha}{\Delta x} - \frac{2D_F^\alpha}{(\Delta x)^2}\right)$$

Equation (3-87) is the Crank-Nicolson finite difference approximation of the fractal (space) advection-dispersion equation.

A *Von Neumann* stability analysis is performed to evaluate the stability of the Crank-Nicolson finite difference approximation applied to Equation (3-87), remembering Equations (3-75) to (3-78), and additionally:

$$\lambda_{i+1}^{k+1} = e^{a(t+\Delta t)} e^{jk(x+\Delta x)} \quad (3\text{-}88)$$

$$\lambda_{i-1}^{k+1} = e^{a(t+\Delta t)} e^{jk(x-\Delta x)} \quad (3\text{-}89)$$

To obtain:

$$e_2 e^{a(t+\Delta t)} e^{jkx} = b_2 e^{at} e^{jkx} + c_2 e^{at} e^{jk(x+\Delta x)} + d_2 e^{at} e^{jk(x-\Delta x)} + c_2 e^{a(t+\Delta t)} e^{jk(x+\Delta x)} + d_2 e^{a(t+\Delta t)} e^{jk(x-\Delta x)} \quad (3\text{-}90)$$

Expanding,

$$e_2 e^{at} e^{a\Delta t} e^{jkx} = b_2 e^{at} e^{jkx} + c_2 e^{at} e^{jkx} e^{jk\Delta x} + d_2 e^{at} e^{jkx} e^{-jk\Delta x} + c_2 e^{at} e^{a\Delta t} e^{jkx} e^{jk\Delta x} + d_2 e^{at} e^{a\Delta t} e^{jkx} e^{-jk\Delta x} \quad (3\text{-}91)$$

Simplifying and rearranging,

$$e^{a\Delta t} = \frac{b_2 + c_2 e^{jk\Delta x} + d_2 e^{-jk\Delta x}}{(e_2 - c_2 e^{jk\Delta x} - d_2 e^{-jk\Delta x})} \quad (3\text{-}92)$$

Applying known identities, simplifying and applying the absolute value of a complex number, where $z = a + ib$ and $|z| = \sqrt{a^2 + b^2}$:

$$\left|e^{a\Delta t}\right| = \frac{\sqrt{[b_2 + (c_2 + d_2)\cos(k\Delta x)]^2 + [(c_1 - d_2)\sin(k\Delta x)]^2}}{\sqrt{[e_2 - (c_2 + d_2)\cos(k\Delta x)]^2 + [(c_1 - d_2)\sin(k\Delta x)]^2}} \leq 1 \quad (3\text{-}93)$$

where,

$$\sqrt{[b_2 + (c_2 + d_2)\cos(k\Delta x)]^2 + [(c_2 - d_2)\sin(k\Delta x)]^2} \leq \sqrt{[e_2 - (c_2 + d_2)\cos(k\Delta x)]^2 + [(c_2 - d_2)\sin(k\Delta x)]^2} \quad (3\text{-}94)$$

Simplifying,

$$\cos(k\Delta x) \leq \frac{e_2 - b_2}{2(c_2 + d_2)} \quad (3\text{-}95)$$

Equation (3-95) is an expression of the stability criteria for Equation (3-85).

## 3.4 Numerical integration methods (fractal integral)

The fractal derivative is a local operator, and thus the numerical solution of fractal derivative equations can be approximated using standard numerical techniques for the integer-order derivative equations (Chen et al., 2010a).

The fractal advection-dispersion equation (Equation (3-41)) is converted to an integral formulation by applying the integral to both sides:

$$\int_0^t \frac{\partial}{\partial \tau} c(x,\tau) = \int_0^t \left( V_F^\alpha \frac{\partial}{\partial x} c(x,\tau) + D_F^\alpha \frac{\partial^2}{\partial x^2} c(x,\tau) \right) \quad (3\text{-}96)$$

Applying the integral to the time derivative,

$$c(x,t) - c(x,0) = \int_0^t \left( V_F^\alpha \frac{\partial}{\partial x} c(x,\tau) + D_F^\alpha \frac{\partial^2}{\partial x^2} c(x,\tau) \right) \quad (3\text{-}97)$$

Rearranging,

$$c(x,t) = c(x,0) + \int_0^t \left( V_F^\alpha \frac{\partial}{\partial x} c(x,\tau) + D_F^\alpha \frac{\partial^2}{\partial x^2} c(x,\tau) \right) \quad (3\text{-}98)$$

To facilitate the numerical integration of the fractal advection and dispersion terms, let $F\big(x,\tau,C(x,\tau)\big)$ be equal to the integral of the advection and dispersion terms, where $F\big(x,\tau,c(x,\tau)\big) = V_F^\alpha \frac{\partial}{\partial x} c(x,\tau) + D_F^\alpha \frac{\partial^2}{\partial x^2} c(x,\tau)$:

$$c(x,t) = c(x,0) + \int_0^t F(x,\tau,c(x,\tau)) \tag{3-99}$$

Considering Equation (3-99) for a specific time ($t^n$):

$$c(x,t_n) = c(x,0) + \int_0^{t_n} F(x,\tau,c(x,\tau)) \tag{3-100}$$

The integral can be approximated applying numerical integration techniques, including the traditional *Trapezoid Rule*, or the alternative methods of *Simpson's 3/8 Rule* and *Boole's Rule*, which are more rigorous. For this reason, the *Simpson's 3/8 Rule* and *Boole's Rule* are applied.

### 3.4.1 *Simpson's 3/8 Rule* of numerical integration

Consider the defined fractal integral over a specific time interval ($t_n$), where, $0 = t_0 < t_1 < t_2 < t_3 \dots < t_n = t$

$$\alpha \int_0^t \tau^{\alpha-1} f(\tau)\, d\tau = \alpha \int_{t_0}^{t_n} \tau^{\alpha-1} f(\tau)\, d\tau \tag{3-101}$$

Applying *Simpson's 3/8 Rule* for the defined fractal integral (Abramowitz and Stegun, 1966):

$$\int_{t_0}^{t_n} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \int_{t_0}^{t_3} \alpha\tau^{\alpha-1} f(\tau)\, d\tau + \int_{t_3}^{t_6} \alpha\tau^{\alpha-1} f(\tau)\, d\tau + \dots + \int_{t_{n-4}}^{t_{n-1}} \alpha\tau^{\alpha-1} f(\tau)\, d\tau \tag{3-102}$$

According to *Simpson's 3/8 Rule* (Abramowitz and Stegun, 1966):

$$\int_a^b f(x)dx = \frac{b-a}{8}\left[f(a) + 3f\left(\frac{2a+b}{3}\right) + 3f\left(\frac{a+2b}{6}\right) + f(b)\right] \tag{3-103}$$

Without losing generality, the integral is considered:

$$\int_{t_0}^{t_3} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \frac{t_3 - t_0}{8}\left[\alpha t_0^{\alpha-1} f(t_0) + 3\alpha t_1^{\alpha-1} f(t_1) + 3\alpha t_2^{\alpha-1} f(t_2) + \alpha t_3^{\alpha-1} f(t_3)\right] \tag{3-104}$$

Simplifying,

$$\int_{t_0}^{t_3} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \alpha\left(\frac{t_3 - t_0}{8}\right)\left[t_0^{\alpha-1} f(t_0) + 3t_1^{\alpha-1} f(t_1) + 3t_2^{\alpha-1} f(t_2) + t_3^{\alpha-1} f(t_3)\right] \tag{3-105}$$

Similarly, the integral $\int_{t_3}^{t_6}$ is considered:

$$\int_{t_3}^{t_6} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \alpha\left(\frac{t_6 - t_3}{8}\right)\left[t_3^{\alpha-1} f(t_3) + 3t_4^{\alpha-1} f(t_4) + 3t_5^{\alpha-1} f(t_5) + t_6^{\alpha-1} f(t_6)\right] \tag{3-106}$$

and, the generalized integral $\int_{t_{n-4}}^{t_{n-1}}$ is considered:

$$\int_{t_{n-4}}^{t_{n-1}} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \alpha\left(\frac{t_{n-1}-t_{n-4}}{8}\right)\left[t_{n-4}^{\alpha-1} f(t_{n-4}) + 3t_{n-1}^{\alpha-1} f(t_{n-3}) + 3t_{n-2}^{\alpha-1} f(t_{n-2}) + t_{n-1}^{\alpha-1} f(t_{n-1})\right] \tag{3-107}$$

Incorporating the integrals back into Equation (3-102), and simplifying:

$$\int_{t_0}^{t_n} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \left(\frac{3\,\Delta t\,\alpha}{8}\right)\begin{Bmatrix} t_0^{\alpha-1} f(t_0) + 3t_1^{\alpha-1} f(t_1) + 3t_2^{\alpha-1} f(t_2) + t_3^{\alpha-1} f(t_3) + \\ t_3^{\alpha-1} f(t_3) + 3t_4^{\alpha-1} f(t_4) + 3t_5^{\alpha-1} f(t_5) + t_6^{\alpha-1} f(t_6) + \cdots + \\ t_{n-4}^{\alpha-1} f(t_{n-4}) + 3t_{n-1}^{\alpha-1} f(t_{n-3}) + 3t_{n-2}^{\alpha-1} f(t_{n-2}) + t_{n-1}^{\alpha-1} f(t_{n-1}) \end{Bmatrix} \tag{3-108}$$

Equation (3-108) is the numerical approximation of the fractal integral using *Simpson's 3/8 Rule* for numerical integration.

Applying the *Simpson's 3/8 Rule* to the integral formulation of the fractal advection-dispersion equation,

$$\int_0^{t_n} F\big(x, t_n, c(x,t_n)\big) d\tau = \int_{t_0}^{t_3} F\big(x, t_n, c(x,t_n)\big) d\tau + \int_{t_3}^{t_6} F\big(x, t_n, c(x,t_n)\big) d\tau + \cdots + \int_{t_{n-4}}^{t_{n-1}} F\big(x, t_n, c(x,t_n)\big) d\tau \tag{3-109}$$

Without losing generality, the integral, $\int_{t_0}^{t_3} F\big(x, t_n, c(x,t_n)\big) d\tau$, is considered:

$$\int_{t_0}^{t_3} F\big(x, t_n, c(x,t_n)\big) d\tau = \frac{t_3 - t_0}{8} \cdot \Big[F\big(x, t_0, c(x,t_0)\big) + 3F\big(x, t_1, v(x,t_1)\big) + 3F\big(x, t_2, c(x,t_2)\big) + F\big(x, t_3, c(x,t_3)\big)\Big] \tag{3-110}$$

Similarly, the integral, $\int_{t_3}^{t_6} F\big(x, t_n, c(x,t_n)\big) d\tau$, is considered:

$$\int_{t_3}^{t_6} F\big(x, t_n, c(x,t_n)\big) d\tau = \frac{t_6 - t_3}{8} \cdot \Big[F\big(x, t_3, c(x,t_3)\big) + 3F\big(x, t_4, c(x,t_4)\big) + 3F\big(x, t_5, c(x,t_5)\big) + F\big(x, t_6, c(x,t_6)\big)\Big] \tag{3-111}$$

and, the generalized integral, $\int_{t_{n-4}}^{t_{n-1}} F\big(x, t_n, c(x,t_n)\big) d\tau$, is considered:

$$\int_{t_{n-4}}^{t_{n-1}} F\big(x, t_n, c(x,t_n)\big) d\tau = \frac{t_{n-1} - t_{n-4}}{8} \cdot \begin{bmatrix} F\big(x, t_{n-4}, c(x,t_{n-4})\big) + 3F\big(x, t_{n-3}, c(x,t_{n-3})\big) + \\ 3F\big(x, t_{n-2}, c(x,t_{n-2})\big) + F\big(x, t_{n-1}, c(x,t_{n-1})\big) \end{bmatrix} \tag{3-112}$$

Incorporating the integrals back into Equation (3-100), and simplifying:

$$c(x,t_n) = c(x,0) + \left(\frac{3\,\Delta t}{8}\right)\left\{\begin{matrix} F\big(x,t_0,c(x,t_0)\big) + 3F\big(x,t_1,c(x,t_1)\big) \\ +3F\big(x,t_2,c(x,t_2)\big) + F\big(x,t_3,c(x,t_3)\big) + \\ F\big(x,t_3,c(x,t_3)\big) + 3F\big(x,t_4,c(x,t_4)\big) \\ +3F\big(x,t_5,c(x,t_5)\big) + F\big(x,t_6,c(x,t_6)\big) + \cdots + \\ F\big(x,t_{n-4},c(x,t_{n-4})\big) + 3F\big(x,t_{n-3},c(x,t_{n-3})\big) \\ +3F\big(x,t_{n-2},c(x,t_{n-2})\big) + F\big(x,t_{n-1},c(x,t_{n-1})\big) \end{matrix}\right\} \tag{3-113}$$

Substituting back the function $F\big(x,\tau,c(x,\tau)\big)$, and expanding $c(x,t_n)$:

$$c(x,t_n) = c(x,0) +$$

$$\left(\frac{3\,\Delta t}{8}\right)\left\{\begin{matrix} \left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_0) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_0)\right) + 3\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_1) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_1)\right) \\ +3\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_2) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_2)\right) + \left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_3) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_3)\right) + \\ + \cdots + \\ \left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-4}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-4})\right) + 3\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-3}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-3})\right) \\ +3\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-2}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-2})\right) + \left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-1}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-1})\right) \end{matrix}\right\} \tag{3-114}$$

Equation (3-114) is the numerical approximation of the integral formulation of the fractal advection-dispersion equation, where the numerical integration of the fractal integral is performed using the *Simpson's 3/8 Rule*.

### 3.4.2 Boole's Rule of numerical integration

Alternatively, the *Boole's Rule* for numerical integration can be applied to the approximation of the fractal integral. Applying *Boole's Rule* for the defined fractal integral (Abramowitz and Stegun, 1966):

$$\int_{t_0}^{t_n} \alpha\tau^{\alpha-1}\, f(\tau)\, d\tau = \int_{t_0}^{t_4} \alpha\tau^{\alpha-1}\, f(\tau)\, d\tau + \int_{t_4}^{t_8} \alpha\tau^{\alpha-1}\, f(\tau)\, d\tau + \cdots + \int_{t_{n-5}}^{t_{n-1}} \alpha\tau^{\alpha-1}\, f(\tau)\, d\tau \tag{3-115}$$

According to *Boole's Rule* (Abramowitz and Stegun, 1966):

$$\int_a^b f(x)dx = \frac{b-a}{90}[7f_0 + 32f_1 + 127f_2 + 32f_3 + 7f_4] \tag{3-116}$$

Without losing generality, the integral $\int_{t_0}^{t_4}$ is considered:

$$\int_{t_0}^{t_4} \alpha\tau^{\alpha-1}\, f(\tau)\, d\tau = \frac{t_4 - t_0}{90}\left[\begin{matrix} 7\alpha t_0^{\alpha-1}\, f(t_0) + 32\alpha t_1^{\alpha-1} f(t_1) + 12\alpha t_2^{\alpha-1} f(t_2) \\ +32\alpha t_3^{\alpha-1} f(t_3) + 7\alpha t_4^{\alpha-1} f(t_4) \end{matrix}\right] \tag{3-117}$$

Simplifying,

$$\int_{t_0}^{t_4} \alpha\tau^{\alpha-1}\, f(\tau)\, d\tau = \alpha\left(\frac{t_4 - t_0}{90}\right)\left[\begin{matrix} 7t_0^{\alpha-1}\, f(t_0) + 32t_1^{\alpha-1} f(t_1) + 12t_2^{\alpha-1} f(t_2) + 32t_3^{\alpha-1} f(t_3) \\ +7t_4^{\alpha-1} f(t_4) \end{matrix}\right] \tag{3-118}$$

Similarly, the integral $\int_{t_4}^{t_8}$ is considered:

$$\int_{t_4}^{t_8} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \alpha\left(\frac{t_8-t_4}{90}\right)\begin{bmatrix} 7t_4^{\alpha-1} f(t_4) \\ +32t_5^{\alpha-1}f(t_5)+12t_6^{\alpha-1}f(t_6)+32t_7^{\alpha-1}f(t_7)+7t_8^{\alpha-1}f(t_8) \end{bmatrix} \quad (3\text{-}119)$$

and, the generalized integral $\int_{t_{n-5}}^{t_{n-1}}$ is considered:

$$\int_{t_{n-5}}^{t_{n-1}} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \alpha\left(\frac{t_{n-5}-t_{n-1}}{90}\right) \times \begin{bmatrix} 7t_{n-5}^{\alpha-1} f(t_{n-5}) \\ +32t_{n-4}^{\alpha-1}f(t_{n-4})+12t_{n-3}^{\alpha-1}f(t_{n-3})+32t_{n-2}^{\alpha-1}f(t_{n-2})+7t_{n-1}^{\alpha-1}f(t_{n-1}) \end{bmatrix} \quad (3\text{-}120)$$

Incorporating the integrals back into Equation (3-115), and simplifying:

$$\int_{t_0}^{t_n} \alpha\tau^{\alpha-1} f(\tau)\, d\tau = \left(\frac{4\,\Delta t\,\alpha}{90}\right)\begin{Bmatrix} 7t_0^{\alpha-1} f(t_0)+32t_1^{\alpha-1}f(t_1)+12t_2^{\alpha-1}f(t_2)+32t_3^{\alpha-1}f(t_3)+7t_4^{\alpha-1}f(t_4)+ \\ 7t_4^{\alpha-1} f(t_4)+32t_5^{\alpha-1}f(t_5)+12t_6^{\alpha-1}f(t_6)+32t_7^{\alpha-1}f(t_7)+7t_8^{\alpha-1}f(t_8)+\cdots+ \\ 7t_{n-5}^{\alpha-1} f(t_{n-5})+32t_{n-4}^{\alpha-1}f(t_{n-4})+12t_{n-3}^{\alpha-1}f(t_{n-3})+32t_{n-2}^{\alpha-1}f(t_{n-2})+7t_{n-1}^{\alpha-1}f(t_{n-1}) \end{Bmatrix} \quad (3\text{-}121)$$

Equation (3-121) is the numerical approximation of the fractal integral using *Boole's Rule* for numerical integration.

*Boole's Rule* of numerical integration is now considered for the solution of integral of the advection and dispersion terms (represented as $F(x,t,c(x,t))$) in Equation (3-100), where (Abramowitz and Stegun, 1966):

$$\int_0^{t_n} F(x,t_n,c(x,t_n))d\tau = \int_{t_0}^{t_4} F(x,\tau,c(x,\tau))\,d\tau + \int_{t_4}^{t_8} F(x,\tau,c(x,\tau))\,d\tau + \cdots + \int_{t_{n-5}}^{t_{n-1}} F(x,\tau,c(x,\tau))\,d\tau \quad (3\text{-}122)$$

Without losing generality, the integral, $\int_{t_0}^{t_4} F(x,\tau,c(x,\tau))\,d\tau$, is considered:

$$\int_{t_0}^{t_4} F(x,\tau,c(x,\tau))d\tau = \frac{t_4-t_0}{90}\begin{bmatrix} 7F(x,t_0,c(x,t_0))+32F(x,t_1,c(x,t_1)) \\ +12F(x,t_2,c(x,t_2))+32F(x,t_3,c(x,t_3))+7F(x,t_4,c(x,t_4)) \end{bmatrix} \quad (3\text{-}123)$$

Similarly, the integral, $\int_{t_4}^{t_8} F(x,\tau,c(x,\tau))\,d\tau$, is considered:

$$\int_{t_4}^{t_8} F(x,\tau,c(x,\tau))d\tau = \frac{t_8-t_4}{90}\begin{bmatrix} 7F(x,t_4,c(x,t_4))+32F(x,t_5,c(x,t_5))+12F(x,t_6,c(x,t_6)) \\ +32F(x,t_7,c(x,t_7))+7F(x,t_8,c(x,t_8)) \end{bmatrix} \quad (3\text{-}124)$$

and, the generalized integral, $\int_{t_{n-5}}^{t_{n-1}} F(x,\tau,c(x,\tau))\,d\tau$, is considered:

$$\int_{t_{n-5}}^{t_{n-1}} F\big(x,\tau,c(x,\tau)\big)d\tau = \frac{t_{n-1}-t_{n-5}}{90}\begin{bmatrix} 7F\big(x,t_{n-5},c(x,t_{n-5})\big)+32F\big(x,t_{n-4},c(x,t_{n-4})\big)+12F\big(x,t_{n-3},c(x,t_{n-3})\big) \\ +32F\big(x,t_{n-2},c(x,t_{n-2})\big)+7F\big(x,t_{n-1},c(x,t_{n-1})\big)\end{bmatrix} \tag{3-125}$$

Incorporating the integrals back into Equation (3-100), and simplifying:

$$(x,t_n) = c(x,0) + \left(\frac{4\,\Delta t}{90}\right)\begin{Bmatrix} 7F\big(x,t_0,c(x,t_0)\big)+32F\big(x,t_1,c(x,t_1)\big)+12F\big(x,t_2,c(x,t_2)\big) \\ +32F\big(x,t_3,c(x,t_3)\big)+7F\big(x,t_4,c(x,t_4)\big)+ \\ 7F\big(x,t_4,c(x,t_4)\big)+32F\big(x,t_5,c(x,t_5)\big)+12F\big(x,t_6,c(x,t_6)\big) \\ +32F\big(x,t_7,c(x,t_7)\big)+7F\big(x,t_8,c(x,t_8)\big)+\cdots+ \\ 7F\big(x,t_{n-5},c(x,t_{n-5})\big)+32F\big(x,t_{n-4},c(x,t_{n-4})\big)+12F\big(x,t_{n-3},c(x,t_{n-3})\big) \\ +32F\big(x,t_{n-2},c(x,t_{n-2})\big)+7F\big(x,t_{n-1},c(x,t_{n-1})\big) \end{Bmatrix} \tag{3-126}$$

Substituting back the function $F\big(x,\tau,c(x,\tau)\big) = V_F^\alpha \frac{\partial}{\partial x}c(x,\tau) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,\tau)$:

$$c(x,t_n) = c(x,0) + \left(\frac{4\,\Delta t}{90}\right)\begin{Bmatrix} 7\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_0) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_0)\right) + 32F\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_1) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_1)\right) \\ +12\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_2) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_2)\right) + 32\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_3) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_3)\right) + \\ 7\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_4) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_4)\right) \\ +\cdots+ \\ 7\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-5}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-5})\right) + 32\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-4}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-4})\right) \\ +12\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-3}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-3})\right) + 32\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-2}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-2})\right) \\ +7\left(V_F^\alpha \frac{\partial}{\partial x}c(x,t_{n-1}) + D_F^\alpha \frac{\partial^2}{\partial x^2}c(x,t_{n-1})\right) \end{Bmatrix} \tag{3-127}$$

Equation (3-127) is the numerical approximation of the fractal advection-dispersion equation, where the numerical integration of the fractal integral is performed using *Boole's Rule*.

The *Simpson's 3/8 Rule* and *Boole's Rule* of numerical integration are both methods from the *Newton-Cotes Quadrature Rules* which are founded on assessing the integral at equally spaced points. The traditionally used *Trapezoid Rule* uses two points of calculation within each larger step of the numerical integration, *Simpson's 3/8 Rule* uses four calculation points, and *Boole's Rule* uses five calculation points. The accuracy of numerical integration is related to the size of the steps used, where the smaller the step the more accurate the solution. Thus, *Simpson's 3/8 Rule* and *Boole's Rule* will have a higher degree of accuracy because smaller sub-steps are considering within each step.

## 3.5 Numerical simulation for different fractal dimensions

The fractal advection-dispersion equation was developed with the fractal derivative in space to account for anomalous diffusion associated with groundwater transport in fractured systems. To corroborate this theory, the equation is applied to a simple one-dimensional transport problem and simulated in the software programme *Maple* (Figure 2-1) (Appendix B). The velocity within the aquifer is constant at 0.05 m/d, the hydrodynamic dispersivity in the x-direction is 0.3 $m^2$/d, and the initial contaminant concentration ($C_0$) is 10 mg/l. The initial condition and boundary conditions for the defined problem are:

$$\left.\begin{aligned} & c(x,0) = C_0 && x \geq 0 \\ & c(0,t) = C_0 \cdot \exp(\lambda t) && t \geq 0 \\ & \frac{\partial c}{\partial x}(L,t) = 0 && t \geq 0 \end{aligned}\right]$$

The fractal advection-dispersion equation is applied to the defined problem, and the fractal dimension varied to investigate the influence this parameter has on the simulated transport (Figure 3-1, Figure 3-2, and Figure 3-3). When the fractal dimension is 1 ($\alpha = 1$), the equation reduces to the traditional advection-dispersion equation and thus forms the basis for comparison. The traditional advection-dispersion simulates an expected movement along the x-directional line, with the contaminant reaching 50 m after 200 days. The concentration spreads out evenly from the source over time as anticipated. From this basecase, the fractal dimension is varied from 0.9 to 0.1, in increments of 0.1. When the fractal dimension is 0.9 ($\alpha = 0.9$), the extent of the transport is increased, where the contaminant now reaches further than 50 m after 200 days. This trend is continued with each increment reduction in the fractal dimension, where the contaminant reaches 140 m after 200 days for the fractal dimension 0.7 ($\alpha = 0.7$), and exceeds the 200 m line in 110 days with a fractal dimension of 0.6 (Figure 3-1). From the fractal dimension of 0.7 to 0.1, there is an exponential increase in the simulated transport along the x-directional line (Figure 3-2). For the fractal dimension 0.1 ($\alpha = 0.1$), the contaminant reaches the 200 m line reach after just 10 days. The fractal dimensions above 0.6 ($\alpha = 0.6$) change the general orientation from perpendicular to the x-direction to parallel, representing the preferential pathway which fractures can provide. A constant groundwater velocity was applied to all models, and thus the simulation validates the use of this equation to develop new models to better simulate groundwater transport in fractured systems, where the specific characterisation of the fractured system is not available.

To further investigate the influence of the fractal dimension, values greater than 1 are considered (Figure 3-3). The fractal dimension has the opposite influence when the fractal order is greater than 1, where now the transport is impeded, slower than the traditional model, representing subdiffusion.

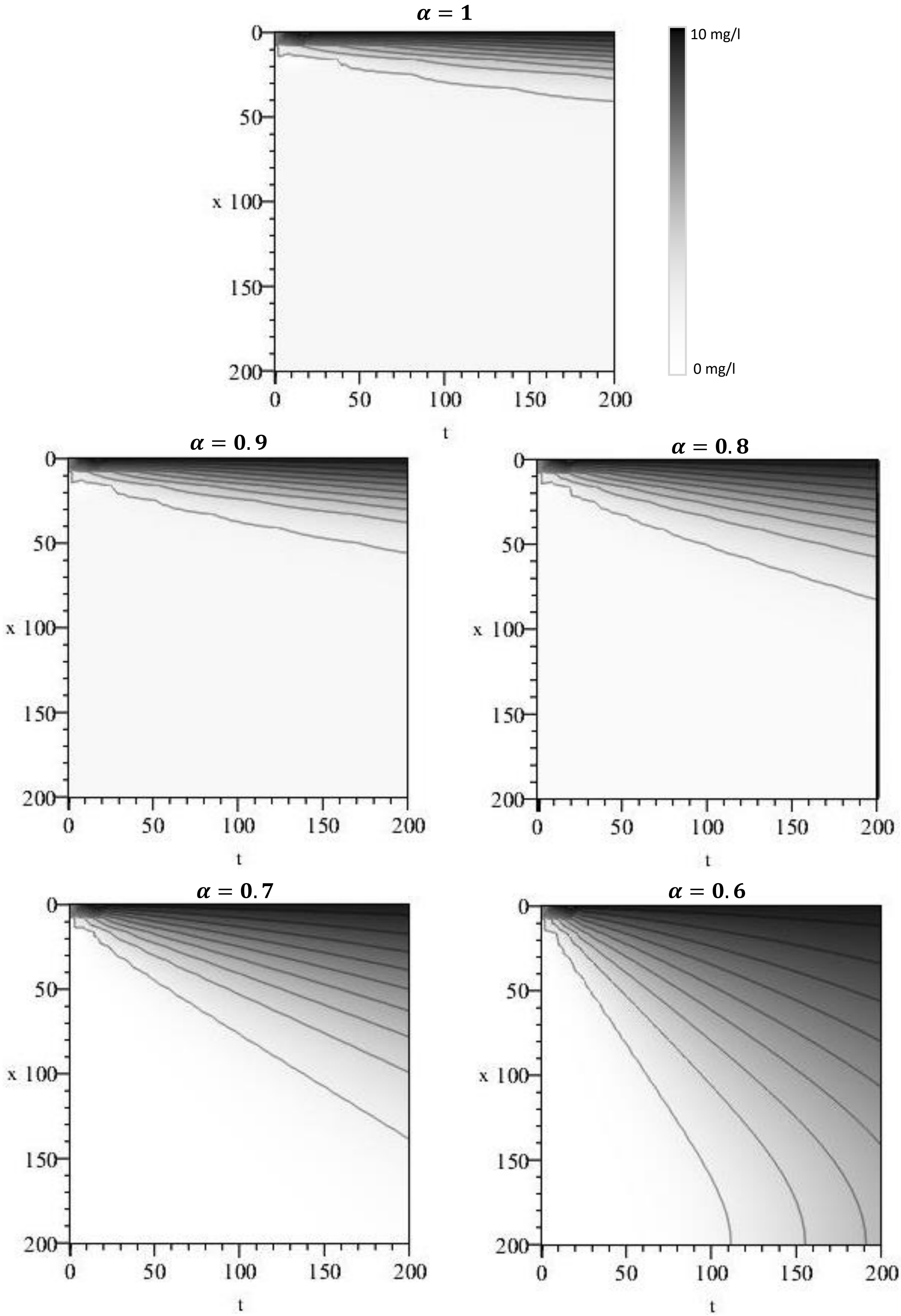


**Figure 3-1 Simulation results for the simple transport problem for variable fractal dimensions ($0.6 \leq \alpha \leq 1$), $x$ is distance in meters, and $t$ is time in days. When $\alpha = 1$, the equation simplifies to the traditional advection-dispersion equation and forms the basis of comparison. Changing the fractal dimension increases the extent of the transport plume along the one-dimensional line in the x-direction, representing superdiffusion.**

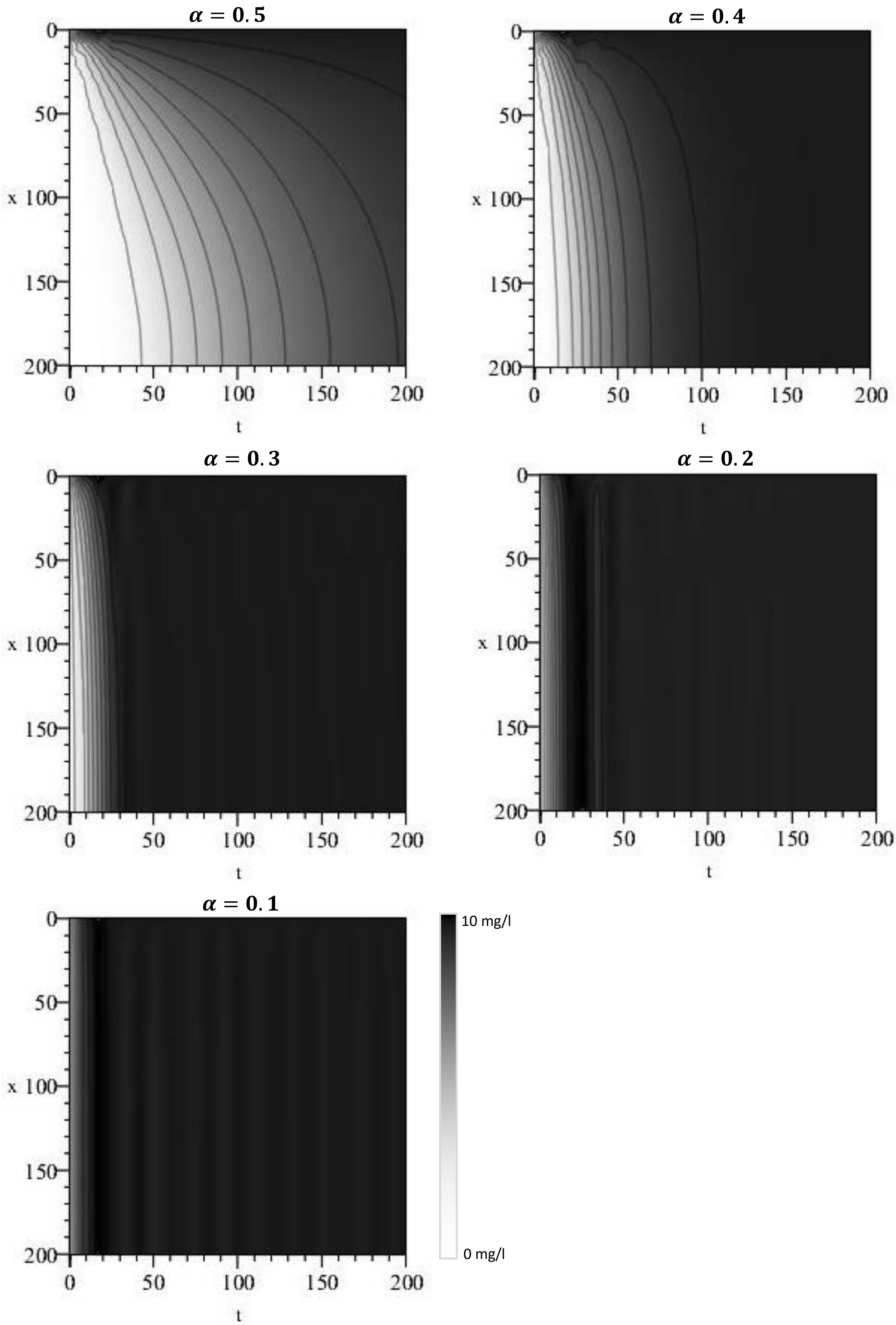


**Figure 3-2 Simulation results for the simple transport problem for variable fractal dimensions ($0.1 \leq \alpha \leq 0.5$). Fractal dimensions below 0.5 result in significant contaminant transport along the line.**

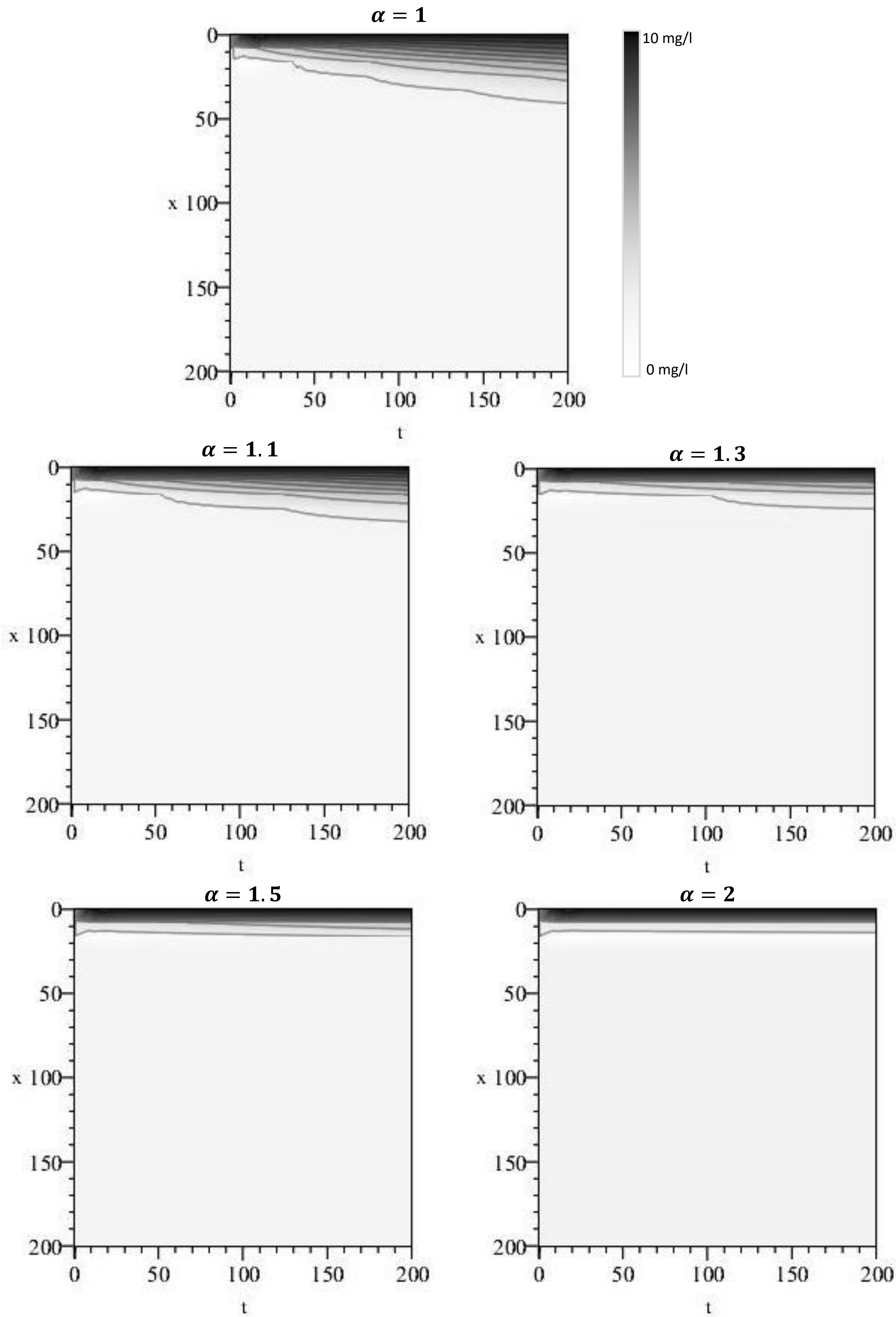


**Figure 3-3 Simulation results for the simple transport problem for variable fractal dimensions ($1 \leq \alpha \leq 2$). When $\alpha = 1$, the equation simplifies to the traditional advection-dispersion equation and forms the basis of comparison. Fractal dimensions greater than 1, impede transport along the x-directional line, representing subdiffusion.**

## 3.6 Investigation of fractal velocity ($V_F^{\alpha}$) and fractal dispersivity ($D_F^{\alpha}$)

The simulation of variable fractal dimensions has validated the use of the model for fractured groundwater systems lacking detailed characterisation of heterogeneity. But, questions arise with respect to the fractal velocity and fractal dispersivity, in terms of the relationship between velocity, dispersivity and the fractal dimension. To understand this relationship, plots of the fractal velocity and fractal dispersivity with respect to the fractal dimension are evaluated on the same scale (Figure 3-5 and Figure 3-4) and on a local scale (Figure 3-6 and Figure 3-7). For a fractal dimension of 1 ($\alpha = 1$), the fractal velocity equals the defined constant velocity of 0.05 m/d. The introduction of the fractal order at $\alpha = 0.9$, slightly changes the set constant velocity to a variable velocity from 0.05 m/d to 0.81 m/d at 50 m. A similar trend of exponential distributions are seen from $\alpha = 0.8$ to $\alpha = 0.6$, until a linear relationship over distance is found at $\alpha = 0.5$. From a fractal order of 0.5, an exponential trend is seen again up to $\alpha = 0.1$.

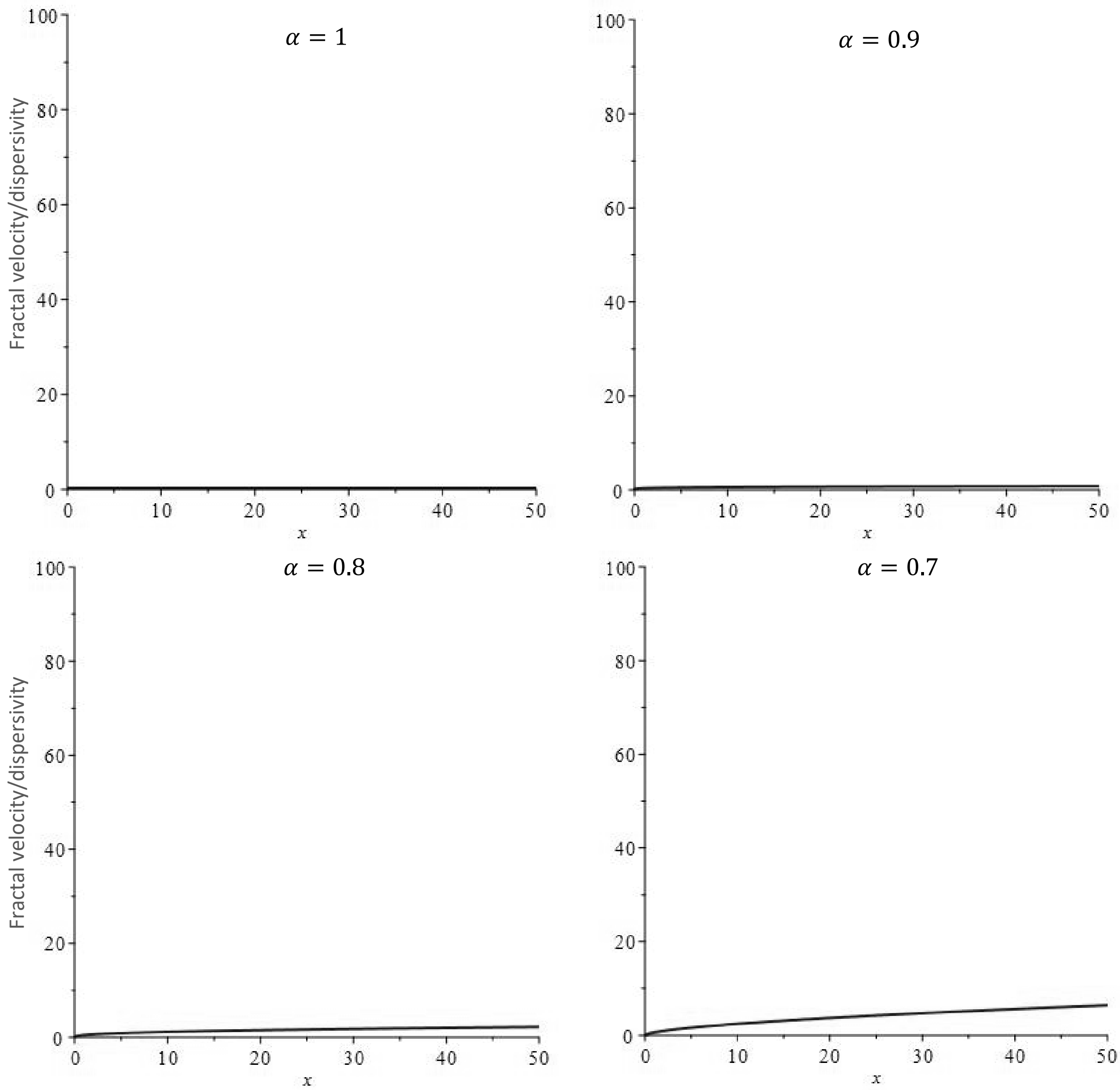


**Figure 3-4 Fractal velocity and dispersivity over space for varying fractal dimensions ($0.7 \leq \alpha \leq 1$) on the same scale.**

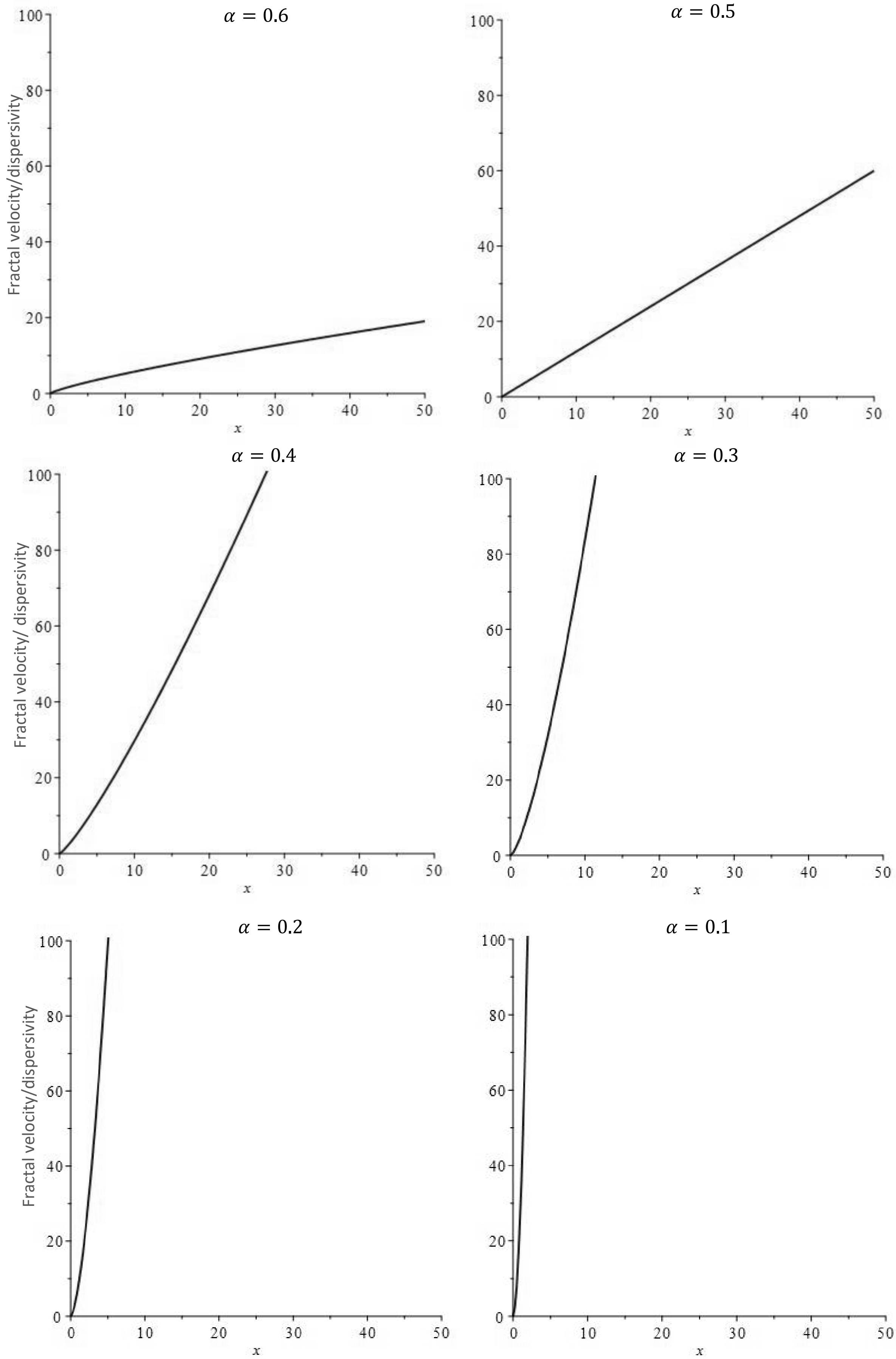


**Figure 3-5 Fractal velocity and dispersivity over space for varying fractal dimensions ($0.1 \leq \alpha \leq 0.6$) on the same scale.**

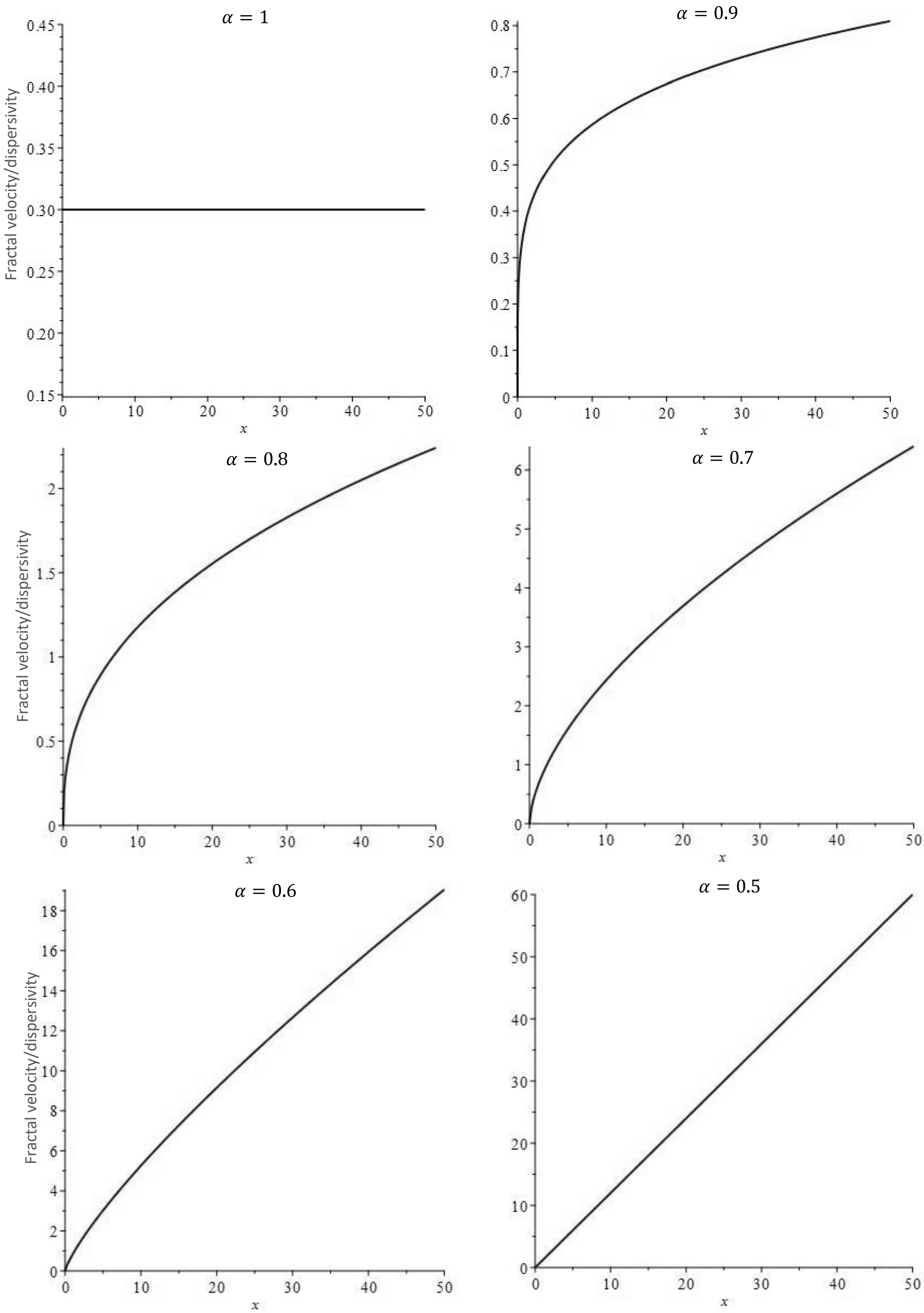


**Figure 3-6 Fractal velocity and dispersivity over space for varying fractal dimensions ($0.5 \leq \alpha \leq 1$) on a local scale for each plot.**

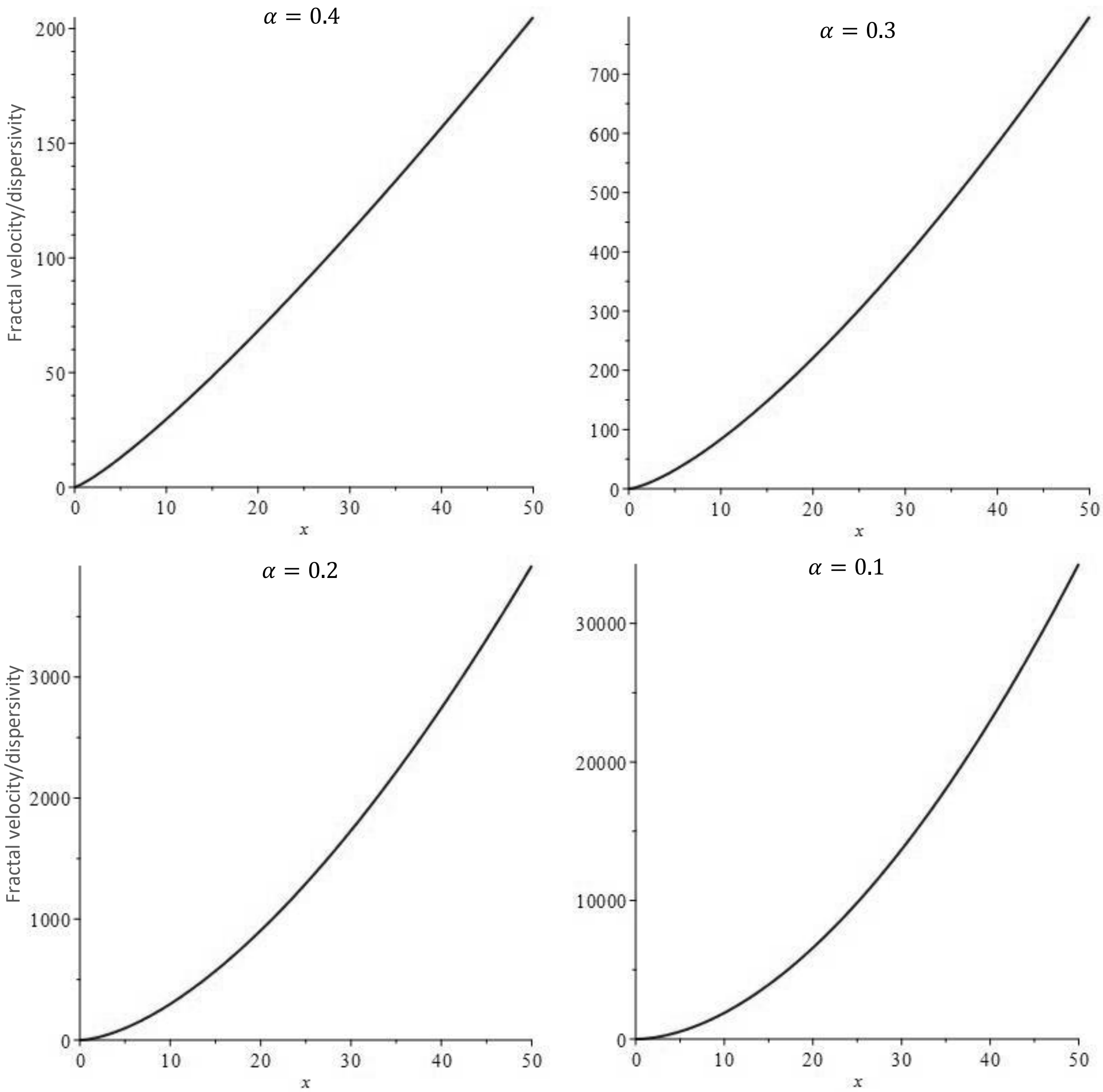


**Figure 3-7 Fractal velocity and dispersivity over space for varying fractal dimensions ($0.1 \leq \alpha \leq 0.4$) on an individual scale for each plot.**

From the plots of fractal velocity and fractal dispersivity, which show the same distributions over the fractal dimensions, it can be seen that there is an exponential increase in the fractal velocity and dispersivity as the fractal dimension decreases. However, from a fractal dimension of 0.5 to 0.1, the increase becomes extreme from a groundwater perspective, where typically groundwater moves slowly. From a practical interpretation, the use of a fractal dimensions below $\alpha = 0.5$ should be used with caution because of this exponential increase in velocity and hydrodynamic dispersivity.

## 3.7 Chapter summary

It is discussed that the use of the classical advection-dispersion equation tends to inaccurately simulate observed contaminant transport because the information required to characterise a fractured system, to an appropriate level of detail, is often not available. This is due to the fact that heterogeneity is not explicitly incorporated into the classical advection-dispersion equation, but rather a constant velocity and dispersivity is considered at each point and heterogeneity is incorporated externally. In response to the current limitations of transport modelling using the advection-dispersion equation, especially in fractured media, a fractal advection-dispersion groundwater transport equation was developed and four methods to solve the fractal advection-dispersion equation are described, namely forward finite differences and Crank-Nicolson finite differences for the fractal derivative formulation, and the Simpson 3/8 and Boole's numerical integration for the fractal integral formulation.

The developed fractal advection-dispersion equation is numerically simulated for a generic groundwater transport model to investigate the effects of varying the fractal dimension in a one-dimensional groundwater flow system. The simulations provided evidence that the fractal formulation of the advection-dispersion equation could possibly model superdiffusion for fractal dimension less than 1, as well as subdiffusion for fractal dimensions greater than 1, without explicitly defining fractures or preferential pathways. Being able to model the effect of fractures or faults without explicitly including the location and specific details in the model has the potential to account for anomalous transport, especially where limited information is available on the preferential pathway causing the discrepancy.

The relationship between the fractal velocity and dispersivity with the fractal dimension is evaluated, and the use of fractal dimensions above 0.5 are recommended for practical use, due to the supersonic increase in velocity and dispersivity for fractal dimensions $0.1 \leq \alpha \leq 0.5$.

# 4 FRACTIONAL DERIVATIVES: SINGULAR AND NON-SINGULAR

A brief introduction to fractional calculus and the various fractional derivative definitions have been discussed in Section 1.2.2. To continue this discussion, the functions required for the definition of fractional integrals and derivatives are presented, followed by the fundamental fractional definitions, including Riemann-Liouville (RL), Caputo (C), Atangana-Baleanu in Caputo sense (ABC), and Atangana-Baleanu in Riemann-Liouville (ABR). The kernel associated with each fractional definition is investigated from the perspective of a convolution of two functions.

Derivatives and integrals are traditionally introduced as the mathematical representation of slopes and areas, yet fractional derivatives are mysterious, as they have no obvious geometric interpretation. Oldham and Spanier (1974) encourage that if one is able to move beyond with this pictorial representation of a classical derivative, fractional-order derivatives and integrals can become equally tangible as a new dimension in mathematics is revealed (Oldham and Spanier, 1974; Loverro, 2004).

## 4.1 Special functions in fractional definitions

The Gamma and Mittag-Leffler functions are well-established extensions of the factorial and exponential function, which service to explain the definitions and use of the fractional integral and derivative (Loverro, 2004; Herrmann, 2011).

### 4.1.1 Gamma function

Euler's Gamma function can be generalised as the factorial for all real numbers, and is intrinsically tied to fractional calculus. The definition of the gamma function is (Loverro, 2004; Petráš, 2010; Herrmann, 2011):

$$\Gamma(z) = \int_0^\infty u^{z-1} e^{-t} \, d\tau \tag{4-1}$$

Applying integration by parts,

$$\Gamma(1+z) = z\,\Gamma(z) \tag{4-2}$$

Applying direct integration $\Gamma(1) = 1$,

$$\Gamma(1+n) = n! \tag{4-3}$$

or

$$\Gamma(n) = (n-1)! \tag{4-4}$$

### 4.1.2 Power Law function

The power law can simply be stated as

$$f(x) = x^a \tag{4-5}$$

where, $a$ is a constant known as the exponent of the power law.

From a statistical perspective, the power law is a relationship between two quantities, where a change in one variable results in a proportional change in the other controlled by the exponential power.

Power-law distributions are commonly found in nature and patterns, ranging from city population trends, magnitude of earthquakes, foraging patterns of various species, to describing the size of craters on the moon (Gutenberg and Richter, 1944; Neukum and Ivanov, 1994; Newman, 2005; Frank, 2009; Humphries et al., 2010).

### 4.1.3 Exponential function

The exponential function can simply be stated as

$$f(x) = e^x \tag{4-6}$$

where, $e$ is a constant, and in this case Euler's constant of 2.71828.

The exponential function describes the relationship where a quantity grows or decays at a rate proportional to its current value. The exponential pattern is a more common than the power law and is widely recognised in nature, from survival times for decaying atomic nuclei, the Boltzmann distribution of energies in statistical mechanics, to the frequency of Korean family names (Kim and Park, 2005; Newman, 2005; Frank, 2009).

The stretched exponential function has been proposed as a complement to the power law distributions, where Laherrere and Sornette (1998) showed stretched exponential functions to describe natural phenomena such as radio and light emissions from galaxies, oilfield reserve sizes, and Vostok temperature variations. Lee et al. (2001) demonstrated that the stretched exponential function could represent the observed autofluorescence decay profiles in biological tissue, producing high-quality contrast and spatial maps.

### 4.1.4 Mittag-Leffler function

The Mittag-Leffler function plays an important role in the solution of non-integer order differential equations, and can be analogously compared to the exponential function, used in the solution of integer-order differential equations. The exponential function ($e^z$) can be defined as (Loverro, 2004; Petráš, 2010; Herrmann, 2011):

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!} \tag{4-7}$$

Considering the defined gamma function ($\Gamma$) (Equation (4-3), the factorial $n!$ can be replaced by $\Gamma(1+n)$:

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+n)} \tag{4-8}$$

The Mittag-Leffler function $E_\alpha(z)$ can be defined as:

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+\alpha n)} \tag{4-9}$$

where, $\alpha$ denotes an arbitrary real number $\alpha > 0$.

The generalised Mittag-Leffler function is a most natural generalisation of the exponential function, and can be expressed as (Shukla and Prajapati, 2007; Mathai and Haubold, 2008),

$$E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n+\beta)} \tag{4-10}$$

The Mittag-Leffler function reduces to the exponential function when $\alpha = 1$, because the function is a direct generalisation of the exponential function. However, the Mittag-Leffler function interpolates between the pure exponential and a hypergeometric function $\left(\frac{1}{1-z}\right)$ for values of $0 < \alpha < 1$ (Shukla and Prajapati, 2007).

The versatility of the Mittag-Leffler function has been fully realised in the last two decades with applications over a wide range, from stress-strength analysis, growth-decay mechanisms, to production of melatonin in the body (Shukla and Prajapati, 2007; Sebastian and Gorenflo, 2016).

## 4.2 Riemann-Liouville fractional definition

The functions required for fractional derivatives have been discussed, and the various definitions of the fractional derivative and integral can be explored, starting with the Riemann-Liouville fractional definition.

An integral can be interpreted as a generalisation of area in integer-order mathematical terms, and is referred to as the antiderivative or primitive. The integer-order integral is analysed and extended to the fractional operator. Let the integral operator be notionally represented by (Herrmann, 2011):

$$ {}_aI(f(x)) = \int_a^x f(\tau)\, d\tau \tag{4-11}$$

and, the multiple integral can be defined as:

$$ {}_aI^n(f(x)) = \int_a^{x_n} \int_a^{x_{n-1}} \dots \int_a^{x_1} f(x_0)\, dx_0 \dots dx_{n-1} \tag{4-12}$$

The multiple integral can be generalised for the $n^{th}$ integration of the function $f(x)$ using Cauchy's formula of repeated integration, on condition that $f(a) = 0$:

$$ {}_aI^n f(x) = \frac{1}{(n+1)!} \int_a^x (x-\tau)^{n-1} f(\tau)\, d\tau \tag{4-13}$$

The Cauchy defined integral can be extended to the fractional case by replacing $n$ with $\alpha$:

$$ {}_aI_+^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-\tau)^{\alpha-1} f(\tau)\, d\tau \tag{4-14}$$

$$ {}_bI_-^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_x^b (\tau-x)^{\alpha-1} f(\tau)\, d\tau \tag{4-15}$$

where, $a$ and $b$ denote the lower and upper boundary of the integral domain and may be arbitrarily chosen. Equation (4-14) is valid where $x > a$, and Equation (4-15) is valid where $x < b$. The choice of these two constants $(a, b)$ determines the value of the integral, and leads to a number of definitions for the fractional integral. The two most commonly applied definitions of the fractional integral include the Liouville and Riemann fractional integral definitions (Debnath, 2004; Loverro, 2004; Herrmann, 2011).

The Liouville fractional integral is defined for $a = -\infty$ and $b = +\infty$ (Herrmann, 2011):

$$ {}_{L}I_{+}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^{x} (x-\tau)^{\alpha-1} f(\tau)\, d\tau \tag{4-16} $$

$$ {}_{L}I_{-}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_{x}^{+\infty} (\tau-x)^{\alpha-1} f(\tau)\, d\tau \tag{4-17} $$

The Riemann fractional integral is defined for $a = 0$ and $b = 0$ (Herrmann, 2011):

$$ {}_{R}I_{+}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_{0}^{x} (x-\tau)^{\alpha-1} f(\tau)\, d\tau \tag{4-18} $$

$$ {}_{R}I_{-}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_{x}^{0} (\tau-x)^{\alpha-1} f(\tau)\, d\tau \tag{4-19} $$

Herrmann (2011) considered the special function $f(x) = e^{kx}$ to compare the Liouville and Riemann fractional integral definitions. When applying the Liouville fractional integral, the function disappears for values of $k > 0$ at the lower boundary of the integral domain, with no further contribution. Conversely, when applying the Riemann fractional integral, the function does not disappear because $a = 0$, and a further contribution is maintained.

The Liouville and Riemann fractional integral definitions are combined to form the general Riemann-Liouville definition of fractional integral (Debnath, 2004; Atangana, 2016):

$$ {}_{a}D_{x}^{-\alpha} f(x) = {}_{a}I_{x}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_{a}^{x} (x-\tau)^{\alpha-1} f(\tau)\, d\tau \tag{4-20} $$

where,

${}_{a}D^{-\alpha} = {}_{a}I^{\alpha}$ is the Riemann-Liouville integral operator,

$a = 0$, the Riemann definition of the fractional integral is valid,

$a = -\infty$, the Liouville definition of the fractional integral is valid

The fractional integral and fractional derivative are inverse operations, and similar to how integer-order derivatives are related to the integer-order integral, so do fractional derivatives share a relationship to fractional integrals. The derivative can be interpreted as the slope of a curve (geometric) or as a rate of change (physical) in integer-order mathematical terms. The integer-order derivative is analysed along with the fractional integral to extend the definition to the fractional derivative (Gootman, 1997; Loverro, 2004; Herrmann, 2011).

Let the derivative to an arbitrary order $(\alpha)$ order be denotes as follows:

$$ \frac{d^n}{dx^n} = D^{\alpha} \tag{0-21} $$

The fractional derivative can be divided into appropriate integer-order derivative and the remaining fractional order derivative (Herrmann, 2011):

$$\begin{aligned} D^{\alpha} &= D^{m} D^{\alpha-m} \qquad\qquad m \in \mathbb{N} \\ &= \frac{d^m}{dx^m} {}_a I^{m-\alpha} \end{aligned} \tag{4-22}$$

where,

$$D^{\alpha} = I^{-\alpha} = \frac{d^{\alpha}}{dx^{\alpha}}$$

Equation (4-22) states the fractional derivative can be represented or defined as a fractional integral followed by an integer-order derivative, where once a fractional integral is defined the fractional derivative is defined as well. This explains why the fractional derivative is referred to as the *differintegral*. The inverted sequence of operators leads to an alternative decomposition of the fractional derivative into an integer-order derivative followed by a fractional integral (Herrmann, 2011):

$$\begin{aligned} D^{\alpha} &= D^{\alpha-m} D^{m} \qquad\qquad m \in \mathbb{N} \\ &= {}_a I^{m-\alpha} \frac{d^m}{dx^m} \end{aligned} \tag{4-23}$$

Equation (4-22) and Equation (4-23) serve to highlight the non-locality of fractional calculus, where the integer-order derivative is a local operator, but the fractional integral is a non-local operator. The fractional derivative is thus a non-local operator, because it is the inverse of the fractional integral, which is a non-local operator (Herrmann, 2011).

The Liouville definition of the fractional derivative is obtained by applying the Liouville definition of the fractional integral (Equation (4-16) and Equation (4-17)) and the operator sequence in Equation (4-22) for the simple case $(0 < \alpha < 1)$ (Herrmann, 2011):

$$\begin{aligned} {}_L D_{+}^{\alpha} f(x) &= \frac{d}{dx} {}_L I_{+}^{1-\alpha} f(x) \\ &= \frac{d}{dx} \frac{1}{\Gamma(1-\alpha)} \int_{-\infty}^{x} (x-\tau)^{-\alpha} f(\tau)\, d\tau \end{aligned} \tag{4-24}$$

and,

$$\begin{aligned} {}_L D_{-}^{\alpha} f(x) &= \frac{d}{dx} {}_L I_{-}^{1-\alpha} f(x) \\ &= \frac{d}{dx} \frac{1}{\Gamma(1-\alpha)} \int_{x}^{+\infty} (\tau-x)^{-\alpha} f(\tau)\, d\tau \end{aligned} \tag{4-25}$$

The Riemann definition of the fractional derivative is obtained by applying the Riemann definition of the fractional integral (Equation (4-18) and Equation (4-19)) and the operator sequence in Equation (4-22) (Herrmann, 2011):

$$
\begin{aligned}
{}_{R}D_{+}^{\alpha}f(x) &= \frac{d}{dx}\,{}_{R}I_{+}^{1-\alpha}f(x) \\
&= \frac{d}{dx}\frac{1}{\Gamma(1-\alpha)}\int_{0}^{x}(x-\tau)^{-\alpha}\,f(\tau)\,d\tau
\end{aligned}
\qquad (4\text{-}26)
$$

and,

$$
\begin{aligned}
{}_{R}D_{-}^{\alpha}f(x) &= \frac{d}{dx}\,{}_{R}I_{-}^{1-\alpha}f(x) \\
&= \frac{d}{dx}\frac{1}{\Gamma(1-\alpha)}\int_{x}^{0}(\tau-x)^{-\alpha}\,f(\tau)\,d\tau
\end{aligned}
\qquad (4\text{-}27)
$$

The Liouville and Riemann fractional derivative definitions are combined to form the general Riemann-Liouville definition of fractional derivative or differintegral for $(n-1<\alpha<n)$ (Oldham and Spanier, 1974; Kisela, 2008; Petráš, 2010; Atangana, 2016):

$$
{}_{a}^{RL}D_{x}^{\alpha}f(x) = \frac{1}{\Gamma(n-\alpha)}\,\frac{d^{n}}{dx^{n}}\int_{\alpha}^{x}(x-\tau)^{-\alpha-n+1}\,f(\tau)\,d\tau
\qquad (4\text{-}28)
$$

where,

$^{RL}D^{\alpha}$ is the Riemann-Liouville differintegral operator,

$a=0$, the Riemann definition of the fractional integral is valid,

$a=-\infty$, the Liouville definition of the fractional integral is valid.

## 4.3 Caputo fractional definition

The Caputo definition of the fractional derivative was developed in response to limitations of the Riemann-Liouville fractional derivative, in terms of an unusual initial condition, $f^{\alpha}(0)$. The Caputo fractional derivative is based on the inverted sequence of operators in Equation (4-23), where an alternative decomposition of the fractional derivative into a fractional integral is followed by an integer-order derivative, $(n-1<\alpha<n)$ (Kisela, 2008; Petráš, 2010; Atangana, 2016):

$$
\begin{aligned}
{}_{a}^{C}D_{x}^{\alpha}f(x) &= {}_{a}I^{n-\alpha}\left[\frac{d^{n}}{dx^{n}}f(x)\right] \\
&= \frac{1}{\Gamma(n-\alpha)}\int_{\alpha}^{x}\frac{d^{n}}{d\tau^{n}}f(\tau)(x-\tau)^{-\alpha-n+1}\;d\tau
\end{aligned}
\qquad (4\text{-}29)
$$

where,

$^{C}D^{\alpha}$ is the Caputo differintegral operator.

The Caputo definition of the fractional derivative is different from the classical Riemann-Liouville definition, because it becomes unnecessary to define the fractional order initial condition with the Caputo definition. The Caputo definition of the fractional derivative can be applied either with the Liouville or Riemann definition of the fractional integral, where when $\alpha=0$ the Riemann definition of the fractional integral is valid (Riemann-Caputo definition), and when $a=-\infty$ the Liouville definition of the fractional integral is valid (Liouville-Caputo definition) (Petráš, 2010; Herrmann, 2011; Atangana, 2016).

The standard Caputo definition fractional derivative for a system $(0 < \alpha < 1)$ containing a singular power-kernel can be expressed as (Sun et al., 2017a):

$$ {}_{a}^{C}D_{x}^{\alpha} f(x) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{x} \frac{d}{d\tau} f(\tau)(x-\tau)^{-\alpha}\, d\tau \tag{4-30} $$

The Caputo type fractional derivative is considered a successful tool to characterise anomalous dynamics, and mathematically this is produced from the standard power-law memory kernel. However, the singularity of the power-law kernel is a source of difficulties with numerical computation and applications of fractional partial differential equations. To overcome these difficulties, a number of authors have proposed new definitions of the fractional derivative, which replaces the singular power-law kernel. Caputo and Fabrizio (2015) define a fractional derivative where the singular power-law kernel $x^{-\alpha}$ is replaced with a non-singular exponential function (Caputo and Fabrizio, 2015; Sun et al., 2017a):

$$ {}_{a}^{CF1}D_{x}^{\alpha} f(x) = \frac{M(\alpha)}{(1-\alpha)} \int_{\alpha}^{x} \frac{d}{d\tau} f(\tau)\, exp\left[-\frac{\alpha(x-\tau)}{1-\alpha}\right] d\tau \tag{4-31} $$

where,

$^{CF1}D$ denotes the Caputo and Fabrizio type derivative, and
$M(\alpha)$ is a normalisation function where $M(0) = M(1) = 1$.

Furthermore, Caputo and Fabrizio (2016) define a fractional derivative where the singular power-law kernel $x^{-\alpha}$ is replaced with a Gaussian-function and Laplace operators $(n = 1)$ (Caputo and Fabrizio, 2016; Sun *et al.*, 2017a):

$$ {}_{a}^{CF2}D_{x}^{\alpha} f(x) = \frac{1+\alpha^2}{\sqrt{\pi^2(1-\alpha)}} \int_{\alpha}^{x} \frac{d}{d\tau} f(\tau)\, exp\left[-\frac{\alpha(x-\tau)^2}{1-\alpha}\right] d\tau \tag{4-32} $$

An investigation on the application of the new Caputo-Fabrizio type derivatives was conducted by Sun et al. (2017), and found that these definitions of the fractional derivative have limitations for characterising complex anomalous relaxation and diffusion processes. Sun *et al*. (2017a) then propose an alternative notion with a stretched exponential-function kernel $(0 < \alpha < 1); n = 1$:

$$ {}_{a}^{SE}D_{x}^{\alpha} f(x) = \frac{M(\alpha)}{(1-\alpha)^{1/\alpha}} \int_{\alpha}^{x} \frac{d}{d\tau} f(\tau)\, exp\left[-\frac{\alpha(x-\tau)^{\alpha}}{1-\alpha}\right] d\tau \tag{4-33} $$

where,

$^{SE}D$ denotes the stretched exponential type Caputo definition fractional derivative operator.

## 4.4 Atangana-Baleanu fractional definitions

An alternative approach to overcome the problems associated with the singular power-law kernel was performed by Atangana and Baleanu (2016). The Atangana and Baleanu definition of the fractional derivative replaces the singular power-law kernel in a similar manner to Caputo and Fabrizio (2015), but rather considers the Mittag-Leffler function (Equation (4-9)) instead of the exponential function. Atangana and Baleanu (2016) define two versions of the Atangana and Baleanu definition of the fractional derivative, namely the Atangana-Baleanu in Caputo sense (ABC) and the Atangana-Baleanu fractional derivative in Riemann-Liouville sense (ABR).

Atangana and Baleanu (2016) state the Atangana-Baleanu fractional derivative definition will be helpful to discuss real world problems, and will have a great advantage when using the Laplace transform to solve physical problems with initial conditions. A number of applications of the Atangana-Baleanu fractional derivative definition have proven its usefulness and its ability to characterise complex anomalous processes, ranging from applications in fundamental physics to geohydrology (Atangana, 2016; Atangana and Baleanu, 2016; Aldhaifallah et al., 2016; Abdeljawad and Baleanu, 2016; Atangana and Koca, 2016; Zafar and Fetecau, 2016; Goufo et al., 2016; Omez-Aguilar and Atangana, 2017).

The Atangana-Baleanu fractional derivative in Riemann-Liouville sense (ABR) is the derivative of a convolution of a given function not necessarily differentiable with the generalized Mittag-Leffler function (Atangana and Baleanu, 2016; Abdeljawad and Baleanu, 2016) ($n = 1$):

$$ {}_{a}^{ABR}D_{t}^{\alpha} f(t) = \frac{AB(\alpha)}{(1-\alpha)} \frac{d}{dt} \int_{\alpha}^{t} f(\tau)\, E_{\alpha}\left[-\frac{\alpha}{1-\alpha}(t-\tau)^{\alpha}\right] d\tau \tag{4-34} $$

where,

$^{ABR}D$ denotes the Atangana-Baleanu in Riemann sense fractional derivative operator,

$E_{\alpha}$ denotes the Mittag-Leffler function $\left(E_{\alpha}(z^{\alpha}) = \sum_{n=0}^{\infty} \frac{z^{\alpha n}}{\Gamma(\alpha n+1)}\right)$, and

$AB(\alpha)$ is a normalization function, where

$$ AB(\alpha) = 1 - \alpha + \frac{\alpha}{\Gamma(\alpha)} \tag{4-35} $$
$$ AB(0) = AB(1) = 1 $$

The Atangana-Baleanu in Caputo sense (ABC) is the convolution of a local derivative of a given function with the generalized Mittag-Leffler function, and is defined as (Atangana and Baleanu, 2016; Aldhaifallah et al., 2016; Abdeljawad and Baleanu, 2016; Sun *et al.*, 2017a):

$$ {}_{a}^{ABC}D_{x}^{\alpha} f(t) = \frac{AB(\alpha)}{(1-\alpha)} \int_{\alpha}^{t} \frac{d}{d\tau} f(\tau)\, E_{\alpha}\left[-\frac{\alpha}{1-\alpha}(t-\tau)^{\alpha}\right] d\tau \tag{4-36} $$

where,

$^{ABC}D$ denotes the Atangana-Baleanu in Caputo sense fractional derivative operator,

### 4.4.1 Properties

Similarly to the local derivative, the properties of the non-local derivative are investigated by analysing the analytical (or exact) solution. Specifically, two fundamental integral transforms are considered, namely the Laplace transform and the Fourier transform.

**Laplace transform**

The Laplace transform of the arbitrary order α for the Riemann-Liouville and Caputo fractional derivatives, under the zero initial conditions is (Petráš, 2010):

$$\mathcal{L}\{\,_0D_t^{\alpha}f(t)\}(s) = s^{\alpha}F(s) \tag{4-37}$$

The Laplace transform of the fractional derivative is similar to the Laplace transform of an integer-order derivative, except that the Laplace space variable ($s$) is to the fractional order ($\alpha$). Considering the Atangana-Baleanu in Caputo sense (ABC) fractional derivative definition (Equation (4-36), let

$$v(t) = \frac{d}{d\tau}f(t) \tag{4-38}$$

and

$$u(t) = E_{\alpha}\left[-\frac{\alpha}{1-\alpha}t^{\alpha}\right] \tag{4-39}$$

Applying the convolution theorem ($con$) for the functions $v(t)$ and $u(t)$, the following is obtained

$$_{a}^{ABC}D_x^{\alpha}f(t) = \frac{AB(\alpha)}{1-\alpha}\left[\frac{d}{d\tau}f(t) * E_{\alpha}\left[-\frac{\alpha}{1-\alpha}t^{\alpha}\right]\right] \tag{4-40}$$

Considering,

$$\mathcal{L}(v * u) = \mathcal{L}(u)\cdot\mathcal{L}(v) \tag{4-41}$$

Then,

$$\mathcal{L}\{\,_{a}^{ABC}D_x^{\alpha}f(t)\}(s) = \frac{AB(\alpha)}{1-\alpha}\cdot\mathcal{L}\left\{\frac{d}{d\tau}f(t)\right\} * \mathcal{L}\left\{E_{\alpha}\left[-\frac{\alpha}{1-\alpha}t^{\alpha}\right]\right\} \tag{4-42}$$

Applying the standard Laplace transforms (Atangana and Koca, 2016),

$$\mathcal{L}\{\,_{a}^{ABC}D_x^{\alpha}f(t)\}(s) = \frac{AB(\alpha)}{1-\alpha}\cdot\frac{s^{\alpha}\mathcal{L}\{f(t)\}(s) - s^{\alpha-1}f(0)}{s^{\alpha}+\dfrac{\alpha}{1-\alpha}} \tag{4-43}$$

where

$\mathcal{L}\{\,_{a}^{ABC}D_t^{\alpha}f(t)\,\}$ represents the Laplace transform of function $f$ with respect to time $t$,

$s$ represents the transform domain or complex number frequency parameter ($s = \sigma + iv$).

Equation (4-43) is the Laplace transform of the ABC fractional derivative. From this analysis, it can been seen that the ABC fractional derivative produces a normal initial condition ($f(0)$), similar to the Caputo fractional derivative.

The Laplace transform of the Atangana-Baleanu fractional derivative in the Riemann-Liouville sense ((4-34) can be defined as (Atangana and Koca, 2016):

$$\mathcal{L}\{ {}_{a}^{ABR}D_t^{\alpha} f(t)\}(s) = \mathcal{L}\left\{\frac{AB(\alpha)}{(1-\alpha)} \frac{d}{dt}\int_0^t f(\tau)\, E_\alpha\left[-\frac{\alpha(t-\tau)^\alpha}{1-\alpha}\right] d\tau\right\}$$
$$= \frac{AB(\alpha)}{(1-\alpha)} \frac{s^\alpha \mathcal{L}\{f(t)\}(s)}{s^\alpha + \frac{\alpha}{1-\alpha}} \tag{4-44}$$

where,

$\mathcal{L}\{ {}_{a}^{ABR}D_t^{\alpha} f(t) \}$ represents the Laplace transform of function $f$ with respect to time $t$,

$s$ represents the transform domain or complex number frequency parameter ($s = \sigma + i\upsilon$).

**Fourier transform**

The Fourier transform of the arbitrary order α for the Riemann-Liouville and Caputo fractional derivatives, under the zero initial conditions is (Kisela, 2008):

$$\mathcal{F}\{ {}_0D_t^{\alpha} f(t)\}(\upsilon) = (i\upsilon)^\alpha F(\upsilon) \tag{4-45}$$

The Fourier transform of the fractional derivative is similar to the Fourier transform of an integer-order derivative, except that the Fourier transform space variable ($i\upsilon$) is now to the fractional order ($\alpha$). The Fourier transform of the Atangana-Baleanu fractional derivative in Caputo sense (Equation (4-36)) has been defined as (Atangana and Koca, 2016):

$$\mathcal{F}\{ {}_{a}^{ABC}D_x^{\alpha} f(t)\}(\upsilon) = \mathcal{F}\left\{\frac{AB(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau)\, E_\alpha\left[-\frac{\alpha(t-\tau)^\alpha}{1-\alpha}\right] d\tau\right\}(\upsilon)$$
$$= \frac{AB(\alpha)}{(1-\alpha)} (j\upsilon)\mathcal{F}\{f(t)\} \times \left(\frac{i\left(-1+e^{2i\alpha}\right)(-1+\alpha)\alpha|\upsilon|^{\alpha-1}(1+sgn[\upsilon])}{2\sqrt{2}(e^{\frac{3i\alpha}{2}}\alpha - |\upsilon|^\alpha + \alpha|\upsilon|^\alpha\left(\alpha - e^{\frac{i\alpha}{2}}|\upsilon|^\alpha + e^{\frac{i\alpha}{2}}|\upsilon|^\alpha\right))}\right) \tag{4-46}$$

where,

$\mathcal{F}\{ {}_{a}^{ABC}D_t^{\alpha} f(t) \}$ represents the Fourier transform of function $f$ with respect to time $t$,

$\upsilon$ represents the transform domain or complex number frequency parameter.

The Fourier transform of the Atangana-Baleanu fractional derivative in Riemann sense (Equation (4-34)) has been defined as (Atangana and Koca, 2016):

$$\mathcal{F}\{ {}_{a}^{ABR}D_t^{\alpha} f(t)\}(\upsilon) = \mathcal{F}\left\{\frac{AB(\alpha)}{(1-\alpha)} \frac{d}{dx}\int_0^x f(x)\, E_\alpha\left[-\frac{\alpha(x-u)^\alpha}{1-\alpha}\right] du\right\}(\upsilon)$$
$$= \frac{AB(\alpha)}{(1-\alpha)} \mathcal{F}\{f(t)\} \times \left(-\frac{i(-1+e^{2i\alpha}(-1+\alpha)\alpha|\upsilon|^{\alpha-1}(1+sgn[\upsilon])}{2\sqrt{2}(e^{\frac{3i\alpha}{2}}\alpha - |\upsilon|^\alpha + \alpha|\upsilon|^\alpha)(\alpha - e^{\frac{i\alpha}{2}}|\upsilon|^\alpha + e^{\frac{i\alpha}{2}}|\upsilon|^\alpha)}\right) \tag{4-47}$$

where,

$\mathcal{F}\{ {}_{a}^{ABR}D_t^{\alpha} f(t) \}$ represents the Fourier transform of function $f$ with respect to time $t$

In summary, the Laplace and Fourier transforms for the fractional derivatives are similar to those of the integer-order derivative, with the exception that the transform space is considered to the fractional order of the fractional derivative. The Laplace and Fourier transforms of the Atangana-Baleanu fractional derivative in the Caputo and Riemann-Liouville senses are presented from literature to illustrate the fractional derivatives can be analytically solved by means of these integral transforms, although they become mathematically complex.

### 4.4.2 Boundary analysis of fractional order $\alpha$

The fractional order is typically defined as $0 < \alpha < 1$, yet the extreme cases of $\alpha = 0$ and $\alpha = 1$ are investigated for the Atangana-Baleanu fractional derivative. The Atangana-Baleanu fractional derivative in the Riemann-Liouville sense when $\alpha = 0$ becomes,

$$ {}_{0}^{ABR}D_t^0 f(t) = \frac{AB(0)}{(1-0)} \frac{d}{dt} \int_0^t f(\tau)\, E_\alpha \left[ -\frac{0}{1-0} (t-\tau)^0 \right] d\tau \tag{4-48} $$

Simplifying,

$$ \begin{aligned} {}_{0}^{ABR}D_t^0 f(t) &= \frac{d}{dt} \int_0^t f(\tau)\, d\tau \\ &= f(t) \end{aligned} \tag{4-49} $$

Thus, when $\alpha = 0$, the Atangana-Baleanu fractional derivative in the Riemann-Liouville sense simplifies to the function $f(t)$.

Before the scenario is considered where $\alpha = 1$, it is stated that as per the definition of the delta Dirac function ($\delta$) (Caputo and Fabrizio, 2015):

$$ \lim_{x \to 0} \frac{1}{x} exp \left[ -\frac{1}{x} t \right] = \delta(t) \tag{4-50} $$

The Atangana-Baleanu fractional derivative in the Riemann-Liouville sense when $\alpha \to 1$,

$$ \lim_{\alpha \to 1} {}_{0}^{ABR}D_t^\alpha f(t) = \lim_{\alpha \to 1} \frac{AB(\alpha)}{(1-\alpha)} \frac{d}{dt} \int_0^t f(\tau)\; E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t-\tau)^\alpha \right] d\tau \tag{4-51} $$

It is known that the Mittag-Leffler function reduces to the exponential function when $\alpha = 1$ (Shukla and Prajapati, 2007), thus

$$ \lim_{\alpha \to 1} {}_{0}^{ABR}D_t^\alpha f(t) = \frac{d}{dt} \int_0^t f(\tau)\; \lim_{\alpha \to 1} \frac{1}{(1-\alpha)} exp \left[ -\frac{1}{1-\alpha} (t-\tau) \right] d\tau \tag{4-52} $$

Let

$$ \varepsilon = 1 - \alpha $$

Substituting in the newly defined variable ($\varepsilon$),

$$\lim_{\alpha \to 1} {}_0^{ABR}D_t^{\alpha} f(t) = \frac{d}{dt} \int_0^t f(\tau) \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} exp\left[-\frac{1}{\varepsilon}(t-\tau)\right] d\tau \tag{4-53}$$

Applying the known property of the Delta Dirac function ($\delta$), given in Equation (4-50)

$$\lim_{\alpha \to 1} {}_0^{ABR}D_t^{\alpha} f(t) = \frac{d}{dt} \int_0^t f(\tau)\, \delta(t-\tau)\, d\tau \tag{4-54}$$

Now considering the property of the Delta Dirac function (Arfken and Weber, 1999), where

$$\int F(t)\delta(t-x)dt = F(x) \tag{4-55}$$

Therefore,

$$\lim_{\alpha \to 1} {}_0^{ABR}D_t^{\alpha} f(t) = \frac{d}{dt} f(t) \tag{4-56}$$

Equation (4-56) confirms that the ABR fractional derivative is valid for the boundary condition $\alpha = 1$. Following a similar procedure the ABC fractional derivative is also found to be valid for the boundary conditions.

## 4.5 Analysis of kernels associated with fractional derivatives

A kernel describes the fundamental component of a system. In computer science, the kernel computer program forms the core of a computers operating system and controls the entire system. Drawing an analogue with computers kernel, the kernel expressed for each fractional derivative in a similar way controls how a fractional derivative operates. The significant fractional derivative definitions have been given, and to facilitate a discussion on the implication of the different definitions, the kernel associated with each definition is analysed.

To define the kernel for each fractional derivative definition, the convolution theorem is considered, which gives the inverse transform of the product of two transforms. Considering two functions $v$ and $u$, which are piecewise continuous on $t \geq 0$, the Laplace transform is (Logan, 2006):

$$\mathcal{L}(v * u)(s) = V(s)U(s) \tag{4-57}$$

The convolution of $v(t)$ and $u(t)$ is:

$$(v * u)(t) \equiv \int_0^t v(\tau)\, u(t-\tau)\, d\tau \tag{4-58}$$

and, the inverse Laplace transform is thus:

$$\mathcal{L}^{-1}\{V(s)U(s)\} = (v * u)(t) \tag{4-59}$$

The Laplace transform is additive, but not multiplicative. This means that the Laplace transform of a product is not the product of the Laplace transforms.

The convolution theorem gives the transform required to get a product of Laplace transforms, i.e. the convolution (Logan, 2006).

The Riemann-Liouville fractional derivative can be expressed for a first order derivative as

$$ {}_{0}^{RL}D_t^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{d\tau} \int_0^t f(\tau)\,(t-\tau)^{-\alpha}\,d\tau \tag{4-60} $$

Let

$$ v(t) = f(t) \tag{4-61} $$

and

$$ u(t) = \frac{1}{\Gamma(1-\alpha)} t^{-\alpha} \tag{4-62} $$

Applying the convolution theorem for the functions $v(t)$ and $u(t)$, the following is obtained

$$ (v * u)(t) = \int_0^t f(\tau) \frac{(t-\tau)^{-\alpha}}{\Gamma(1-\alpha)}\,d\tau \tag{4-63} $$

Taking the derivative,

$$ \frac{d}{dt}(v * u)(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t f(\tau)\,(t-\tau)^{-\alpha}\,d\tau \tag{4-64} $$

Equation (4-64) is the Riemann-Liouville fractional derivative, and it can thus be concluded that the convolution of functions $v(t)$ and $u(t)$ is representative of the Riemann-Liouville fractional derivative and function $u(t)$ is an expression of the Riemann-Liouville kernel.

From this perspective, it becomes clear why the Riemann-Liouville kernel is considered a singularity,

$$ \frac{1}{\Gamma(1-\alpha)} t^{-\alpha} \tag{4-65} $$

where, for values where $t = 0$, the kernel becomes undefined.

The Caputo fractional derivative can be expressed for a first order derivative as

$$ {}_{0}^{C}D_t^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau)\,(t-\tau)^{-\alpha}\,d\tau \tag{4-66} $$

Following a similar procedure as for the Riemann-Liouville fractional derivative, the Caputo kernel is also a found to contain a singularity (Equation (4-65)).

The Caputo-Fabrizio fractional derivative can be expressed for a first order derivative as

$$ {}_{0}^{CF}D_t^{\alpha} f(x) = \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau)\, exp\left[-\frac{\alpha(t-\tau)}{1-\alpha}\right] d\tau \tag{4-67} $$

Following a similar procedure, the following is found:

$$(v * u)(t) = \frac{M(\alpha)}{(1-\alpha)} \int_0^t \frac{d}{d\tau} f(\tau)\, exp\left[-\frac{\alpha(t-\tau)}{1-\alpha}\right] d\tau \tag{4-68}$$

Equation (4-68) is the Caputo-Fabrizio fractional derivative, and it can thus be concluded that the convolution of functions $v(t)$ and $u(t)$ is representative of the Caputo-Fabrizio fractional derivative, and function $u(t)$ is an expression of the Caputo-Fabrizio kernel. From this perspective, the Caputo-Fabrizio kernel is non-singular:

$$\frac{M(\alpha)}{(1-\alpha)} exp\left[-\frac{\alpha}{1-\alpha} t\right]$$

where, alpha ($\alpha$) is constrained $0 < \alpha < 1$.

The Atangana-Baleanu in Riemann sense (ABR) fractional derivative can be expressed for a first order derivative as

$${}_{a}^{ABR}D_t^{\alpha} f(t) = \frac{AB(\alpha)}{(1-\alpha)} \frac{d}{dt} \int_{\alpha}^{t} f(\tau)\, E_{\alpha}\left[-\frac{\alpha}{1-\alpha}(t-\tau)^{\alpha}\right] d\tau \tag{4-69}$$

From a similar convolution perspective, the Atangana-Baleanu in Riemann sense (ABR) kernel is found to be non-singular:

$$\frac{AB(\alpha)}{(1-\alpha)}\, E_{\alpha}\left[-\frac{\alpha}{1-\alpha} t^{\alpha}\right]$$

where, alpha ($\alpha$) is constrained $0 < \alpha < 1$.

The Atangana-Baleanu in Caputo sense (ABC) fractional derivative can be expressed for a first order derivative as

$${}_{a}^{ABC}D_x^{\alpha} f(t) = \frac{AB(\alpha)}{(1-\alpha)} \int_{\alpha}^{t} \frac{d}{d\tau} f(\tau)\, E_{\alpha}\left[-\frac{\alpha}{1-\alpha}(t-\tau)^{\alpha}\right] d\tau \tag{4-70}$$

From a similar convolution perspective, the Atangana-Baleanu in Caputo sense (ABC) kernel is the same as the ABR kernel and non-singular. The respective kernels for each fractional derivative are summarised in Table 4-1. The Riemann-Liouville and Caputo definitions of the fractional derivative contain a potential singularity within the power-law defined kernel, while the Caputo-Fabrizio and Atangana-Baleanu definitions of the fractional derivative do not contain any potential singularities within their respective exponential and Mittag-Leffler function defined kernels. The Riemann-Liouville and Caputo definitions do house a potential singularity, yet the formulation is non-local. Conversely, the Caputo-Fabrizio definition removes the potential singularity, but is considered a local operator because the variable ($t$) has no associated fractional order ($\alpha$). From this perspective, the significance of the Atangana-Baleanu definitions of the fractional derivative becomes clear, where the potential singularity is removed and the formulation retains a non-local operator.

The fractional order exponent can be interpreted as an indication of the memory capacity in empirical systems (Du et al., 2013; Tateishi et al., 2017). Additionally, the fractional order exponent introduces a non-linear time dependence in the mean square displacement of the system (Metzler and Klafter, 2000; Tateishi et al., 2017). Tateishi et al. (2017) explored this property by considering the relationship between the random walk concept and the diffusion equation. The usual random walk is characterised by Gaussian, Markovian and ergodic properties, which is related to a linear time dependence of the mean squared displacement $(\Delta x)^2 \sim t$. On the other hand, the continuous time random walk concept is characterised by non-Gaussian, non-Markovian and non-ergodic properties, which is related to non-linear dependence of the mean squared displacement $(\Delta x)^2 \sim t^{\alpha}$. Here, sub-diffusion is expressed where $\alpha < 1$, and superdiffusion where $\alpha > 1$ (Tateishi et al., 2017). From this perspective, it becomes clear why the Caputo-Fabrizio fractional derivative is local and has no memory component, because the exponential kernel has no fractional order exponent, which is an indication of the memory and non-linear time dependence. On the other hand, the Riemann-Liouville, Caputo and Atangana-Baleanu fractional derivatives are non-local and have a memory because the fractional order exponent is present in the kernel and associated with time ($t$).

**Table 4-1 Summary of kernels associated with each fractional derivative definition**

<table>
<tr><th>Fractional derivative</th><th>Kernel</th><th>Distribution</th><th>Singularity/ non-Singularity</th><th>Locality</th><th>Memory</th></tr>
<tr><td>Riemann-Liouville</td><td rowspan="2">$\frac{1}{\Gamma(1-\alpha)} t^{-\alpha}$</td><td rowspan="2">Power Law</td><td rowspan="2">Singularity</td><td rowspan="2">Non-Local</td><td rowspan="2">Yes</td></tr>
<tr><td>Caputo</td></tr>
<tr><td>Caputo-Fabrizio</td><td>$\frac{M(\alpha)}{(1-\alpha)} exp\left[-\frac{\alpha}{1-\alpha} t\right]$</td><td>Exponential</td><td>Non-Singularity</td><td>Local</td><td>No</td></tr>
<tr><td>Atangana-Baleanu in Riemann sense (ABR)</td><td rowspan="2">$\frac{AB(\alpha)}{(1-\alpha)} E_{\alpha}\left[-\frac{\alpha}{1-\alpha} t^{\alpha}\right]$</td><td rowspan="2">Mittag-Leffler</td><td rowspan="2">Non-Singularity</td><td rowspan="2">Non-Local</td><td rowspan="2">Yes</td></tr>
<tr><td>Atangana-Baleanu in Caputo sense (ABC)</td></tr>
</table>

The question is why the Riemann-Liouville and Caputo fractional derivatives contain a potential singularity within the power-law defined kernel, while Caputo-Fabrizio and Atangana-Baleanu derivatives do not. One possible explanation for this could be the order in which the fractional derivative and integral were formulated (Equation (4-23) and Equation (4-29)). The Riemann-Liouville fractional integral was first formulated, and from the integral, the derivative was derived. On the other hand, the Atangana-Baleanu fractional derivative was first formulated and then the integral was derived. Considering the natural properties of a derivative (discrete) and an integral (continuous), perhaps "squeezing" an integral into a derivative formulation could have triggered the singularity in the Riemann-Liouville and Caputo fractional definition.

For further analysis of the various fractional derivative kernels, the associated statistical probability distributions are investigated. The statistical probability distribution of finding a particle in any one place is commonly correlated to simulating the transport of a contaminant or particle. The Riemann-Liouville and Caputo fractional derivatives are associated with a power law distribution, the Caputo-Fabrizio fractional derivative is associated with an exponential function distribution, and the Atangana-Baleanu fractional derivative is associated with a Mittag-Leffler function distribution (Table 4-1). Investigating the statistical properties of each of these distributions, can provide an insight into how the kernels control the behaviour of each fractional derivative definition.

The power law probability distribution, also called the Pareto distribution, uses the power law to describe certain phenomena (See Section 4.1.2). The various statistical properties of the Pareto distribution are discussed herein. The Pareto (type I) distribution can be defined by the survival function, where the probability of a random variable ($X$) being greater than some number $x$ is expressed as (Arnold, 2008; Arnold, 2015a; Arnold, 2015b):

$$\bar{F}(x) = \Pr(X > x) = \begin{cases} \left(\frac{x_m}{x}\right)^{\alpha} & x \geq x_m, \\ 1 & x < x_m, \end{cases} \quad (4\text{-}71)$$

where,

$x_m$ is the minimum possible value of $X$ (scale parameter), and

$\alpha$ is the shape parameter (positive parameter).

Based on this definition, the cumulative distribution function has been defined as (Arnold, 2015a):

$$F_x(x) = \begin{cases} 1 - \left(\frac{x_m}{x}\right)^{\alpha} & x \geq x_m, \\ 0 & x < x_m, \end{cases} \quad (4\text{-}72)$$

Considering the differentiation of the cumulative distribution function, the probability density function has been defined as (Arnold, 2015a):

$$f(x) = \begin{cases} \frac{\alpha x_m^\alpha}{x^{\alpha+1}} & x \geq x_m, \\ 0 & x < x_m, \end{cases} \tag{4-73}$$

Therefore, the expected value of a random variable has been defined as (Arnold, 2015a):

$$E(X) = \begin{cases} \infty & \alpha \leq 1 \\ \frac{\alpha x_m}{\alpha - 1} & \alpha > 1 \end{cases} \tag{4-74}$$

The variance of a random variable has been defined as (Arnold, 2015a):

$$Var(X) = \begin{cases} \infty & \alpha \in (1,2) \\ \left(\frac{x_m}{\alpha - 1}\right)^2 \frac{\alpha}{\alpha - 1} & \alpha > 2 \end{cases} \tag{4-75}$$

From the properties of the power law distribution, it becomes clear that the expected value is undefined for values of $\alpha \leq 1$, and the variance is undefined for values of $\alpha \in (1,2)$. If the distribution is related back to the Riemann-Liouville and Caputo fractional derivative definitions, where the traditional values of the fractional order ($\alpha$) are $0 < \alpha < 1$, there is a fundamental disagreement. This disparity could be the answer to the question posed, why the Riemann-Liouville and Caputo fractional derivatives contain a potential singularity within the power-law defined kernel.

The exponential probability distribution uses the exponential function to describe certain phenomena (See Section 4.1.3). The various statistical properties of the exponential distribution are discussed herein. The general probability density function can be defined as (NIST/SEMATECH, 2003):

$$f(x) = \frac{1}{\beta} e^{-(x-\mu)/\beta} \quad x \geq \mu;\ \beta > 0 \tag{4-76}$$

where,

$\mu$ is the location parameter, and

$\beta$ is the scale parameter, often expressed as $\lambda$, which equals $\frac{1}{\beta}$.

The standard exponential distribution has been expressed for the case where $\mu = 0$ and $\beta = 1$:

$$f(x) = e^{-x} \quad x \geq 0 \tag{4-77}$$

Based on this definition, the cumulative distribution function has been defined as (NIST/SEMATECH, 2003):

$$F(x) = 1 - e^{-x/\beta} \quad x \geq 0;\ \beta > 0 \tag{4-78}$$

The expected value of a random variable following an exponential distribution has been defined as:

$$E(X) = \frac{1}{\lambda} = \beta \tag{4-79}$$

The variance of a random variable has been defined as:

$$Var(X) = \frac{1}{\lambda^2} = \beta^2 \tag{4-80}$$

From the properties of the exponential distribution, the parameter restrictions are only that $x \geq 0$; $\beta > 0$, which do not represent any fundamental disagreements when related back to the Caputo-Fabrizio fractional derivative definition.

The Mittag-Leffler probability distribution uses the Mittag-Leffler function to describe certain phenomena (See Section 4.1.4). The various statistical properties of the Mittag-Leffler distribution are discussed herein. A Mittag-Leffler statistical distribution was first explored by Pillai (1990), where the distribution function or cumulative density function was defined as (Mathai, 2010; Haubold et al., 2011, Atangana and Gómez-Aguilar, 2018):

$$G_x(x) = 1 - E_\alpha(-x^\alpha) \qquad 0 < \alpha \leq 1, x > 0 \tag{4-81}$$

Differentiating with respect to $x$, the density function $f(x)$ is obtained:

$$f(x) = \frac{dG(x)}{dx} = \sum_{n=1}^{\infty} \frac{(-1)^{n+1} x^{\alpha n}}{\Gamma(1 + \alpha n)} \tag{4-82}$$

Rearranging and replacing $n$ with $n + 1$:

$$f(x) = \frac{dG(x)}{dx} = \sum_{n=1}^{\infty} \frac{(-1)^n x^{\alpha + \alpha n - 1}}{\Gamma(1 + \alpha n)} = x^{\alpha - 1} E_{\alpha,\alpha}(-x^\alpha) \qquad 0 < \alpha \leq 1, x > 0 \tag{4-83}$$

Considering the following probability density function (Atangana and Gómez-Aguilar, 2018),

$$\cap_\alpha = \frac{1}{t} \int_0^\infty \exp[-y] \frac{\sin[\alpha\pi]}{\pi \left[ \left( \frac{\alpha t}{(1-\alpha)y} \right)^\alpha + \left( \frac{\alpha t}{(1-\alpha)y} \right)^{-\alpha} + 2\cos(\pi\alpha) \right]} dy \tag{4-84}$$

The tail probability distribution associated with the waiting time $T$ can be defined from the Equation (4-84) (Atangana and Gómez-Aguilar, 2018):

$$P(T > t) = \int_t^\infty \cap_\alpha(x) dx = E_\alpha \left[ -\frac{\alpha}{1-\alpha} t^\alpha \right] \tag{4-85}$$

From Equation (4-85) the inter-arrival time density can be defined as (Atangana and Gómez-Aguilar, 2018):

$$\chi_\alpha(t) = \frac{\alpha t^{\alpha-1}}{1-\alpha} E_{\alpha,\alpha} \left[ -\frac{\alpha}{1-\alpha} t^\alpha \right] \qquad t \geq 0 \tag{4-86}$$

It follows that when considering the n-arrival time, the corresponding probability density function can be defined as (Atangana and Gómez-Aguilar, 2018):

$$f_n^{\alpha}(t) = \frac{\alpha^{n+1}}{(1-\alpha)^n} \frac{t^{\alpha n-1}}{\Gamma(n)} E_{\alpha}^{n} \left[-\frac{\alpha}{1-\alpha} t^{\alpha}\right] \tag{4-87}$$

The moment generating function can be defined from Equation (4-87) (Atangana and Gómez-Aguilar, 2018):

$$\Omega_{\alpha}(p,t) = \sum_{j=0}^{\infty} \frac{\left(\left(\frac{\alpha}{1-\alpha} t^{\alpha}(\exp[-p]-1)\right)^{j}\right)}{\Gamma(\alpha j+1)} \tag{4-88}$$

Applying the classical formula, Equation (4-88) can be used to calculate the corresponding moment (Atangana and Gómez-Aguilar, 2018):

$$E[N(t)]^{l} = \lim_{p\to 0} \left\{ (-1)^n \frac{\partial^l}{\partial p^l} \sum_{j=0}^{\infty} \frac{\left(\left(\frac{\alpha}{1-\alpha} t^{\alpha}(\exp[-p]-1)\right)^{j}\right)}{\Gamma(\alpha j+1)} \right\} \tag{4-89}$$

Therefore, the mean of the corresponding process can be defined as (Atangana and Gómez-Aguilar, 2018):

$$\bar{m}_{\frac{\alpha}{1-\alpha}} = \sum_{n=0}^{\infty} n\, P_n^{\alpha}(t) = \frac{\alpha t^{\alpha}}{(1-\alpha)\Gamma(\alpha+1)} \tag{4-90}$$

The second moment, or variance, is thus given as (Atangana and Gómez-Aguilar, 2018):

$$\bar{m}^2{}_{\frac{\alpha}{1-\alpha}} = \sum_{n=0}^{\infty} n^2\, P_n^{\alpha}(t) = \frac{\alpha t^{\alpha}}{(1-\alpha)\Gamma(\alpha+1)} \left\{ 1 + \frac{\alpha t^{\alpha}}{(1-\alpha)\Gamma(\alpha+1)} \left[ \frac{\alpha \frac{\Gamma(\alpha)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\alpha+\frac{2}{2}\right)}}{2^{2\alpha-1}} - 1 \right] \right\} \tag{4-91}$$

From the properties of the Mittag-Leffler distribution, restrictions associated with the statistical properties do not form any fundamental disagreements with the values for $\alpha$ in the Atangana-Baleanu fractional derivative definitions.

The statistical properties associated with the respective kernel of each fractional derivative definition provides a potential explanation on the presence of a singularity in the Riemann-Liouville and Caputo fractional derivatives, while the Caputo-Fabrizio and Atangana-Baleanu contain non-singularities. The explanation being the distribution associated with the controlling kernel should not only satisfy the fractional derivative boundaries of the fractional order, but also the associated statistical boundaries.

The Riemann-Liouville and Caputo fractional derivatives have a disagreement between the fractional order boundaries and the statistical property boundaries.

In a final analysis of the fractional derivative definitions, the results of the work performed by Tateishi et al. (2017) are considered. The usual diffusion equation was generalised by means of the Riemann-Liouville, Caputo-Fabrizio and Atangana-Baleanu fractional derivatives, and the effect each kernel had on the simulated results analysed by a comparison with a continuous random walk framework. The results obtained by Tateishi et al. (2017) are in Table 4-2, where the Caputo-Fabrizio and Atangana-Baleanu fractional derivatives modify the behaviour of the waiting time distribution, as well as introduce non-Gaussian distributions and different diffusive regimes depending on the time scale. The Caputo-Fabrizio fractional derivative has a waiting time distribution described by an exponential distribution, and the probability distribution displays a stationary state as well as saturated diffusion for long times. Tateishi et al. (2017) comments that this finding is remarkable because the fractional diffusion equation is solved without external force and subject to free diffusion boundary conditions. The Atangana-Baleanu fractional derivative produces a waiting time distribution described by stretch exponential for small times, and by a power law (similar to Riemann-Liouville) for long times. Additionally, the Atangana-Baleanu fractional derivative has a probability distribution indicating a cross-over from usual diffusion for small times, and sub-diffusive for long times. It was concluded that the new fractional derivatives definitions have the potential to incorporate different memory effects, which could change the way anomalous diffusion is modelled.

**Table 4-2 Summary of results obtained by Tateishi et al. (2017) on influence on different fractional derivative definitions on the Diffusion Equation**

| Fractional derivative | Waiting time distribution / kernel distribution | Mean square displacement | Probability distribution |
|---|---|---|---|
| **Riemann-Liouville** | Power Law | Power Law and Scale invariant | Non-Gaussian |
| **Caputo-Fabrizio** | Exponential | Cross-over from usual to confined diffusion | Cross-over from Gaussian to non-Gaussian with steady state |
| **Atangana-Baleanu** | Mittag-Leffler (cross-over between a stretch Exponential to Power Law) | Cross-over from usual to sub-diffusion | Cross-over from Gaussian to non-Gaussian |

## 4.6 Fractional derivatives application to the Advection-Dispersion Equation

Following on from the work performed by Tateishi et al. (2017), which found that the new fractional derivatives could be effective in modelling anomalous diffusion, the new fractional derivatives are applied to the advection-dispersion equation to model not only anomalous diffusion, but potentially *anomalous advection* in the form of preferential pathways in fractures within the groundwater system.

It has been conceptualised that within an aquifer, water is moving within the porous media at a predictable rate, but the flow can also be faster than expected within unknown fractures or faults, and/or slower than expected in other areas. This discrepancy in the manner groundwater flows is correlated to the discrepancy in diffusion (anomalous diffusion), referred to as super-diffusion (faster than traditional methods predict) and sub-diffusion (slower than traditional methods predict).

An analogy is drawn with the conceptual groundwater flow within a fractured aquifer, where *super-advection* is defined as flow faster than traditional methods predict, and *sub-advection* as flow slower than traditional methods predict. For this reason, the fractional derivative will be applied to space for the advection term of the advection-dispersion equation.

The fractional derivative will also be applied to time because of the properties of the fractional derivatives discussed, where the waiting time distribution is defined. Incorporating the fractional derivative for time, allows these features to be activated in the advection-dispersion equation solution, i.e. for the Caputo derivative a power law distribution and for the Atangana-Baleanu derivative a Mittag-Leffler distribution, including a cross-over between a stretch exponential to power Law.

The traditional advection-dispersion equation,

$$\frac{\partial}{\partial t}c(x,t) = -v_x\frac{\partial}{\partial x}c(x,t) + D_L\frac{\partial^2}{\partial x^2}c(x,t) \tag{4-92}$$

Incorporating the fractional derivative for time and advection components,

$$D_t^{\alpha}\{c(x,t)\} = -v_x\, D_x^{\alpha}\{c(x,t)\} + D_L\frac{\partial^2}{\partial x^2}c(x,t) \tag{4-93}$$

where, $D_t^{\alpha}$ indicates the use of a fractional derivative with a fractional order $\alpha$.

This approach differs from the usual that incorporates the fractional derivative either in time (Liu et al., 2003; Povstenko, 2014; Rubbab et al., 2016), in space (but only for the diffusion/dispersion term) (Benson, 1998; Benson et al., 2000; Su et al., 2010; Wang and Wang, 2011), or in time and space (diffusion-dispersion term) (Huang and Liu, 2005; Povstenko, 2015; Javadi et al., 2016).

## 4.7 Chapter summary

Fractional calculus is outlined by presenting the functions required for the definition of fractional integrals and derivatives, fundamental fractional derivative definitions, and an analysis of the kernels associated with each fractional definition. The kernel analysis found that the Riemann-Liouville and Caputo definitions of the fractional derivative contain a potential singularity within the power-law defined kernel, while the Caputo-Fabrizio and Atangana-Baleanu definitions of the fractional derivative do not contain any potential singularities within their respective exponential and Mittag-Leffler function defined kernels. Yet, the Caputo-Fabrizio definition removes the potential singularity, but is considered a local operator, and thus the significance of the Atangana-Baleanu definitions of the fractional derivative is highlighted. Research performed by Tateishi et al. (2017) is evaluated, and it is found that the Atangana-Baleanu fractional derivative has a probability distribution indicating a cross-over from usual diffusion for small times and sub-diffusive for long times; and correlated to the potential to incorporate different memory effects, which could change the way anomalous diffusion is modelled. Lastly, a case for anomalous advection in fractured systems is made, with an application of the fractional derivative in space for the advective term and in time to activate the waiting time distribution properties.

# 5 FRACTIONAL ADVECTION-DISPERSION EQUATION WITH CAPUTO DERIVATIVE

The applicability of fractional derivative in modelling anomalous diffusion has been established by several authors (Wyss, 1986; Schneider and Wyss, 1989; Metzler et al., 1994; Metzler and Klafter, 2000; Meerschaert, 2012). Following this research, a case was made for the application of fractional derivatives to the advection-dispersion equation for modelling transport specifically in a fractured groundwater network (Benson, 1998; Benson et al., 2000). In Section 4.6, incorporating a fractional derivative for the advective term has been conceptualised.

The developed fractional advection-dispersion equation requires a solution to be of use. A myriad of methods are available to solve fractional differentials, including Laplace transform methods, Fourier transform methods, Adomian's decomposition method, Homotopy analysis method, finite difference methods, finite element methods and many more (Meerschaert and Tadjeran, 2004; Huang et al., 2008; Jafari and Tajadodi, 2015; Pang et al., 2015; Li et a., 2017). The complex nature of the formulated fractional advection-dispersion equation results in an analytical solution being challenging, and thus numerical solutions will be employed (Sousa, 2009; Meerschaert and Tadjeran, 2004; Jafari and Tajadodi, 2015). Diethelm et al. (2005) reported a need for readily usable tools to numerically solve fractional derivative problems. However, at that time only a limited collection of algorithms had been developed.

Finite difference methods for numerically solving fractional partial differential equations will be considered for the developed fractional advection-dispersion equation. A review of available finite difference numerical schemes for fractional partial differential equations is performed. A finite difference numerical method for the space fractional advection-dispersion equation, with the fractional derivative applied to the dispersion term, was presented by Meerschaert and Tadjeran (2004). Making use of the standard Grünwald estimates, Meerschaert and Tadjeran (2004) describe unconditionally stable explicit and implicit Euler methods, and a Crank-Nicolson method. Lynch et al. (2003) proposed a simple explicit method and a semi-implicit method for the space fractional diffusion equation, which are analysed for efficiency and accuracy. The semi-implicit method was found to be more effective than the explicit method. Liu et al. (2007) considered the space-time fractional advection-dispersion equation, describing an explicit and implicit difference numerical solution method. The implicit difference method was found to be unconditionally stable and convergent, while the explicit difference method was conditionally stable and convergent. Sousa (2009) generalised explicit finite difference approximations for a fractional advection-diffusion problem, where the fractional derivative was used to replace the second order derivative in the problem, were described. One of these generalisations makes use of the finite difference upwind scheme for the advection term but with a classical derivative. An original numerical approximation of the space fractional advection-dispersion equation was presented by Shen et al. (2014), where a fractional centred difference scheme was applied to the Riesz fractional derivatives. The scheme was found to have second-order accuracy, unconditionally stable, consistent and convergent. Since, the development and analysis of numerical solutions for the fractional advection-dispersion equation has remained relevant (Su et al., 2010; Wang and Wang, 2011; Sousa and Li, 2015; Liu and Hou, 2017; Owolabi and Atangana, 2017; Atangana and Owolabi, 2018; Fazio and Jannelli, 2018; Li and Rui, 2018; Liu and Li, 2018).

Upwind finite difference numerical methods have been applied to fractional partial differential equations (Yuan, 2003; Yirang et al., 2014; Yuan et al., 2017), and following on this research, the augmented upwind schemes presented in Chapter 2 for the local advection-dispersion equation will be applied to the Fractional advection-dispersion equation with Caputo fractional derivative. These numerical schemes were found to be an improvement on the traditional upwind approach, and thus selected for application on the fractional advection-dispersion equation to investigate their suitability for anomalous advection in fractured systems.

The numerical approximation schemes for the fractional advection-dispersion equation with Caputo fractional derivatives are developed using the new upwind advection Crank-Nicolson and weighted upwind-downwind schemes, as well as the traditional upwind schemes. The traditional upwind schemes serve to form a base of comparison in terms of numerical stability for the developed schemes.

## 5.1 Upwind numerical approximation schemes

The augmented upwind schemes are applied to the fractional advection-dispersion equation for numerical approximation (Equation (4-93)). Applying the Caputo definition to the fractional advection-dispersion equation,

$$ {}_{0}^{C}D_{t}^{\alpha}\left(c(x,t)\right) = -v_{x}\, {}_{0}^{C}D_{x}^{\alpha}\left(c(x,t)\right) + D_{L}\frac{\partial^{2}}{\partial x^{2}}\left(c(x,t)\right) \tag{5-1} $$

where,

$$ {}_{0}^{C}D_{t}^{\alpha}f(x) = \frac{1}{\Gamma(1-\alpha)}\int_{0}^{t}\frac{d}{d\tau}\, f(\tau)(t-\tau)^{-\alpha}\, d\tau $$

A forward difference scheme in time is applied to the Caputo fractional derivative to demonstrate the numerical approximation approach for the Caputo fractional derivative. The Caputo fractional derivative is considered for a specific time ($t_n$),

$$ {}_{a}^{C}D_{t}^{\alpha}f(t_n) = \frac{1}{\Gamma(1-\alpha)}\int_{0}^{t_n}\frac{d}{d\tau}f(\tau)\,(t_n-\tau)^{-\alpha}\, d\tau \tag{5-2} $$

The time integer-order derivative $\tau$ is replaced with the forward differences approximation at specific points in time ($t$), and a summation is used to express the integral performed for each time step,

$$ {}_{a}^{C}D_{t}^{\alpha}f(t_n) = \frac{1}{\Gamma(1-\alpha)}\left[\sum_{k=0}^{n-1}\int_{t_k}^{t_{k+1}}\frac{f_i^{k+1}-f_i^{k}}{\Delta t}\,(t_n-\tau)^{-\alpha}\, d\tau\right] \tag{5-3} $$

The approximation of the continuous $\tau$ function, results in two specific points of the function with respect to time ($t$), which allows the approximated derivative to be taken out of the integral:

$$ {}_{a}^{C}D_{t}^{\alpha}f(t_n) = \frac{1}{\Gamma(1-\alpha)}\left[\sum_{k=0}^{n-1}\frac{f_i^{k+1}-f_i^{k}}{\Delta t}\int_{t_k}^{t_{k+1}}(t^{n}-\tau)^{-\alpha}\, d\tau\right] \tag{5-4} $$

The fractional integral still requires approximation, let function $y$ represent $(t^{n}-\tau)$, $dy=-d\tau$; and the integral is reversed to consider a single time step:

$$ {}_{a}^{C}D_{t}^{\alpha}f(t_n) = \frac{1}{\Gamma(1-\alpha)}\left[\sum_{k=0}^{n-1}\frac{f_i^{k+1}-f_i^{k}}{\Delta t}\left\{-\int_{t_n-t_k}^{t_n-t_{k+1}}y^{-\alpha}\, dy\right\}\right] \tag{5-5} $$

Integrating,

$$ {}_{a}^{C}D_t^{\alpha} f(t_n) = \frac{1}{\Gamma(1-\alpha)} \left[ \sum_{k=0}^{n-1} \frac{f_i^{k+1} - f_i^k}{\Delta t} \left\{ -\frac{y^{1-\alpha}}{1-\alpha} \bigg|_{t_n - t_k}^{t_n - t_{k+1}} \right\} \right] \tag{5-6} $$

$$ {}_{a}^{C}D_t^{\alpha} f(t_n) = \frac{1}{\Gamma(1-\alpha)} \left[ \sum_{k=0}^{n-1} \frac{f_i^{k+1} - f_i^k}{\Delta t} \left\{ \frac{(t_n - t_k)^{1-\alpha} - (t_n - t_{k+1})^{1-\alpha}}{1-\alpha} \right\} \right] \tag{5-7} $$

Considering the specific time can be represented as the number of time steps required to reach that time ($t^n = \Delta t \cdot n$) and similarly, $t^k = \Delta t \cdot k$. Thus, the same can be applied to achieve $t^n - t^k = \Delta t(n-k)$ and $t^n - t^{k+1} = \Delta t(n-k-1)$:

$$ {}_{a}^{C}D_t^{\alpha} f(t_n) = \frac{1}{\Gamma(1-\alpha)} \left[ \sum_{k=0}^{n-1} \frac{f_i^{k+1} - f_i^k}{\Delta t} \left\{ -\frac{(\Delta t(n-k)\,)^{1-\alpha} - (\Delta t(n-k-1))^{1-\alpha}}{1-\alpha} \right\} \right] \tag{5-8} $$

Simplifying by moving the constant $\Delta t$, $\Delta t^{1-\alpha}$ and $1-\alpha$ out from the summation, and considering the properties of the gamma function, where $\Gamma(2-\alpha) = (1-\alpha)\Gamma(1-\alpha)$ when using integration by parts and *L'Hôpital*s rule:

$$ {}_{a}^{C}D_t^{\alpha} f(t_n) = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{k=0}^{n-1} \left( f_i^{k+1} - f_i^k \right) \{ (n-k)^{1-\alpha} - (n-k-1)^{1-\alpha} \} \right] \tag{5-9} $$

Equation (5-9) is the numerically approximated Caputo fractional derivative, where the function is considered at two discrete points in time, yet additionally the fractional components are included to account for changes in between those two discrete points in time.

### 5.1.1 Explicit upwind

The numerical approximation of the Caputo fractional derivative with respect to time has been presented in Equations (5-2) to (5-9), with the resulting scheme applied specifically to the fractional advection dispersion equation:

$$ {}_{0}^{C}D_t^{\alpha} \left( c(x_m, t_n) \right) = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{k=0}^{n-1} \left( c_m^{k+1} - c_m^k \right) \{ (n-k)^{1-\alpha} - (n-k-1)^{1-\alpha} \} \right] \tag{5-10} $$

where, a function $\delta_{n,k}^{\alpha}$ is applied to simplify,

$$ \delta_{n,k}^{\alpha} = (n-k)^{1-\alpha} - (n-k-1)^{1-\alpha} $$

Thus,

$$ {}_{0}^{C}D_t^{\alpha} \left( c(x_m, t_n) \right) = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{k=0}^{n-1} \left( c_m^{k+1} - c_m^k \right) \delta_{n,k}^{\alpha} \right] \tag{5-11} $$

Similarly, the Caputo fractional derivative with respect to space (explicit) and the upwind scheme is,

$$ {}_0^C D_x^{\alpha}\big(c(x_m,t_n)\big) = \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m}\left(c_i^{n-1}-c_{i-1}^{n-1}\right)\{(m-i)^{1-\alpha}-(m-i-1)^{1-\alpha}\}\right] \tag{5-12} $$

where, a function $\delta_{m,i}^{\alpha}$ is applied to simplify,

$$ \delta_{m,i}^{\alpha} = (m-i)^{1-\alpha} - (m-i-1)^{1-\alpha} $$

Thus,

$$ {}_0^C D_x^{\alpha}\big(c(x_m,t_n)\big) = \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m}\left(c_i^{n-1}-c_{i-1}^{n-1}\right)\delta_{m,i}^{\alpha}\right] \tag{5-13} $$

And, the local second order derivative is approximated using the traditional finite difference approach:

$$ D_L\frac{\partial^2}{\partial x^2}\big(c(x_m,t_n)\big) = D_L\left(\frac{c_{m+1}^{n-1}-2c_m^{n-1}+c_{m-1}^{n-1}}{(\Delta x)^2}\right) \tag{5-14} $$

Substituting back into Equation (5-1),

$$ \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{k=0}^{n-1}\left(c_m^{k+1}-c_m^{k}\right)\delta_{n,k}^{\alpha}\right] + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m}\left(c_i^{n-1}-c_{i-1}^{n-1}\right)\delta_{m,i}^{\alpha}\right] - D_L\left(\frac{c_{m+1}^{n-1}-2c_m^{n-1}+c_{m-1}^{n-1}}{(\Delta x)^2}\right) = 0 \tag{5-15} $$

Reformulating the following can be obtained,

$$ \begin{aligned} &\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(c_m^{n}-c_m^{n-1}\right)\delta_{n,n-1}^{\alpha} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^{k}\right)\delta_{n,k}^{\alpha}\right) \\ &\quad + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(c_m^{n-1}-c_{m-1}^{n-1}\right)\delta_{n,m}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m-1}\left(c_i^{n-1}-c_{i-1}^{n-1}\right)\delta_{m,i}^{\alpha}\right] \\ &\quad - D_L\left(\frac{c_{m+1}^{n-1}-2c_m^{n-1}+c_{m-1}^{n-1}}{(\Delta x)^2}\right) = 0 \end{aligned} \tag{5-16} $$

Rearranging,

$$ \begin{aligned} \left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right)c_m^{n} &= \left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right)c_m^{n-1} \\ &\quad + \left(v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right)c_{m-1}^{n-1} + \left(\frac{D_L}{(\Delta x)^2}\right)c_{m+1}^{n-1} \\ &\quad - \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^{k}\right)\delta_{n,k}^{\alpha}\right) - v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m-1}\left(c_i^{n-1}-c_{i-1}^{n-1}\right)\delta_{m,i}^{\alpha}\right] \end{aligned} \tag{5-17} $$

Equation (5-17) is the explicit upwind finite difference scheme for the one-dimensional, non-reactive fractional advection-dispersion equation with Caputo fractional derivatives. The numerical scheme can be simplified by substituting functions as followings,

$$b_3 c_m^{n-1} + d_3 c_{m-1}^{n-1} + f_3 c_{m+1}^{n-1} - h_3 \left( \sum_{k=0}^{n-2} \left( c_m^{k+1} - c_m^k \right) \delta_{n,k}^{\alpha} \right) - l_3 \left( \sum_{i=1}^{m-1} \left( c_i^{n-1} - c_{i-1}^{n-1} \right) \delta_{m,i}^{\alpha} \right) = a_3 c_m^n \quad (5\text{-}18)$$

where,

$$a_3 = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,n-1}^{\alpha},$$

$$b_3 = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,n-1}^{\alpha} + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2},$$

$$d_3 = v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2},$$

$$f_3 = \frac{D_L}{(\Delta x)^2},$$

$$h_3 = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)},$$

$$l_3 = v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}$$

### 5.1.2 Implicit upwind

Following the same approach, the following is obtained for the implicit upwind scheme,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{k=0}^{n-1} \left( c_m^{k+1} - c_m^k \right) \delta_{n,k}^{\alpha} \right] + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{i=1}^{m} \left( c_i^n - c_{i-1}^n \right) \delta_{m,i}^{\alpha} \right] - D_L \left( \frac{c_{m+1}^n - 2c_m^n + c_{m-1}^n}{(\Delta x)^2} \right) = 0 \quad (5\text{-}19)$$

Reformulating the following can be obtained,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left( c_m^n - c_m^{n-1} \right) \delta_{n,n-1}^{\alpha} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left( \sum_{k=0}^{n-2} \left( c_m^{k+1} - c_m^k \right) \delta_{n,k}^{\alpha} \right) + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left( c_m^n - c_{m-1}^n \right) \delta_{n,m}^{\alpha} + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{i=1}^{m-1} \left( c_i^n - c_{i-1}^n \right) \delta_{m,i}^{\alpha} \right] - D_L \left( \frac{c_{m+1}^n - 2c_m^n + c_{m-1}^n}{(\Delta x)^2} \right) = 0 \quad (5\text{-}20)$$

Rearranging,

$$\left( \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,n-1}^{\alpha} + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} \right) c_m^n = \left( \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,n-1}^{\alpha} \right) c_m^{n-1} + \left( v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} \right) c_{m-1}^n + \left( \frac{D_L}{(\Delta x)^2} \right) c_{m+1}^n - \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left( \sum_{k=0}^{n-2} \left( c_m^{k+1} - c_m^k \right) \delta_{n,k}^{\alpha} \right) - v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{i=1}^{m-1} \left( c_i^n - c_{i-1}^n \right) \delta_{m,i}^{\alpha} \right] \quad (5\text{-}21)$$

Equation (5-21) is the implicit upwind finite difference scheme for the fractional advection-dispersion equation with Caputo fractional derivatives. The numerical scheme is simplified by substituting the following functions (Equation (5-18)),

$$a_3 c_m^{n-1} = b_3 c_m^n - d_3 c_{m-1}^n - f_3 c_{m+1}^n + h_3 \left( \sum_{k=0}^{n-2} (c_m^{k+1} - c_m^k) \delta_{n,k}^{\alpha} \right) + l_3 \left( \sum_{i=1}^{m-1} (c_i^n - c_{i-1}^n)\, \delta_{m,i}^{\alpha} \right) \tag{5-22}$$

### 5.1.3 Upwind advection Crank-Nicolson scheme

The first-order upwind advection Crank-Nicolson finite difference scheme is applied, where the time component remains the same as with the first-order implicit and explicit schemes (Equation (5-10)), but the space components change to,

$${}_0^C D_x^{\alpha}\big(c(x_m, t_n)\big) = \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{i=1}^{m} \left[0.5\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + 0.5\left(c_i^n - c_{i-1}^n\right)\right] \{(m-i)^{1-\alpha} - (m-i-1)^{1-\alpha}\} \right] \tag{5-23}$$

Simplifying using the function $\delta_{m,i}^{\alpha}$,

$${}_0^C D_x^{\alpha}\big(c(x_m, t_n)\big) = \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{i=1}^{m} \left( 0.5\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + 0.5\left(c_i^n - c_{i-1}^n\right) \right) \delta_{m,i}^{\alpha} \right] \tag{5-24}$$

Substituting back into Equation (5-1),

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{k=0}^{n-1} (c_m^{k+1} - c_m^k) \delta_{n,k}^{\alpha} \right] + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{i=1}^{m} \left( 0.5\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + 0.5\left(c_i^n - c_{i-1}^n\right) \right) \delta_{m,i}^{\alpha} \right] - D_L \left( \frac{c_{m+1}^{n-1} - 2c_{im}^{n-1} + c_{m-1}^{n-1}}{(\Delta x)^2} \right) = 0 \tag{5-25}$$

Reformulating the following can be obtained,

$$\begin{aligned} &\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} (c_m^n - c_m^{n-1}) \delta_{n,n-1}^{\alpha} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left( \sum_{k=0}^{n-2} (c_m^{k+1} - c_m^k) \delta_{n,k}^{\alpha} \right) \\ &\quad + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left( 0.5(c_m^{n-1} - c_{m-1}^{n-1}) + 0.5(c_m^n - c_{m-1}^n) \right) \delta_{n,m}^{\alpha} \\ &\quad + v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{i=1}^{m-1} \left( 0.5\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + 0.5\left(c_i^n - c_{i-1}^n\right) \right) \delta_{m,i}^{\alpha} \right] \\ &\quad - D_L \left( \frac{c_{m+1}^{n-1} - 2c_m^{n-1} + c_{m-1}^{n-1}}{(\Delta x)^2} \right) = 0 \end{aligned} \tag{5-26}$$

Rearranging,

$$\left( \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,n-1}^{\alpha} + 0.5 v_x \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \delta_{n,m}^{\alpha} \right) c_m^n = \tag{5-27}$$

$$\left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} - 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2}\right)c_m^{n-1}$$
$$+\left(0.5\ v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2}\right)c_{m-1}^{n-1} + 0.5v_x\left(\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta^{\alpha}_{n,m}\right)c_{m-1}^{n}$$
$$+\left(\frac{D_L}{(\Delta x)^2}\right)c_{m+1}^{n-1} - \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{k=0}^{n-2}\left(c_m^{k+1} - c_m^k\right)\delta^{\alpha}_{n,k}\right)$$
$$- v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{i=1}^{m-1}\left(0.5\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + 0.5\left(c_i^n - c_{i-1}^n\right)\right)\delta^{\alpha}_{m,i}\right)$$

Equation (5-27) is the upwind advection Crank-Nicolson finite difference scheme for the one-dimensional, non-reactive fractional advection-dispersion equation (Caputo). The numerical scheme can be simplified by substituting functions as follows,

$$p_3c_m^{n-1} + q_3c_{m-1}^{n-1} + r_3c_{m-1}^{n} + f_3c_{m+1}^{n-1}$$
$$-h_3\left(\sum_{k=0}^{n-2}\left(c_m^{k+1} - c_m^k\right)\delta^{\alpha}_{n,k}\right) - l_3\left(\sum_{i=1}^{m-1}\left(0.5\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + 0.5\left(c_i^n - c_{i-1}^n\right)\right)\delta^{\alpha}_{m,i}\right) = o_3c_m^n \tag{5-28}$$

where,

$$o_3 = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m},$$
$$p_3 = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} - 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2},$$
$$q_3 = 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2},$$
$$r_3 = 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta^{\alpha}_{n,m},$$

### 5.1.4 Explicit upwind-downwind weighted scheme

The first-order explicit upwind-downwind weighted scheme, as described in Section 2.2.5, is applied and results in the following changes in the space fractional derivative approximation, where the ratio of upwind to downwind is controlled by $\theta$, where $0 \le \theta \le 1$,

$${}_0^C D_x^{\alpha}\left(c(x_m, t_n)\right) = \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m}\left[\theta\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + (1-\theta)\left(c_{i+1}^{n-1} - c_i^{n-1}\right)\right]\delta^{\alpha}_{m,i}\right] \tag{5-29}$$

Substituting into Equation (5-1),

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{k=0}^{n-1}\left(c_m^{k+1} - c_m^k\right)\delta^{\alpha}_{n,k}\right]$$
$$+ v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m}\left[\theta\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + (1-\theta)\left(c_{i+1}^{n-1} - c_i^{n-1}\right)\right]\delta^{\alpha}_{m,,i}\right] \tag{5-30}$$
$$-D_L\left(\frac{c_{m+1}^{n-1} - 2c_{im}^{n-1} + c_{m-1}^{n-1}}{(\Delta x)^2}\right) = 0$$

Reformulating the following can be obtained,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}(c_m^n - c_m^{n-1})\delta_{n,n-1}^{\alpha} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{k=0}^{n-2}(c_m^{k+1} - c_m^k)\delta_{n,k}^{\alpha}\right)$$
$$+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(\theta(c_m^{n-1} - c_{m-1}^{n-1}) + (1-\theta)(c_{m+1}^{n-1} - c_m^{n-1})\right)\delta_{n,m}^{\alpha}$$
$$+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m-1}\left(\theta(c_i^{n-1} - c_{i-1}^{n-1}) + (1-\theta)(c_{i+1}^{n-1} - c_i^{n-1})\right)\delta_{m,i}^{\alpha}\right]$$
$$-D_L\left(\frac{c_{m+1}^{n-1} - 2c_m^{n-1} + c_{m-1}^{n-1}}{(\Delta x)^2}\right) = 0 \tag{5-31}$$

Rearranging,

$$\left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right)c_m^n = \left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right)c_m^{n-1}$$
$$+\left(v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right)c_{m-1}^{n-1} + \left(v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right)c_{m+1}^{n-1}$$
$$-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{k=0}^{n-2}(c_m^{k+1} - c_m^k)\delta_{n,k}^{\alpha}\right)$$
$$-v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m-1}\left(\theta(c_i^{n-1} - c_{i-1}^{n-1}) + (1-\theta)(c_{i+1}^{n-1} - c_i^{n-1})\right)\delta_{m,i}^{\alpha}\right] \tag{5-32}$$

Equation (5-32) is the explicit upwind-downwind weighted finite difference scheme for the fractional advection-dispersion equation (Caputo). The numerical scheme can be simplified by substituting functions as shown,

$$s_3 c_m^{n-1} + u_3 c_{m-1}^{n-1} + v_3 c_{m+1}^{n-1} - h_3\left(\sum_{k=0}^{n-2}(c_m^{k+1} - c_m^k)\delta_{n,k}^{\alpha}\right)$$
$$-l_3\left[\sum_{i=1}^{m-1}\left(\theta\left(c_i^{n-1} - c_{i-1}^{n-1}\right) + (1-\theta)(c_{i+1}^{n-1} - c_i^{n-1})\right)\delta_{m,i}^{\alpha}\right] = a_3 c_m^n \tag{5-33}$$

where,

$$s_3 = \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}$$

$$u_3 = v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}$$

$$v_3 = v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}$$

### 5.1.5 Implicit upwind-downwind weighted scheme

Similarly, the implicit upwind-downwind weighted scheme, presented in Section 2.2.6, is applied, where the ratio of upwind to downwind is controlled by $\theta$, where $0 \leq \theta \leq 1$,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{k=0}^{n-1}\left(c_m^{k+1}-c_m^k\right)\delta_{n,k}^{\alpha}\right]+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m}[\theta(c_i^n-c_{i-1}^n)+(1-\theta)(c_{i+1}^n-c_i^n)]\,\delta_{m,,i}^{\alpha}\right] -D_L\left(\frac{c_{m+1}^n-2c_{im}^n+c_{m-1}^n}{(\Delta x)^2}\right)=0 \quad (5\text{-}34)$$

Reformulating the following can be obtained,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}(c_m^n-c_m^{n-1})\delta_{n,n-1}^{\alpha}+\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^k\right)\delta_{n,k}^{\alpha}\right) + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(\theta(c_m^n-c_{m-1}^n)+(1-\theta)(c_{m+1}^n-c_m^n)\right)\delta_{n,m}^{\alpha}+ v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m-1}\left(\theta(c_i^n-c_{i-1}^n)+(1-\theta)(c_{i+1}^n-c_i^n)\right)\delta_{m,i}^{\alpha}\right]-D_L\left(\frac{c_{m+1}^n-2c_m^n+c_{m-1}^n}{(\Delta x)^2}\right)=0 \quad (5\text{-}35)$$

Rearranging,

$$\left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}-\frac{2D_L}{(\Delta x)^2}\right)c_m^n=\left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right)c_m^{n-1} +\left(v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right)c_{m-1}^n+\left(v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right)c_{m+1}^n -\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left(\sum_{k=0}^{n-2}(c_m^{k+1}-c_m^k)\delta_{n,k}^{\alpha}\right)-v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{i=1}^{m-1}\left(\theta(c_i^n-c_{i-1}^n)+(1-\theta)(c_{i+1}^n-c_i^n)\right)\delta_{m,i}^{\alpha}\right] \quad (5\text{-}36)$$

Equation (5-36) is the implicit upwind-downwind weighted finite difference scheme for the fractional advection-dispersion equation with Caputo fractional derivative. The numerical scheme is simplified with the following functions (Equations (5-33) and (5-18)),

$$a_3c_m^{n-1}-\ h_3\left(\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^k\right)\delta_{n,k}^{\alpha}\right)-l_3\left[\sum_{i=1}^{m-1}\left(\theta\ (c_i^n-c_{i-1}^n)+(1-\theta)(c_{i+1}^n-c_i^n)\right)\delta_{m,i}^{\alpha}\right] =s_3c_m^n-u_3c_{m-1}^n-v_3c_{m+1}^n \quad (5\text{-}37)$$

This concludes the formulation of the numerical approximations schemes to be investigated for the fractional advection-dispersion equation with Caputo fractional derivative. In the following section, the numerical stability of each scheme will be analysed.

## 5.2 Numerical stability analysis

The numerical stability method used in Section 2.3 for the local operator numerical approximation schemes, will also be applied to the developed numerical approximation schemes for the fractional advection-dispersion equation with Caputo fractional derivative. The numerical stability for the upwind schemes are evaluated to validate their use in solving the fractional advection-dispersion equation with a Caputo fractional definition.

### 5.2.1 Explicit upwind

The developed finite difference explicit upwind numerical scheme presented in Section 5.1.1 is applied. Substituting induction method terms results in:

$$\begin{aligned} b_3\hat{c}_{n-1}e^{jk_ix} + d_3\hat{c}_{n-1}e^{jk_i(x-\Delta x)} + f_3\hat{c}_{n-1}e^{jk_ix(x+\Delta x)} - h_3\left(\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_mx} - \hat{c}_ke^{jk_mx}\right)\delta_{n,k}^{\alpha}\right) \\ - l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_{n-1}e^{jk_ix} - \hat{c}_{n-1}e^{jk_i(x-\Delta x)}\right)\delta_{m,i}^{\alpha}\right) = a_3\hat{c}_ne^{jk_ix} \end{aligned} \tag{5-38}$$

Multiple out,

$$\begin{aligned} & b_3\hat{c}_{n-1}e^{jk_ix} + d_3\hat{c}_{n-1}e^{jk_ix}e^{-jk_i\Delta x} + f_3\hat{c}_{n-1}e^{jk_ix}e^{jk_i\Delta x} \\ & -h_3\left(\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_mx} - \hat{c}_ke^{jk_mx}\right)\delta_{n,k}^{\alpha}\right) - l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_{n-1}e^{jk_ix} - \hat{c}_{n-1}e^{jk_ix}e^{-jk_i\Delta x}\right)\delta_{m,i}^{\alpha}\right) \\ & = a_3\hat{c}_ne^{jk_ix} \end{aligned} \tag{5-39}$$

Divide by $e^{jk_ix}$,

$$\begin{aligned} a_3\hat{c}_n = {} & b_3\hat{c}_{n-1} + d_3\hat{c}_{n-1}e^{-jk_i\Delta x} + f_3\hat{c}_{n-1}e^{jk_i\Delta x} \\ & -h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) - l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_{n-1} - \hat{c}_{n-1}e^{-jk_i\Delta x}\right)\delta_{m,i}^{\alpha}\right) \end{aligned} \tag{5-40}$$

The induction numerical stability analysis is performed in two parts; firstly it is proved for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 1$, then

$$a_3\hat{c}_1 = b_3\hat{c}_0 + d_3\hat{c}_0e^{-jk_i\Delta x} + f_3\hat{c}_0e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_0 - \hat{c}_0e^{-jk_i\Delta x}\right)\delta_{m,i}^{\alpha}\right) \tag{5-41}$$

A subset for $m$ is now considered, where $m = 1$,

$$a_3\hat{c}_1 = b_3\hat{c}_0 + d_3\hat{c}_0e^{-jk_i\Delta x} + f_3\hat{c}_0e^{jk_i\Delta x} \tag{5-42}$$

Simplifying,

$$a_3\hat{c}_1 = \left(b_3 + d_3e^{-jk_i\Delta x} + f_3e^{jk_i\Delta x}\right)\hat{c}_0 \tag{5-43}$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{b_3 + d_3e^{-jk_i\Delta x} + f_3e^{jk_i\Delta x}}{a_3} \tag{5-44}$$

Apply a norm on both sides,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|b_3| + \left|-d_3e^{-jk_i\Delta x}\right| + \left|-f_3e^{jk_i\Delta x}\right|}{|a_3|} \tag{5-45}$$

The condition thus becomes,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, the condition becomes

$$\frac{|b_3| + |d_3| + |f_3|}{|a_3|} < 1$$

It can be concluded that $|\hat{c}_1| < |\hat{c}_o|$, when

$$\frac{|b_3| + |d_3| + |f_3|}{|a_3|} < 1$$

The term is expanded using the simplification terms associated with Equation (5-18),

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right|} < 1 \tag{5-46}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2} \tag{5-47}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}} < 1 \tag{5-48}$$

Simplifying, under this assumption (Equation (5-47)), the explicit upwind numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unstable.

When the complementary assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2} \tag{5-49}$$

Then,

$$\frac{-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}} < 1 \tag{5-50}$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2} < \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} \tag{5-51}$$

Under this assumption, the finite difference first-order upwind (explicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

A subset for $m$ is now considered for all $m > 1$,

$$a_3\hat{c}_1 = b_3\hat{c}_0 + d_3\hat{c}_0 e^{-jk_i\Delta x} + f_3\hat{c}_0 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_0 - \hat{c}_0 e^{-jk_i\Delta x}\right)\delta_{m,i}^{\alpha}\right) \tag{5-52}$$

Simplifying,

$$a_3\hat{c}_1 = \left(b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(1 - e^{-jk_i\Delta x}\right)\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\hat{c}_0 \tag{5-53}$$

Remembering $\delta_{m,i}^{\alpha} = (m-i)^{1-\alpha} - (m-i-1)^{1-\alpha}$, and substitute back into Equation (5-53),

$$a_3\hat{c}_1 = \left(b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(1 - e^{-jk_i\Delta x}\right)\sum_{i=1}^{m-1}(m-i)^{1-\alpha} - (m-i-1)^{1-\alpha}\right)\hat{c}_0 \tag{5-54}$$

where, expanding the summation the following is obtained

$$\begin{aligned}\sum_{i=1}^{m-1}((m-i)^{1-\alpha} - (m-i-1)^{1-\alpha}) &= \{m^{1-\alpha} - (m-1)^{1-\alpha}\} + \{(m-1)^{1-\alpha} - (m-2)^{1-\alpha}\}\\ &+\{(m-2)^{1-\alpha} - (m-3)^{1-\alpha}\}\\ &+\{(m-3)^{1-\alpha} - (m-4)^{1-\alpha}\} + \cdots + \{-(-1)^{1-\alpha}\}\\ &= m^{1-\alpha} - (-1)^{1-\alpha}\end{aligned}$$

Simplifying and substituting,

$$a_3\hat{c}_1 = \left(b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(1 - e^{-jk_i\Delta x}\right)(m^{1-\alpha} - (-1)^{1-\alpha})\right)\hat{c}_0 \tag{5-55}$$

Let a new function simplify to,

$$\phi = k_i\Delta x$$

where,

$$e^{-j\phi} = e^{-jk_i\Delta x}$$

Remembering Euler's formula for complex numbers,

$$1 - \cos\phi + i\,sin\,\phi = 1 - e^{-i\phi}$$

Substituting back into Equation (5-55):

$$a_3\hat{c}_1 = \left(b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right)\hat{c}_0 \tag{5-56}$$

A norm is applied on both sides,

$$\begin{aligned}|a_3||\hat{c}_1| = \big(|b_3| + \left|d_3 e^{-jk_i\Delta x}\right| + \left|f_3 e^{jk_i\Delta x}\right|\\ + |-l_3|\,(|1 - \cos\phi| + i\,|sin\,\phi|)|m^{1-\alpha} - (-1)^{1-\alpha}|\big)|\hat{c}_0|\end{aligned} \tag{5-57}$$

Remembering $|e^n| = 1$,

$$|a_3||\hat{c}_1| = (|b_3| + |d_3| + |f_3| + |l_3|\,(|1 - \cos\phi| + i\,|sin\,\phi|)|m^{1-\alpha} - (-1)^{1-\alpha}|)|\hat{c}_0| \tag{5-58}$$

and,

$$\begin{aligned}|1 - \cos\phi| + i\,|sin\,\phi| &= (1 - \cos\phi)^2 + \,sin^2\,\phi\\ &= 1 - 2\cos\phi + \cos^2\phi + \,sin^2\,\phi\\ &= 2 - 2\cos\phi\end{aligned}$$

Thus,

$$|a_3||\hat{c}_1| = (|b_3| + |d_3| + |f_3| + |l_3|\,(2 - 2\cos\phi)|\beta_m|)|\hat{c}_0| \tag{5-59}$$

where,

$$\beta_m = m^{1-\alpha} - (-1)^{1-\alpha}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|b_3| + |d_3| + |f_3| + |l_3|(2 - 2\cos\phi)|\beta_m|}{|a_3|} \tag{5-60}$$

The condition required can be expressed as,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

The condition becomes,

$$\frac{|b_3| + |d_3| + |f_3| + |l_3|(2 - 2\cos\phi)|\beta_m|}{|a_3|} < 1 \tag{5-61}$$

The term is expanded using the simplification terms associated with Equation (5-18),

$$\frac{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right| \\ + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(2 - 2\cos\phi)(|\beta_m|)\end{array}\right)}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right|} < 1 \tag{5-62}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2} \tag{5-63}$$

Then,

$$\frac{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} \\ + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2 - 2\cos\phi)\beta_m\end{array}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}} < 1 \tag{5-64}$$

Simplifying, under this assumption (Equation (5-63)), the finite difference first-order upwind (explicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unstable.

When the opposite assumption is made,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2} \tag{5-65}$$

Then,

$$\frac{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}-v\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{2D_L}{(\Delta x)^2}+v\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2}\\ +v\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m\end{array}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}}<1 \tag{5-66}$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2}<\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \tag{5-67}$$

Under this assumption, the finite difference first-order upwind (explicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

Furthermore, making the assumption that $|\hat{c}_{n-1}|<|\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n\geq 1$, that

$$|\hat{c}_n|<|\hat{c}_o|$$

Rearranging Equation (5-40) for $\hat{c}_n$,

$$\begin{aligned}a_3\hat{c}_n=&\left(b_3+d_3e^{-jk_i\Delta x}+f_3e^{jk_i\Delta x}-l_3\left(1-e^{-jk_i\Delta x}\right)\left(\sum_{i=1}^{m-1}\delta^{\alpha}_{m,i}\right)\right)\hat{c}_{n-1}\\&-h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta^{\alpha}_{n,k}\right)\end{aligned} \tag{5-68}$$

Following a similar process as previously (Equation (5-56)),

$$\begin{aligned}a_3\hat{c}_n=&\left(b_3+d_3e^{-jk_i\Delta x}+f_3e^{jk_i\Delta x}-l_3(1-\cos\phi+i\sin\phi)\left(m^{1-\alpha}-(-1)^{1-\alpha}\right)\right)\hat{c}_{n-1}\\&-h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta^{\alpha}_{n,k}\right)\end{aligned} \tag{5-69}$$

Taking the norm on both sides,

$$|a_3\hat{c}_n|=\left|\begin{array}{c}\left(b_3+d_3e^{-jk_i\Delta x}+f_3e^{jk_i\Delta x}-l_3(1-\cos\phi+i\sin\phi)(m^{1-\alpha}-(-1)^{1-\alpha})\right)\hat{c}_{n-1}\\ -h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta^{\alpha}_{n,k}\right)\end{array}\right| \tag{5-70}$$

Thus,

$$\begin{aligned}|a_3||\hat{c}_n|<&\left|b_3+d_3e^{-jk_i\Delta x}+f_3e^{jk_i\Delta x}-l_3(1-\cos\phi+i\sin\phi)(m^{1-\alpha}-(-1)^{1-\alpha})\right||\hat{c}_{n-1}|\\&+|h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta^{\alpha}_{n,k}\right|\end{aligned} \tag{5-71}$$

Remembering that it has been proved that for a set $\forall\, n\geq 1$,

$$|\hat{c}_{n-1}|<|\hat{c}_o|$$

Thus,

$$
\begin{aligned}
|a_3||\hat{c}_n| &< \left|b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(1-\cos\phi + i\sin\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right||\hat{c}_{n-1}| \\
&\quad + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \\
&< \left|b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(1-\cos\phi + i\sin\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right||\hat{c}_0| \\
&\quad + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right|
\end{aligned} \tag{5-72}
$$

and, it can be inferred that,

$$
\begin{aligned}
|a_3||\hat{c}_n| < \left|b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(1-\cos\phi + i\sin\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right||\hat{c}_0| \\
+|h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right|
\end{aligned} \tag{5-73}
$$

The remaining summation is considered at the upper limit,

$$
\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| < \sum_{k=0}^{n-2}|\hat{c}_{k+1}|\left(\left|1 - \frac{\hat{c}_k}{\hat{c}_{k+1}}\right|\right)\delta_{n,k}^{\alpha} \tag{5-74}
$$

Subset $k$ will follow the same assumption made for a set $\forall\ n \geq 1$, where

$$
\sum_{k=0}^{n-2}\hat{c}_{k+1}\left(1 - \frac{\hat{c}_k}{\hat{c}_{k+1}}\right)\delta_{n,k}^{\alpha} < |\hat{c}_0|\sum_{k=0}^{n-2}\delta_{n,k}^{\alpha} \tag{5-75}
$$

Substituting back into Equation (5-73),

$$
\begin{aligned}
|a_3||\hat{c}_n| < \left|b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(1-\cos\phi + i\sin\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right||\hat{c}_0| \\
+|h_3||\hat{c}_0|\sum_{k=0}^{n-2}\delta_{n,k}^{\alpha}
\end{aligned} \tag{5-76}
$$

Expanding the summation,

$$
\begin{aligned}
\sum_{k=0}^{n-2}\delta_{n,k}^{\alpha} &= \sum_{k=0}^{n-2}((n-k)^{1-\alpha} - (n-k-1)^{1-\alpha}) \\
&= \{n^{1-\alpha} - (n-1)^{1-\alpha}\} + \{(n-1)^{1-\alpha} - (n-2)^{1-\alpha}\} + \{(n-2)^{1-\alpha} - (n-3)^{1-\alpha}\} \\
&\quad + \{(n-3)^{1-\alpha} - (n-4)^{1-\alpha}\} + \cdots + \{2^{1-\alpha} - 1^{1-\alpha}\} \\
&= n^{1-\alpha} + 2^{1-\alpha} - 1^{1-\alpha}
\end{aligned} \tag{5-77}
$$

Substituting back into Equation (5-76) and simplifying,

$$
|a_3||\hat{c}_n| < \left|b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(1-\cos\phi + i\sin\phi)\beta_m\right||\hat{c}_0| + |h_3||\hat{c}_0|\beta_n \tag{5-78}
$$

where,

$$
\beta_n = n^{1-\alpha} + 2^{1-\alpha} - 1^{1-\alpha}
$$
$$
\beta_m = m^{1-\alpha} - (-1)^{1-\alpha}
$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{\left|b_3 + d_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(1 - \cos\phi + i\, sin\,\phi)\beta_m\right| + |h_3|\beta_n}{|a_3|} \tag{5-79}$$

Remembering $|e^n| = 1$ and simplifying,

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{|b_3| + |d_3| + |f_3| + |l_3|(|1 - \cos\phi| + i\,|sin\,\phi|)\beta_m + |h_3|\beta_n}{|a_3|}$$

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{|b_3| + |d_3| + |f_3| + |l_3|(2 - 2\cos\phi)\beta_m + |h_3|\beta_n}{|a_3|} \tag{5-80}$$

Thus, the solution will be stable when,

$$\frac{|b| + |d_3| + |f_3| + |l_3|(2 - 2\cos\phi)\beta_m + |h_3|\beta_n}{|a_3|} < 1 \tag{5-81}$$

The term is expanded using the simplification terms associated with Equation (5-18),

$$\frac{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2}\right| \\ + \left|\frac{D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(2 - 2\cos\phi)\beta_m + \left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\right|\beta_n\end{array}\right)}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}\right|} < 1 \tag{5-82}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} > \frac{2D_L}{(\Delta x)^2} \tag{5-83}$$

Then,

$$\frac{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(\alpha)}(2 - 2\cos\phi)\beta_m + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n\end{array}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}} < 1 \tag{5-84}$$

Simplifying, under this assumption (Equation (5-83)), the explicit upwind numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unstable.

When the complementary assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} < \frac{2D_L}{(\Delta x)^2} \tag{5-85}$$

Then,

$$\frac{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} - v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2 - 2\cos\phi)\beta_m + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n\end{array}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}} < 1 \tag{5-86}$$

Simplifying,

$$(2+\beta_n)\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} < \frac{4D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \tag{5-87}$$

where,

$$\delta_{n,n-1}^{\alpha} = \big(n-(n-1)\big)^{1-\alpha} - (n-(n-1)-1)^{1-\alpha}$$
$$= 1^{1-\alpha}$$

Under this assumption (Equation (5-85)), the finite difference first-order upwind (explicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

It has been proved by means of the induction method that the explicit upwind finite difference scheme for the one-dimensional, non-reactive fractional advection-dispersion equation (Caputo) has the following stability criterion,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} < \frac{2D_L}{(\Delta x)^2}$$

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\big(2\delta_{n,m}^{\alpha} + (2-2\cos\phi)\beta_m\big)$$

and,

$$(2+\beta_n)\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} < \frac{4D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m$$

According to the stability analysis method applied, under these conditions, the error of the approximation is not propagated throughout the solution, but rather decreases with each time step.

### 5.2.2 Implicit upwind

The developed implicit upwind numerical scheme discussed in Section 5.1.2 (Equation (5-22)) is applied, and substituting induction method terms provides:

$$b_3\hat{c}_n e^{jk_i x} = a_3\hat{c}_{n-1}e^{jk_i x} + d_3\hat{c}_n e^{jk_i(x-\Delta x)} + f_3\hat{c}_n e^{jk_i x(x+\Delta x)}$$
$$-h_3\left(\sum_{k=0}^{n-2}\big(\hat{c}_{k+1}e^{jk_m x} - \hat{c}_k e^{jk_m x}\big)\delta_{n,k}^{\alpha}\right) - l_3\left(\sum_{i=1}^{m-1}\big(\hat{c}_n e^{jk_i x} - \hat{c}_n e^{jk_i(x-\Delta x)}\big)\,\delta_{m,i}^{\alpha}\right) \tag{5-88}$$

Multiple out,

$$b_3\hat{c}_n e^{jk_i x} = a_3\hat{c}_{n-1}e^{jk_i x} + d_3\hat{c}_n e^{jk_i x}e^{-jk_i\Delta x} + f_3\hat{c}_n e^{jk_i x}e^{jk_i\Delta x}$$
$$-h_3\left(\sum_{k=0}^{n-2}\big(\hat{c}_{k+1}e^{jk_m x} - \hat{c}_k e^{jk_m x}\big)\delta_{n,k}^{\alpha}\right) - l_3\left(\sum_{i=1}^{m-1}\big(\hat{c}_n e^{jk_i x} - \hat{c}_n e^{jk_i x}e^{-jk_i\Delta x}\big)\,\delta_{m,i}^{\alpha}\right) \tag{5-89}$$

Divide by $e^{jk_i x}$,

$$b_3\hat{c}_n = a_3\hat{c}_{n-1} + d_3\hat{c}_n e^{-jk_i\Delta x} + f_3\hat{c}_n e^{jk_i\Delta x} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) - l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_n - \hat{c}_n e^{-jk_i\Delta x}\right)\delta_{m,i}^{\alpha}\right) \tag{5-90}$$

The induction numerical stability analysis is performed in two parts; firstly it is proved for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 1$, then

$$b_3\hat{c}_1 = a_3\hat{c}_0 + d_3\hat{c}_1 e^{-jk_i\Delta x} + f_3\hat{c}_1 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_1 - \hat{c}_1 e^{-jk_i\Delta x}\right)\delta_{m,i}^{\alpha}\right) \tag{5-91}$$

A subset for $m$ is now considered, where $m = 1$,

$$b_3\hat{c}_1 = a_3\hat{c}_0 + d_3\hat{c}_1 e^{-jk_i\Delta x} + f_3\hat{c}_1 e^{jk_i\Delta x} \tag{5-92}$$

Simplifying,

$$\left(b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x}\right)\hat{c}_1 = a_3\hat{c}_0 \tag{5-93}$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{a_3}{(b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x})} \tag{5-94}$$

Applying a norm,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|a_3|}{(|b_3| + |-d_3 e^{-jk_i\Delta x}| + |-f_3 e^{jk_i\Delta x}|)} \tag{5-95}$$

The condition thus becomes:

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, it can be concluded that $|\hat{c}_1| < |\hat{c}_o|$, when

$$\frac{|a_3|}{(|b_3| + |d_3| + |f_3|)} < 1$$

The term is expanded using the simplification terms associated with Equation (5-22),

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right|}{\left(\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|\right)} < 1 \tag{5-96}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2} \tag{5-97}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}-\frac{2D_L}{(\Delta x)^2}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2}}<1 \tag{5-98}$$

Simplifying,

$$2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}>0 \tag{5-99}$$

Under this assumption (Equation (5-97)), the finite difference first-order upwind (implicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unconditionally stable.

When the corresponding assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}<\frac{2D_L}{(\Delta x)^2} \tag{5-100}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}}{-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}-v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2}}<1 \tag{5-101}$$

Simplifying,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}<\frac{2D_L}{(\Delta x)^2} \tag{5-102}$$

Under this assumption (Equation (5-100)), the implicit upwind numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

A subset for $m$ is now considered for all $m>1$,

$$b_3\hat{c}_1=a_3\hat{c}_0+d_3\hat{c}_1e^{-jk_i\Delta x}+f_3\hat{c}_1e^{jk_i\Delta x}-l_3\left(\sum_{i=1}^{m-1}\left(\hat{c}_1-\hat{c}_1e^{-jk_i\Delta x}\right)\delta_{m,i}^{\alpha}\right) \tag{5-103}$$

Simplifying,

$$\left(b_3-d_3e^{-jk_i\Delta x}-f_3e^{jk_i\Delta x}+l_3\left(1-e^{-jk_i\Delta x}\right)\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\hat{c}_1=a_3\hat{c}_0 \tag{5-104}$$

Following the same procedure as in Section 5.2.1,

$$(|b_3|+|d_3|+|f_3|+|l_3|\,(2-2\cos\phi)|\beta_m|)|\hat{c}_1|=|a_3||\hat{c}_0| \tag{5-105}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|}=\frac{|a_3|}{(|b_3|+|d_3|+|f_3|+|l_3|\,(2-2\cos\phi)|\beta_m|)} \tag{5-106}$$

The condition thus becomes,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

And, substituting the following is found,

$$\frac{|a_3|}{\left(|b_3| + |d_3| + |f_3| + |l|\,(2 - 2\cos\phi)(|\beta_m|)\right)} < 1 \tag{5-107}$$

The term is expanded using the simplification terms associated with Equation (5-22),

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}\right|}{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right| \\ + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(2 - 2\cos\phi)(|\beta_m|)\end{array}\right)} < 1 \tag{5-108}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} > \frac{2D_L}{(\Delta x)^2} \tag{5-109}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}}{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2} + v\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} \\ + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2 - 2\cos\phi)\beta_m\end{array}\right)} < 1 \tag{5-110}$$

Simplifying,

$$v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(2\delta^{\alpha}_{n,m} + (2 - 2\cos\phi)\beta_m\right) > 0 \tag{5-111}$$

Under this assumption (Equation (5-109)), the implicit upwind numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unconditionally stable.

When the complementary assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} < \frac{2D_L}{(\Delta x)^2} \tag{5-112}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}}{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} - v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} \\ + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2 - 2\cos\phi)(\beta_m)\end{array}\right)} < 1 \tag{5-113}$$

Simplifying,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} < \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1 - 1\cos\phi)\beta_m \tag{5-114}$$

Under this assumption (Equation (5-112)), the finite difference first-order upwind (implicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

It is assumed that $|\hat{c}_{n-1}| < |\hat{c}_o|$ is true for all time steps is made, and the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_n| < |\hat{c}_o|$$

Rearranging Equation (5-90) for $\hat{c}_n$,

$$\left(b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3\left(1 - e^{-jk_i\Delta x}\right)\left(\sum_{i=1}^{m-1} \delta_{m,i}^{\alpha}\right)\right)\hat{c}_n = a_3\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) \tag{5-115}$$

Following a similar process as previously (Equation (5-105)),

$$\left(b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right)\hat{c}_n = a_3\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) \tag{5-116}$$

Taking the norm on both sides,

$$\left|\left(b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right)\hat{c}_n\right| = \left|a_3\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right)\right| \tag{5-117}$$

Thus,

$$\left|b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right||\hat{c}_n| < |a_3||\hat{c}_{n-1}| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{5-118}$$

Remembering that it has been proved that for a set $\forall\, n \geq 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Thus,

$$\left|b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right||\hat{c}_n| < |a_3||\hat{c}_{n-1}| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| < |a_3||\hat{c}_0| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{5-119}$$

and, it can be inferred that,

$$\left|b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right||\hat{c}_n| < |a_3||\hat{c}_0| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{5-120}$$

The remaining summation is considered at the upper limit and simplifying as in Section 5.2.1,

$$\left|b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3(1 - \cos\phi + i\,sin\,\phi)\beta_m\right||\hat{c}_n| < |a_3||\hat{c}_0| + |h_3||\hat{c}_0|\beta_n \tag{5-121}$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{|a_3| + |h_3|\beta_n}{\left|\left|b_3 - d_3 e^{-jk_i\Delta x} - f_3 e^{jk_i\Delta x} + l_3(1 - \cos\phi + i\,sin\,\phi)\beta_m\right|\right|} \tag{5-122}$$

Remembering $|e^n| = 1$ and simplifying,

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{|a_3| + |h_3|\beta_n}{|b_3| + |d_3| + |f_3| + |l_3|(2 - 2\cos\phi)\beta_m} \tag{5-123}$$

Thus, the solution will be stable when,

$$\frac{|a_3| + |h_3|\beta_n}{|b_3| + |d_3| + |f_3| + |l_3|(2 - 2\cos\phi)\beta_m} < 1 \tag{5-124}$$

The term is expanded using the simplification terms associated with Equation (5-22),

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}\right| + \left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\right|\beta_n}{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(\alpha)}\delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2}\right| \\ + \left|\frac{D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(2 - 2\cos\phi)\beta_m\end{array}\right)} < 1 \tag{5-125}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} > \frac{2D_L}{(\Delta x)^2} \tag{5-126}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n}{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} - \frac{2D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} + \frac{D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2 - 2\cos\phi)\beta_m\end{array}\right)} < 1 \tag{5-127}$$

Simplifying,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(2\delta^{\alpha}_{n,m} + (2 - 2\cos\phi)\beta_m\right) \tag{5-128}$$

Under this assumption (Equation (5-126)), the implicit upwind numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

When the opposite assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m} < \frac{2D_L}{(\Delta x)^2} \tag{5-129}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}+\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n}{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}-v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\\ +\frac{D_L}{(\Delta x)^2}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m\end{array}\right)}<1 \tag{5-130}$$

Simplifying,

$$(2+\beta_n)\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}<\frac{4D_L}{(\Delta x)^2}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \tag{5-131}$$

Under this assumption (Equation (5-129)), the implicit upwind numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

It has been proven by means of the induction method that the first-order implicit upwind finite difference scheme for the fractional advection-dispersion equation (Caputo) has the following stability criterion,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}<\frac{2D_L}{(\Delta x)^2}$$

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n<v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(2\delta_{n,m}^{\alpha}+(2-2\cos\phi)\beta_m\right)$$

and

$$(2+\beta_n)\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}<\frac{4D_L}{(\Delta x)^2}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m$$

Under these conditions, the error of the approximation decreases with each time step, as according to the induction method, where for all values of n, $|\hat{c}_{n+1}|<|\hat{c}_o|$.

### 5.2.3 Upwind advection Crank-Nicolson scheme

The developed upwind advection Crank-Nicolson numerical scheme offered in Section 5.1.3 (Equation (5-28) is applied, and the substituting induction method terms results in,

$$\begin{aligned}o_3\hat{c}_n e^{jk_ix} &= p_3\hat{c}_{n-1}e^{jk_ix}+q_3\hat{c}_{n-1}e^{jk_i(x-\Delta x)}-r_3\hat{c}_n e^{jk_i(x-\Delta x)}\\ &+f_3\hat{c}_{n-1}e^{jk_i(x+\Delta x)}-h_3\left(\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_mx}-\hat{c}_k e^{jk_mx}\right)\delta_{n,k}^{\alpha}\right)\\ &-l_3\left(\sum_{i=1}^{m-1}\left(0.5\left(\hat{c}_{n-1}e^{jk_ix}-\hat{c}_{n-1}e^{jk_i(x-\Delta x)}\right)+0.5\left(\hat{c}_n e^{jk_ix}-\hat{c}_n e^{jk_i(x-\Delta x)}\right)\right)\delta_{m,i}^{\alpha}\right)\end{aligned} \tag{5-132}$$

Multiple out,

$$o_3\hat{c}_n e^{jk_ix} = p_3\hat{c}_{n-1}e^{jk_ix} + q_3\hat{c}_{n-1}e^{jk_ix}e^{-jk_i\Delta x} - r_3\hat{c}_n e^{jk_ix}e^{-jk_i\Delta x} + f_3\hat{c}_{n-1}e^{jk_ix}e^{jk_i\Delta x} - h_3\left(\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_mx} - \hat{c}_k e^{jk_mx}\right)\delta_{n,k}^{\alpha}\right) - l_3\left(\sum_{i=1}^{m-1}\left(0.5\left(\hat{c}_{n-1}e^{jk_ix} - \hat{c}_{n-1}e^{jk_ix}e^{-jk_i\Delta x}\right) + 0.5\left(\hat{c}_n e^{jk_ix} - \hat{c}_n e^{jk_ix}e^{-jk_i\Delta x}\right)\right)\delta_{m,i}^{\alpha}\right) \quad (5\text{-}133)$$

Divide by $e^{jk_ix}$,

$$o_3\hat{c}_n = p_3\hat{c}_{n-1} + q_3\hat{c}_{n-1}e^{-jk_i\Delta x} - r_3\hat{c}_n e^{-jk_i\Delta x} + f_3\hat{c}_{n-1}e^{jk_i\Delta x} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) - l_3\left(\sum_{i=1}^{m-1}\left(0.5\left(\hat{c}_{n-1} - \hat{c}_{n-1}e^{-jk_i\Delta x}\right) + 0.5\left(\hat{c}_n - \hat{c}_n e^{-jk_i\Delta x}\right)\right)\delta_{m,i}^{\alpha}\right) \quad (5\text{-}134)$$

The induction numerical stability analysis is performed in two parts; firstly it is proved for a set $\forall\, n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 1$, then

$$o_3\hat{c}_1 = p_3\hat{c}_0 + q_3\hat{c}_0 e^{-jk_i\Delta x} - r_3\hat{c}_1 e^{-jk_i\Delta x} + f_3\hat{c}_0 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(0.5\left(\hat{c}_0 - \hat{c}_0 e^{-jk_i\Delta x}\right) + 0.5\left(\hat{c}_1 - \hat{c}_1 e^{-jk_i\Delta x}\right)\right)\delta_{m,i}^{\alpha}\right) \quad (5\text{-}135)$$

A subset for $m$ is now considered, where $m = 1$,

$$o_3\hat{c}_1 = p_3\hat{c}_0 + q_3\hat{c}_0 e^{-jk_i\Delta x} - r_3\hat{c}_1 e^{-jk_i\Delta x} + f_3\hat{c}_0 e^{jk_i\Delta x} \quad (5\text{-}136)$$

Simplifying,

$$\left(o_3 + f e^{-jk_i\Delta x}\right)\hat{c}_1 = \left(p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x}\right)\hat{c}_0 \quad (5\text{-}137)$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x}}{o_3 + r_3 e^{-jk_i\Delta x}} \quad (5\text{-}138)$$

Applying the norm,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|p_3| + \left|q_3 e^{-jk_i\Delta x}\right| + \left|f_3 e^{jk_i\Delta x}\right|}{|o_3| + |r_3 e^{-jk_i\Delta x}|} \quad (5\text{-}139)$$

The condition required can be expressed as,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, it can be established that $|\hat{c}_1| < |\hat{c}_o|$, when

$$\frac{|p_3| + |q_3| + |f_3|}{|o_3| + |r_3|} < 1$$

The term is expanded using the simplification terms associated with Equation (5-28),

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}\right| + \left|0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha}\right|} < 1 \quad (5\text{-}140)$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} > 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \quad (5\text{-}141)$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}} < 1 \quad (5\text{-}142)$$

Simplifying,

$$v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > 0 \quad (5\text{-}143)$$

Under this assumption (Equation (5-141)), the upwind advection Crank-Nicolson scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unconditionally stable.

The complementary assumption is made,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} < 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \quad (5\text{-}144)$$

Then,

$$\frac{-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha}} < 1 \quad (5\text{-}145)$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2} < \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \quad (5\text{-}146)$$

Under the assumption made in Equation (5-144), the upwind advection Crank-Nicolson numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

A subset for $m$ is now considered for all $m > 1$,

$$o_3\hat{c}_1 = p_3\hat{c}_0 + q_3\hat{c}_0e^{-jk_i\Delta x} - r_3\hat{c}_1e^{-jk_i\Delta x} + f_3\hat{c}_0e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(0.5\left(\hat{c}_0 - \hat{c}_0e^{-jk_i\Delta x}\right) + 0.5\left(\hat{c}_1 - \hat{c}_1e^{-jk_i\Delta x}\right)\right)\delta_{m,i}^{\alpha}\right) \quad (5\text{-}147)$$

Simplifying,

$$\left(o_3 + r_3 e^{-jk_i\Delta x} + 0.5 l_3\left(1 - e^{-jk_i\Delta x}\right)\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\hat{c}_1 = \left(p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - 0.5 l_3\left(1 - e^{-jk_i\Delta x}\right)\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\hat{c}_0 \tag{5-148}$$

Following the same procedure as in Section 5.2.1,

$$\left(o_3 + r_3 e^{-jk_i\Delta x} + 0.5 l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right)\hat{c}_1 = \left(p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - 0.5 l_3(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right)\hat{c}_0 \tag{5-149}$$

Applying a norm on both sides,

$$\left(|o_3| + \left|r_3 e^{-jk_i\Delta x}\right| + 0.5|l_3|(|1 - \cos\phi| + i\,|sin\,\phi|)(|m^{1-\alpha} - (-1)^{1-\alpha}|)\right)|\hat{c}_1| = \left(|p_3| + \left|q_3 e^{-jk_i\Delta x}\right| + \left|f_3 e^{jk_i\Delta x}\right| + 0.5|l_3|(|1 - \cos\phi| + i\,|sin\,\phi|)(|m^{1-\alpha} - (-1)^{1-\alpha}|)\right)|\hat{c}_0| \tag{5-150}$$

Remembering $|e^n| = 1$ and the procedure followed in Section 5.2.1,

$$(|o_3| + |r_3| + 0.5|l_3|(2 - 2\cos\phi)\beta_m)|\hat{c}_1| = (|p_3| + |q_3| + |f_3| + 0.5|l_3|(2 - 2\cos\phi)\beta_m)|\hat{c}_0| \tag{5-151}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|p_3| + |q_3| + |f_3| + 0.5|l_3|(2 - 2\cos\phi)\beta_m}{(|o_3| + |r_3| + 0.5|l_3|(2 - 2\cos\phi)\beta_m)} \tag{5-152}$$

The condition required can be expressed as:

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Thus, the condition becomes,

$$\frac{|p_3| + |q_3| + |f_3| + 0.5|l_3|(2 - 2\cos\phi)\beta_m}{(|o_3| + |r_3| + 0.5|l_3|(2 - 2\cos\phi)\beta_m)} < 1 \tag{5-153}$$

The term is expanded using the simplification terms associated with Equation (5-28),

$$\frac{\left(\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - 0.5 v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5 v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right| + 0.5\left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(2 - 2\cos\phi)\beta_m\right)}{\left(\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5 v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}\right| + \left|0.5 v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha}\right| + 0.5\left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(2 - 2\cos\phi)\beta_m\right)} < 1 \tag{5-154}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} > 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \tag{5-155}$$

Then,

$$\frac{\left(\begin{matrix}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(\alpha)}(2-2\cos\phi)\beta_m\end{matrix}\right)}{\left(\begin{matrix}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} \\ +0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m\end{matrix}\right)} < 1 \tag{5-156}$$

Simplifying,

$$v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > 0 \tag{5-157}$$

Under the assumption made in Equation (5-155), the upwind advection Crank-Nicolson scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unconditionally stable.

When the complementary assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} < 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \tag{5-158}$$

Then,

$$\frac{\left(\begin{matrix}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m\end{matrix}\right)}{\left(\begin{matrix}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{0.5(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + v_x\frac{0.5(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} \\ +0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m\end{matrix}\right)} < 1 \tag{5-159}$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2} < \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \tag{5-160}$$

Under this assumption (Equation (5-158)), the upwind advection Crank-Nicolson scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

Secondly, it is assumed that $|\hat{c}_{n-1}| < |\hat{c}_o|$ is true for all time steps, and the second component of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_n| < |\hat{c}_o|$$

Rearranging Equation (5-134) for $\hat{c}_n$,

$$\left(o_3 + r_3 e^{-jk_i\Delta x} + \ l\left(0.5\left(1 - e^{-jk_i\Delta x}\right)\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\right)\hat{c}_n$$
$$= \left(p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(0.5\left(1 - e^{-jk_i\Delta x}\right)\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\right)\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) \quad (5\text{-}161)$$

Following a similar process as previously,

$$\left(o_3 + r_3 e^{-jk_i\Delta x} + l_3\left(0.5(1 - \cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right)\hat{c}_n$$
$$= \left(p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(0.5(1 - \cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right)\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) \quad (5\text{-}162)$$

Taking the norm on both sides,

$$\left|\left(o_3 + r_3 e^{-jk_i\Delta x} + l_3\left(0.5(1 - \cos\phi + i\,sin\,\phi)(m^{1-\alpha} - (-1)^{1-\alpha})\right)\right)\hat{c}_n\right|$$
$$= \left|\left(p_3 + q_3 e^{jk_i\Delta x}... \right.\right.$$

Thus,

$$\left|o_3 + r_3 e^{-jk_i\Delta x} + l_3\left(0.5(1 - \cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right||\hat{c}_n|$$
$$< \left|p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(0.5(1 - \cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right||\hat{c}_{n-1}| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \quad (5\text{-}164)$$

Remembering that it has been proved that for a set $\forall\ n \geq 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Thus,

$$\left|o_3 + r_3 e^{-jk_i\Delta x} + l_3\left(0.5(1 - \cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right||\hat{c}_n|$$
$$< \left|p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(0.5(1 - \cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right||\hat{c}_{n-1}| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \quad (5\text{-}165)$$

$$< \left|p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(0.5(1-\cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right| |\hat{c}_0| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right|$$

and, it can be inferred that,

$$\left|o_3 + r_3 e^{-jk_i\Delta x} + l_3\left(0.5(1-\cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right| |\hat{c}_n| < \left|p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3\left(0.5(1-\cos\phi + i\,sin\,\phi)\left(m^{1-\alpha} - (-1)^{1-\alpha}\right)\right)\right| |\hat{c}_0| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{5-166}$$

A simplification is performed as in Section 5.2.1,

$$\left|o_3 + r_3 e^{-jk_i\Delta x} + l_3(0.5(1-\cos\phi + i\,sin\,\phi)\beta_m)\right||\hat{c}_n| < \left|p_3 + q_3 e^{-jk_i\Delta x} + f_3 e^{jk_i\Delta x} - l_3(0.5(1-\cos\phi + i\,sin\,\phi)\beta_m)\right||\hat{c}_0| + |h_3||\hat{c}_0|\beta_n \tag{5-167}$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{|p_3| + |q_3| + |f_3| + 0.5|l_3|(2-2\cos\phi)\beta_m + |h_3|\beta_n}{|o_3| + |r_3| + |l_3|(2-2\cos\theta)\beta_m} \tag{5-168}$$

Thus, the solution will be stable when,

$$\frac{|p_3| + |q_3| + |f_3| + 0.5|l_3|(2-2\cos\phi)\beta_m + |h_3|\beta_n}{|o_3| + |r_3| + |l_3|(2-2\cos\phi)\beta_m} < 1 \tag{5-169}$$

The term is expanded using the simplification terms associated with Equation (5-28),

$$\frac{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\;\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\;\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| \\ + \left|\frac{D_L}{(\Delta x)^2}\right| + 0.5\left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|\left((2-2\cos\phi)\beta_m\right) + \left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\right|\beta_n\end{array}\right)}{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}\right| + \left|0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\;\delta_{n,m}^{\alpha}\right| \\ + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(2-2\cos\phi)\beta_m\end{array}\right)} < 1 \tag{5-170}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} > v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \tag{5-171}$$

Then,

$$\frac{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - v_x\frac{0.5(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + v_x\frac{0.5(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\\ + \frac{D_L}{(\Delta x)^2} + \ 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\Big((2-2\cos\phi)\beta_m\Big) + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n\end{array}\right)}{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{0.5(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + v_x\frac{0.5(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha}\\ +v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m\end{array}\right)} < 1 \qquad (5\text{-}172)$$

Simplifying,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\Big(\delta_{n,m}^{\alpha} \ + 0.5\beta_m(2-2\cos\phi)\Big) \qquad (5\text{-}173)$$

The assumption made in Equation (5-171), leads to a conditionally stable result for the upwind advection Crank-Nicolson scheme.

When the complementary assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \qquad (5\text{-}174)$$

Then,

$$\frac{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\\ + \frac{D_L}{(\Delta x)^2} + \ 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\Big((2-2\cos\phi)\beta_m\Big) + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n\end{array}\right)}{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\ \delta_{n,m}^{\alpha}\\ +v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m\end{array}\right)} < 1 \qquad (5\text{-}175)$$

Simplifying,

$$\frac{4D_L}{(\Delta x)^2} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < \frac{2(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \qquad (5\text{-}176)$$

Under this assumption (Equation (5-174)), the upwind advection Crank-Nicolson scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

The stability criterion for the upwind advection Crank-Nicolson finite difference scheme for the fractional advection-dispersion equation (Caputo) has been determined by the induction method. The stability criteria are thus as follows,

$$\frac{2D_L}{(\Delta x)^2} < \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)},$$

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\Big(\delta_{n,m}^{\alpha} \ + \beta_m(1-\cos\phi)\Big),$$

and,

$$\frac{4D_L}{(\Delta x)^2}+\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n<\frac{2(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(\alpha)}(1-\cos\phi)\beta_m$$

Under these conditions, the error of the approximation is not propagated throughout the solution, but rather decreases with each time step, where for all values of n, $|\hat{c}_{n+1}|<|\hat{c}_o|$.

### 5.2.4 Explicit upwind-downwind weighted scheme

To perform the stability analysis, induction method terms are substituted into the explicit upwind-downwind weighted numerical scheme presented in Section 5.1.4,

$$\begin{aligned}a_3\hat{c}_n e^{jk_ix} &= s_3\hat{c}_{n-1}e^{jk_ix}+u_3\hat{c}_{n-1}e^{jk_i(x-\Delta x)}+v_3\hat{c}_{n-1}e^{jk_i(x+\Delta x)}\\ &\quad -h_3\left(\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_mx}-\hat{c}_ke^{jk_mx}\right)\delta_{n,k}^{\alpha}\right)\\ &\quad -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_{n-1}e^{jk_ix}-\hat{c}_{n-1}e^{jk_i(x-\Delta x)}\right)+(1-\theta)\left(\hat{c}_{n-1}e^{jk_i(x+\Delta x)}-\hat{c}_{n-1}e^{jk_ix}\right)\right)\delta_{m,i}^{\alpha}\right)\end{aligned} \tag{5-177}$$

Multiple out,

$$\begin{aligned}a_3\hat{c}_n e^{jk_ix} &= s_3\hat{c}_{n-1}e^{jk_ix}+u_3\hat{c}_{n-1}e^{jk_ix}e^{-jk_i\Delta x}+v_3\hat{c}_{n-1}e^{jk_ix}e^{jk_i\Delta x}\\ &\quad -h_3\left(\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_mx}-\hat{c}_ke^{jk_mx}\right)\delta_{n,k}^{\alpha}\right)\\ &\quad -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_{n-1}e^{jk_ix}-\hat{c}_{n-1}e^{jk_ix}e^{-jk_i\Delta x}\right)+(1-\theta)\left(\hat{c}_{n-1}e^{jk_ix}e^{jk_i\Delta x}-\hat{c}_{n-1}e^{jk_ix}\right)\right)\delta_{m,i}^{\alpha}\right)\end{aligned} \tag{5-178}$$

Divide by $e^{jk_ix}$,

$$\begin{aligned}a_3\hat{c}_n &= s_3\hat{c}_{n-1}+u_3\hat{c}_{n-1}e^{-jk_i\Delta x}+v_3\hat{c}_{n-1}e^{jk_i\Delta x}-h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right)\\ &\quad -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_{n-1}-\hat{c}_{n-1}e^{-jk_i\Delta x}\right)+(1-\theta)\left(\hat{c}_{n-1}e^{jk_i\Delta x}-\hat{c}_{n-1}\right)\right)\delta_{m,i}^{\alpha}\right)\end{aligned} \tag{5-179}$$

The induction numerical stability analysis is performed in two parts; firstly it is proved for a set $\forall\, n>1$,

$$|\hat{c}_n|<|\hat{c}_o|$$

If $n=1$, then

$$a_3\hat{c}_1=s_3\hat{c}_0+u_3\hat{c}_0e^{-jk_i\Delta x}+v_3\hat{c}_0e^{jk_i\Delta x}-\ l_3\left(\sum_{i=1}^{m-1}\left(\theta(\hat{c}_0-\hat{c}_0e^{-jk_i\Delta x})+(1-\theta)(\hat{c}_0e^{jk_i\Delta x}-\hat{c}_0)\right)\delta_{m,i}^{\alpha}\right) \tag{5-180}$$

A subset for $m$ is now considered, where $m=1$,

$$a_3\hat{c}_1=s_3\hat{c}_0+u_3\hat{c}_0e^{-jk_i\Delta x}+v_3\hat{c}_0e^{jk_i\Delta x} \tag{5-181}$$

Simplifying,

$$a_3\hat{c}_1 = \left(s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x}\right)\hat{c}_0 \tag{5-182}$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x}}{a_3} \tag{5-183}$$

Applying the norm on both sides,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|s_3| + \left|u_3 e^{-jk_i\Delta x}\right| + \left|v_3 e^{-jk_i\Delta x}\right|}{|a_3|} \tag{5-184}$$

The condition can thus be represented as,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

And, remembering $|e^n| = 1$, the condition is,

$$\frac{|s_3| + |u_3| + |v_3|}{|a_3|} < 1$$

The term is expanded using the simplification terms associated with Equation (5-33),

$$\frac{\left(\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right|\right)}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right|} < 1 \tag{5-185}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2} \tag{5-186}$$

Then,

$$\frac{\left(\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}} < 1 \tag{5-187}$$

Under this assumption (Equation (5-186)), the explicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unstable.

When the opposite assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2} \tag{5-188}$$

Then,

$$\frac{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}-v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\\ +v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\end{array}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}}<1 \tag{5-189}$$

Simplifying,

$$v_x(1-2\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{2D_L}{(\Delta x)^2}<\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \tag{5-190}$$

Under this assumption (Equation (5-188)), the explicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

A subset for $m$ is now considered for all $m>1$,

$$\begin{aligned}a_3\hat{c}_1 &= s_3\hat{c}_0+u_3\hat{c}_0e^{-jk_i\Delta x}+v_3\hat{c}_0e^{jk_i\Delta x}\\ &\qquad -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_0-\hat{c}_0e^{-jk_i\Delta x}\right)+(1-\theta)\left(\hat{c}_0e^{jk_i\Delta x}-\hat{c}_0\right)\right)\delta_{m,i}^{\alpha}\right)\end{aligned} \tag{5-191}$$

Simplifying,

$$a_3\hat{c}_1=\left(\begin{array}{c}s_3+u_3e^{-jk_i\Delta x}+v_3e^{jk_i\Delta x}-l_3\theta\left(1-e^{-jk_i\Delta x}\right)\left(\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\\ -l_3(1-\theta)\left(e^{jk_i\Delta x}-1\right)\left(\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\end{array}\right)\hat{c}_0 \tag{5-192}$$

Considering,

$$\begin{aligned}\left\|e^{jk_i\Delta x}-1\right\| &= (\cos\phi-1)^2+\ sin^2\phi\\ &= \cos^2\phi+sin^2\phi-2\cos\phi+1\\ &= 2-2\cos\phi\end{aligned}$$

Thus,

$$|a_3||\hat{c}_1|=(|s_3|+|u_3|+|v_3|+|l_3|\theta(2-2\cos\phi)\beta_m+\ |l_3|(1-\theta)(2-2\cos\phi)\beta_m)|\hat{c}_0| \tag{5-193}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|}=\frac{|s_3|+|u_3|+|v_3|+|l_3|\theta(2-2\cos\phi)\beta_m+\ |l_3|(1-\theta)(2-2\cos\phi)\beta_m}{|a_3|} \tag{5-194}$$

The stability condition required transforms to,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|}<1$$

The condition becomes,

$$\frac{|s_3|+|u_3|+|v_3|+|l_3|\theta(2-2\cos\phi)\beta_m+\ |l_3|(1-\theta)(2-2\cos\phi)\beta_m}{|a_3|}<1 \tag{5-195}$$

The term is expanded using the simplification terms associated with Equation (5-33),

$$\frac{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}-\frac{2D_L}{(\Delta x)^2}\right|+\left|v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right| \\ +\left|v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right|+\left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|\theta(2-2\cos\phi)\beta_m \\ +\left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(1-\theta)(2-2\cos\phi)\beta_m\end{array}\right)}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\right|}<1 \tag{5-196}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}>\frac{2D_L}{(\Delta x)^2} \tag{5-197}$$

Then,

$$\frac{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}-\frac{2D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2} \\ +v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \\ +v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m\end{array}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}}<1 \tag{5-198}$$

Simplifying, it becomes clear that the upwind-downwind weighted (explicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unstable.

Making the complementary assumption,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+2v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}<\frac{2D_L}{(\Delta x)^2} \tag{5-199}$$

Then,

$$\frac{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}-2v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+2v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2} \\ +2v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}+2v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \\ +2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m\end{array}\right)}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}}<1 \tag{5-200}$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2}<\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(\delta_{n,m}^{\alpha}(\theta+1)+\beta_m\left(1-(\cos\phi)\right)\right) \tag{5-201}$$

Under this assumption (Equation (5-199)), the explicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

Next, making the assumption that $|\hat{c}_{n-1}| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\, n \geq 1$, that

$$|\hat{c}_n| < |\hat{c}_o|$$

Rearranging Equation (5-179) for $\hat{c}_n$,

$$a_3\hat{c}_n = \left(\begin{matrix} s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x} \\ - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1 - e^{-jk_i\Delta x}\right) + (1-\theta)(e^{jk_i\Delta x} - 1)\right)\delta_{m,i}^{\alpha}\right)\end{matrix}\right)\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right) \tag{5-202}$$

Applying a norm on both sides,

$$|a_3\hat{c}_n| = \left|\begin{matrix}\left(\begin{matrix} s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x} \\ - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1 - e^{-jk_i\Delta x}\right) + (1-\theta)(e^{jk_i\Delta x} - 1)\right)\delta_{m,i}^{\alpha}\right)\end{matrix}\right)\hat{c}_{n-1} \\ -h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right)\end{matrix}\right| \tag{5-203}$$

Thus,

$$|a_3||\hat{c}_n| < \left|\left(\begin{matrix} s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x} \\ - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1 - e^{-jk_i\Delta x}\right) + (1-\theta)\left(e^{jk_i\Delta x} - 1\right)\right)\delta_{m,i}^{\alpha}\right)\end{matrix}\right)\right||\hat{c}_{n-1}| - |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{5-204}$$

Remembering that it has been proved that for a set $\forall\, n \geq 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Thus,

$$\begin{aligned} |a_3||\hat{c}_n| &< \left|\left(s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta(1 - e^{-jk_i\Delta x}) + (1-\theta)(e^{jk_i\Delta x} - 1)\right)\delta_{m,i}^{\alpha}\right)\right)\right||\hat{c}_{n-1}| \\ &\quad + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \\ &< \left|\left(s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta(1 - e^{-jk_i\Delta x}) + (1-\theta)(e^{jk_i\Delta x} - 1)\right)\delta_{m,i}^{\alpha}\right)\right)\right||\hat{c}_0| \\ &\quad + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \end{aligned} \tag{5-205}$$

and, it can be inferred that,

$$|a_3||\hat{c}_n| < \left|\left(s_3 + u_3 e^{-jk_i\Delta x} + v_3 e^{jk_i\Delta x} \;\; - l_3\left(\sum_{i=1}^{m-1}\left(\theta(1-e^{-jk_i\Delta x}) + (1-\theta)(e^{jk_i\Delta x}-1)\right)\delta_{m,i}^{\alpha}\right)\right)\right||\hat{c}_0| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{5-206}$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{|s_3| + |u_3| + |v_3| + \; |l_3|\theta(2-2\cos\phi)\beta_m + \; |l_3|(1-\theta)(2-2\cos\phi)\beta_m + |h_3|\beta_n}{|a_3|} \tag{5-207}$$

Thus, the solution will be stable when,

$$\frac{|s_3| + |u_3| + |v_3| + \; |l_3|\theta(2-2\cos\phi)\beta_m + \; |l_3|(1-\theta)(2-2\cos\phi)\beta_m + |h_3|\beta_n}{|a_3|} < 1 \tag{5-208}$$

The term is expanded using the simplification terms associated with Equation (5-33),

$$\frac{\begin{gathered}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| \\ + \left|v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| \\ + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|\theta(2-2\cos\phi)\beta_m + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(1-\theta)(2-2\cos\phi)\beta_m + \left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\right|\beta_n\end{gathered}}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right|} < 1 \tag{5-209}$$

The assumption is made for the norm where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2} \tag{5-210}$$

Then,

$$\frac{\begin{gathered}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} \\ + v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} \\ + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\theta(2-2\cos\phi)\beta_m + \; v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n\end{gathered}}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}} < 1 \tag{5-211}$$

Multiplying out and simplifying, it is found that the explicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unstable under the assumption made in Equation (5-210).

When the complementary assumption is made,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2} \tag{5-212}$$

Then,

$$\frac{\begin{gathered}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}-v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{2D_L}{(\Delta x)^2}\\ +v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}+v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\\ +v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\theta(2-2\cos\phi)\beta_m+v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m+\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n\end{gathered}}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}}<1 \tag{5-213}$$

Simplifying,

$$2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{4D_L}{(\Delta x)^2}+\ 2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m(1-\cos\phi)+\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}(\beta_n-2)<0 \tag{5-214}$$

Conversely, the explicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is also unstable under the complementary assumption made in Equation (5-212). Thus, the second assumption, $|\hat{c}_n|<|\hat{c}_o|$, has failed to produce a stable solution.

### 5.2.5 Implicit upwind-downwind weighted scheme

The developed implicit upwind-downwind weighted scheme discussed in Section 5.1.5 (Equation (5-37)) is applied and induction method terms substituted,

$$\begin{gathered}a_3\hat{c}_n e^{jk_ix}=s_3\hat{c}_{n-1}e^{jk_ix}+u_3\hat{c}_n e^{jk_i(x-\Delta x)}+v_3\hat{c}_n e^{jk_i(x+\Delta x)}\\ -h_3\left(\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_mx}-\hat{c}_k e^{jk_mx}\right)\delta_{n,k}^{\alpha}\right)\\ -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_n e^{jk_ix}-\hat{c}_n e^{jk_i(x-\Delta x)}\right)+(1-\theta)\left(\hat{c}_n e^{jk_i(x+\Delta x)}-\hat{c}_n e^{jk_ix}\right)\right)\delta_{m,i}^{\alpha}\right)\end{gathered} \tag{5-215}$$

Multiple out and dividing by $e^{jk_ix}$,

$$\begin{aligned}a_3\hat{c}_n=s_3\hat{c}_{n-1}+u_3\hat{c}_n e^{-jk_i\Delta x}+v_3\hat{c}_n e^{jk_i\Delta x}-h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right)&\\ -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_n-\hat{c}_n e^{-jk_i\Delta x}\right)+(1-\theta)\left(\hat{c}_n e^{jk_i\Delta x}-\hat{c}_n\right)\right)\delta_{m,i}^{\alpha}\right)&\end{aligned} \tag{5-216}$$

The induction numerical stability analysis is performed in two parts; firstly it is proved for a set $\forall\ n>1$,

$$|\hat{c}_n|<|\hat{c}_o|$$

If $n=1$, then

$$\begin{aligned}a_3\hat{c}_1=s_3\hat{c}_0+u_3\hat{c}_1 e^{-jk_i\Delta x}+v_3\hat{c}_1 e^{jk_i\Delta x}&\\ -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_1-\hat{c}_1 e^{-jk_i\Delta x}\right)+(1-\theta)\left(\hat{c}_1 e^{jk_i\Delta x}-\hat{c}_1\right)\right)\delta_{m,i}^{\alpha}\right)&\end{aligned} \tag{5-217}$$

A subset for $m$ is now considered, where $m = 1$,

$$a_3\hat{c}_1 = s_3\hat{c}_0 + u_3\hat{c}_1 e^{-jk_i\Delta x} + v_3\hat{c}_1 e^{jk_i\Delta x} \tag{5-218}$$

Simplifying,

$$\left(a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x}\right)\hat{c}_1 = s_3\hat{c}_0 \tag{5-219}$$

Rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{s_3}{a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x}} \tag{5-220}$$

Taking a norm on both sides,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|s_3|}{|a_3| + |u_3 e^{-jk_i\Delta x}| + |v_3 e^{-jk_i\Delta x}|} \tag{5-221}$$

The stability condition is:

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} < 1$$

Remembering $|e^n| = 1$, the condition becomes

$$\frac{|s_3|}{|a_3| + |u_3| + |v_3|} < 1$$

The term is expanded using the simplification functions accompanying Equation (5-37),

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right|}{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| \\ + \left|v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right|\end{array}\right)} < 1 \tag{5-222}$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2} \tag{5-223}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}}{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} \\ + v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\end{array}\right)} < 1 \tag{5-224}$$

Simplifying,

$$2v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > 0 \tag{5-225}$$

Under the assumption Equation (5-223), the implicit upwind-downwind weighted numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unconditionally stable, where $\theta > 0$.

Making the complementary assumption,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}<\frac{2D_L}{(\Delta x)^2} \tag{5-226}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}}{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}-v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\\ +v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{D_L}{(\Delta x)^2}\end{array}\right)}<1 \tag{5-227}$$

Simplifying,

$$v_x(2-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}+\frac{4D_L}{(\Delta x)^2}>\frac{2(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \tag{5-228}$$

Under this assumption (Equation (5-226)), the implicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

A subset for $m$ is now considered for all $m>1$,

$$\begin{aligned}a_3\hat{c}_1 &= s_3\hat{c}_0+u_3\hat{c}_1e^{-jk_i\Delta x}+v_3\hat{c}_1e^{jk_i\Delta x}\\ &\quad -l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(\hat{c}_1-\hat{c}_1e^{-jk_i\Delta x}\right)+(1-\theta)\left(\hat{c}_1e^{jk_i\Delta x}-\hat{c}_1\right)\right)\delta_{m,i}^{\alpha}\right)\end{aligned} \tag{5-229}$$

Simplifying,

$$\left(\begin{array}{c}a_3+u_3e^{-jk_i\Delta x}+v_3e^{jk_i\Delta x}-l_3\theta\left(1-e^{-jk_i\Delta x}\right)\left(\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\\ -l_3(1-\theta)\left(e^{jk_i\Delta x}-1\right)\left(\sum_{i=1}^{m-1}\delta_{m,i}^{\alpha}\right)\end{array}\right)\hat{c}_1=s_3\hat{c}_0 \tag{5-230}$$

Thus,

$$(|a_3|+|u_3|+|v_3|+|l_3|\theta(2-2\cos\phi)\beta_m+\ |l_3|(1-\theta)(2-2\cos\phi)\beta_m)|\hat{c}_1|=|s_3||\hat{c}_0| \tag{5-231}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|}=\frac{|s_3|}{|a_3|+|u_3|+|v_3|+|l_3|\theta(2-2\cos\phi)\beta_m+\ |l_3|(1-\theta)(2-2\cos\phi)\beta_m} \tag{5-232}$$

The condition required $|\hat{c}_n|<|\hat{c}_o|$, becomes,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|}<1$$

The condition becomes,

$$\frac{|s_3|}{|a_3|+|u_3|+|v_3|+|l_3|\theta(2-2\cos\phi)\beta_m+\ |l_3|(1-\theta)(2-2\cos\phi)\beta_m}<1 \tag{5-233}$$

The simplification terms associated with Equation (5-37) are incorporated,

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}\right|}{\left(\begin{array}{c}\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}-\frac{2D_L}{(\Delta x)^2}\right|+\left|v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{D_L}{(\Delta x)^2}\right| \\ +\left|v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{D_L}{(\Delta x)^2}\right|+\left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|\theta(2-2\cos\phi)\beta_m \\ +\left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(1-\theta)(2-2\cos\phi)\beta_m\end{array}\right)}<1 \tag{5-234}$$

An assumption for the norm is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}>\frac{2D_L}{(\Delta x)^2} \tag{5-235}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}}{\left(\begin{array}{c}\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}-\frac{2D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{D_L}{(\Delta x)^2} \\ +v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \\ +v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m\end{array}\right)}<1 \tag{5-236}$$

Simplifying,

$$2v\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}\;+2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m\big(1-3\theta(\cos\phi)\big)>0 \tag{5-237}$$

Under this assumption (Equation (5-235)), the finite difference first-order upwind-downwind weighted (implicit) numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is unconditionally stable.

Making the complementary assumption,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}+v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}<\frac{2D_L}{(\Delta x)^2} \tag{5-238}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}}{\left(\begin{array}{c}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,n-1}-v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{2D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{D_L}{(\Delta x)^2} \\ +v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta^{\alpha}_{n,m}+\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \\ +v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m\end{array}\right)}<1 \tag{5-239}$$

Simplifying,

$$v_x(1-\theta)\;\left(\delta^{\alpha}_{n,m}+\beta_m\big(3(\cos\phi)\big)\right)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}+\frac{2D_L}{(\Delta x)^2}>\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \tag{5-240}$$

Under the assumption made in Equation (5-238), the implicit upwind-downwind weighted numerical scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

Secondly, making the assumption that $|\hat{c}_{n-1}| < |\hat{c}_o|$ is true for all time steps, the second part of the numerical stability analysis is to demonstrate for a set $\forall\ n \geq 1$, that

$$|\hat{c}_n| < |\hat{c}_o|$$

Rearranging Equation (5-216) for $\hat{c}_n$,

$$\left(a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1 - e^{-jk_i\Delta x}\right) + (1-\theta)\left(e^{jk_i\Delta x} - 1\right)\right)\delta_{m,i}^{\alpha}\right)\right)\hat{c}_n = s_3\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right)$$

Taking the norm on both sides,

$$\left|\left(a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1 - e^{-jk_i\Delta x}\right) + (1-\theta)\left(e^{jk_i\Delta x} - 1\right)\right)\delta_{m,i}^{\alpha}\right)\right)\hat{c}_n\right| = \left|s_3\hat{c}_{n-1} - h_3\left(\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right)\right| \tag{5-241}$$

Thus,

$$\left|\left(a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1 - e^{-jk_i\Delta x}\right) + (1-\theta)\left(e^{jk_i\Delta x} - 1\right)\right)\delta_{m,i}^{\alpha}\right)\right)\right||\hat{c}_n| < |s_3||\hat{c}_{n-1}| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{5-242}$$

Remembering that it has been proved that for a set $\forall\ n \geq 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Hence,

$$\begin{aligned}\left|\left(a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1 - e^{-jk_i\Delta x}\right) + (1-\theta)\left(e^{jk_i\Delta x} - 1\right)\right)\delta_{m,i}^{\alpha}\right)\right)\right||\hat{c}_n| &< |s_3||\hat{c}_{n-1}| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \\ &< |s_3||\hat{c}_0| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right|\end{aligned} \tag{5-243}$$

and, it can be inferred that,

$$\left|\left(a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1-e^{-jk_i\Delta x}\right)+(1-\theta)\left(e^{jk_i\Delta x}-1\right)\right)\delta_{m,i}^{\alpha}\right)\right)\right||\hat{c}_n| < |s_3||\hat{c}_0| + |h_3|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \quad (5\text{-}244)$$

Simplifying and rearranging,

$$\left|\left(a_3 - u_3 e^{-jk_i\Delta x} - v_3 e^{jk_i\Delta x} - l_3\left(\sum_{i=1}^{m-1}\left(\theta\left(1-e^{-jk_i\Delta x}\right)+(1-\theta)\left(e^{jk_i\Delta x}-1\right)\right)\delta_{m,i}^{\alpha}\right)\right)\right||\hat{c}_n| < (|s_3| + |h_3|\beta_n)|\hat{c}_0| \quad (5\text{-}245)$$

$$\frac{|\hat{c}_n|}{|\hat{c}_0|} < \frac{|s_3| + |h_3|\beta_n}{|a_3| + |u_3| + |v_3| + |l_3|\theta(2-2\cos\phi)\beta_m + |l_3|(1-\theta)(2-2\cos\phi)\beta_m}$$

Thus, the solution will be stable when,

$$\frac{|s_3| + |h_3|\beta_n}{|a_3| + |u_3| + |v_3| + |l_3|\theta(2-2\cos\phi)\beta_m + |l_3|(1-\theta)(2-2\cos\phi)\beta_m} < 1 \quad (5\text{-}246)$$

The term is expanded using the simplification terms associated with Equation (5-37),

$$\frac{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha}\right| + \left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\right|\beta_n}{\left|\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|\theta(2-2\cos\phi)\beta_m + \left|v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\right|(1-\theta)(2-2\cos\phi)\beta_m} < 1 \quad (5\text{-}247)$$

The assumption is made where,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2} \quad (5\text{-}248)$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n}{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} - \frac{2D_L}{(\Delta x)^2} + v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m} < 1 \quad (5\text{-}249)$$

Multiplying out and simplifying,

$$v_x(\theta+1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 2v_x(1-\cos\phi)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m > \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n \quad (5\text{-}250)$$

Thus, the implicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable under the assumption made in Equation (5-248).

When the corresponding assumption is made,

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2} \tag{5-251}$$

Then,

$$\frac{\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n}{\begin{gathered}-\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} - v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} \\ +v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x\theta\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m \\ +v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(1-\theta)(2-2\cos\phi)\beta_m\end{gathered}} < 1 \tag{5-252}$$

Simplifying,

$$2v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 2v_x(1-\cos\phi)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m + \frac{4D_L}{(\Delta x)^2} > (2+\beta_n)\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \tag{5-253}$$

Under this assumption (Equation (5-251)), the implicit upwind-downwind weighted scheme for the fractional advection-dispersion equation with Caputo fractional derivative is conditionally stable.

The implicit upwind-downwind weighted finite difference scheme for the fractional advection-dispersion equation (Caputo) has the following stability criterion, as proven by the induction method,

$$v_x(2-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{4D_L}{(\Delta x)^2} > \frac{2(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)},$$

$$v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + v_x\big(1-3\theta(\cos\phi)\big)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m + \frac{2D_L}{(\Delta x)^2} > \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)},$$

$$v_x(\theta+1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 2v_x(1-\cos\phi)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m > \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n,$$

and,

$$2v_x(1-\theta)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + 2v_x(1-\cos\phi)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m + \frac{4D_L}{(\Delta x)^2} > (2+\beta_n)\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}$$

Because under these conditions, the error of the approximation is not propagated throughout the solution, but rather decreases with each time step, as according to the induction method, where for all values of n, $|\hat{c}_{n+1}| < |\hat{c}_o|$.

### 5.2.6 Evaluation of numerical stability results

Upwind numerical schemes are developed for the one-dimensional, non-reactive space-time fractional advection-dispersion equation (Caputo), including the traditional upwind as well as the newly proposed upwind Crank-Nicolson and a weighted upwind-downwind scheme. The numerical schemes were subjected to numerical stability analysis using the recursive method, with a summary of these results tabulated in Table 5-1.

The traditional upwind (explicit) numerical scheme for the space-time fractional advection-dispersion equation (Caputo) is found to be unstable under certain assumptions, while the traditional upwind (implicit) numerical scheme is conditionally stable under all assumptions. The upwind Crank-Nicolson scheme, which has a half weighted approach to implicit and explicit for the advection term, is found to be conditionally stable under all assumptions. The weighted upwind-downwind (explicit) scheme is found to be unstable under certain assumptions, similarly to the traditional upwind (explicit) numerical scheme. The weighted upwind-downwind (implicit) scheme is conditionally stable under all assumptions, again similar to the traditional upwind (implicit) scheme. This trend of implicit numerical scheme formulations being more stable than the corresponding explicit formulation has been found by other researchers (Lynch et al., 2003; Meerschaert and Tadjeran, 2004; Liu et al., 2007).

The new weighted upwind-downwind (explicit) scheme is not more applicable than the traditional upwind (explicit) scheme, because the new weighted (explicit) scheme tends to be unstable under more assumptions. On the other hand, the weighted (implicit) scheme does provide an improvement on the traditional upwind (implicit) scheme in terms of stability, where the inclusion of the weighting factor ($\theta$) provides a means to improve the likelihood of upholding the stability condition. Thus, the upwind Crank-Nicolson and weighted upwind-downwind (implicit) schemes are applicable for solution of the space-time fractional advection-dispersion equation (Caputo), if the stability criterion are upheld.

## 5.3 Chapter summary

The space-time fractional advection-dispersion equation with Caputo fractional derivatives is defined, and the upwind numerical schemes developed in Chapter 2 are applied to numerically approximate the solution. Each scheme is analysed for stability, where it is found that the implicit weighted scheme is an improvement on the traditional implicit upwind scheme in terms of stability, where the inclusion of the weighting factor ($\theta$) provides a means to improve the likelihood of upholding the stability condition. It was concluded that the upwind advection Crank-Nicolson and implicit weighted upwind-downwind schemes are applicable for solution of the space-time fractional advection-dispersion equation (Caputo), when the stability criterion are upheld.

**Table 5-1 Summary of the assumptions made and corresponding stability condition for each numerical approximation scheme for the fractional advection-dispersion equation with Caputo fractional derivative**

| Scheme | Assumptions | Stability condition |
|---|---|---|
| **Explicit Upwind** | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2}$ | Unstable |
| | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2}$ | $\frac{4D_L}{(\Delta x)^2} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < \frac{2(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}$<br>Conditionally stable |
| **Implicit Upwind** | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2}$ | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(2\delta_{n,m}^{\alpha} + (2-2\cos\phi)\beta_m\right)$<br>Unconditionally stable / Conditionally stable |
| | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2}$ | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}(2+\beta_n) < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m + \frac{4D_L}{(\Delta x)^2}$<br>Conditionally stable |
| **Upwind Crank-Nicolson** | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} > v_x 0.5\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2}$ | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(\delta_{n,m}^{\alpha} + 0.5\beta_m(2-2\cos\phi)\right)$<br>Unconditionally stable / Conditionally stable |
| | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} < v_x 0.5\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} + \frac{2D_L}{(\Delta x)^2}$ | $\frac{2D_L}{(\Delta x)^2} < \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}$<br>$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\left(\delta_{n,m}^{\alpha} + 0.5\beta_m(2-2\cos\phi)\right)$<br>$\frac{4D_L}{(\Delta x)^2} + \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < \frac{2(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} + 0.5v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}(2-2\cos\phi)\beta_m$<br>Conditionally stable |
| **Explicit weighted upwind-downwind** | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2}$ | Unstable |
| | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2}$ | Conditionally stable / Unstable |
| **Implicit weighted upwind-downwind** | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} > \frac{2D_L}{(\Delta x)^2}$ | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\beta_n < v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}(\theta+1) + 2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m(1-\cos\phi)$<br>Unconditionally stable / conditionally stable |
| | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,n-1}^{\alpha} + v_x(2\theta-1)\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha} < \frac{2D_L}{(\Delta x)^2}$ | $\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}(2+\beta_n) < 2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\delta_{n,m}^{\alpha}(1-\theta) + 2v_x\frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)}\beta_m(1-\cos\phi) + \frac{4D_L}{(\Delta x)^2}$<br>Conditionally stable |

# 6 FRACTIONAL ADVECTION-DISPERSION EQUATION WITH ATANGANA-BALEANU IN CAPUTO SENSE (ABC) DERIVATIVE

It has been discussed that modelling groundwater transport in fractured aquifer systems is complicated due to the uncertainty associated with defining preferential pathways along which water and potential contaminants can be transported along. Misrepresenting an expected movement of a potential contaminant in a groundwater system can lead to environmental implications due to inadequate mitigation or remediation measures (Schmelling and Ross, 1990; Zimmerman et al., 1998; Fomin et al., 2005; Goode et al., 2007; Cello et al., 2009; Shapiro, 2011; Masciopinto and Palmiotta, 2013). To minimise misrepresentations in fractured systems, the newest fractional derivative definition, Atangana-Baleanu, is used to develop an advection-focused fractional advection-dispersion equation. The Atangana-Baleanu fractional derivative definition is presented in Chapter 4, along with the potential advantages of using this definition, where it was concluded that the new fractional derivatives definitions have the potential to incorporate different memory effects, which could change the way anomalous diffusion is modelled. The applicability of this particular formulation and fractional derivative definition is investigated for groundwater transport within fractured aquifers.

The Caputo fractional derivative definition was applied in Chapter 5, and a similar process is followed for the application of the Atangana-Baleanu in Caputo sense (ABC) fractional derivative definition. Firstly, the numerical approximation schemes are developed using the augmented upwind schemes, as well as the traditional upwind schemes, presented in Chapter 2. A numerical stability analysis is performed for each scheme, where the traditional upwind schemes serve to form a base of comparison in terms of numerical stability for the developed schemes.

## 6.1 Advection-focused transport model with Atangana-Baleanu in Caputo sense (ABC) derivative

The advection-focused fractional advection-dispersion equation with the Atangana-Baleanu in Caputo sense (ABC) fractional derivative definition is,

$$ {}^{ABC}_{0}D^{\alpha}_{t}\left(c(x,t)\right) = -v_x\, {}^{ABC}_{0}D^{\alpha}_{x}\left(c(x,t)\right) + D_L \frac{\partial^2}{\partial x^2}\left(c(x,t)\right) \tag{6-1} $$

To investigate the qualitative properties of the formulated equation, the boundedness, existence and uniqueness of the fractional advection-dispersion equation with ABC fractional derivative is determined using the Picard-Lindelöf theorem. Additionally, the stability of the defined fractional advection-dispersion equation is evaluated in time.

### 6.1.1 Picard-Lindelöf theorem for existence and uniqueness

Applying the AB integral to both sides of the fractional advection-dispersion equation with Atangana-Baleanu in Caputo sense (ABC) derivative, to obtain:

$$ \begin{aligned} c(x,t) - c(x,0) &= {}^{AB}_{0}I^{\alpha}_{x}\left\{-v_x\, {}^{ABC}_{0}D^{\alpha}_{x}\left(c(x,\tau)\right) + D_L \frac{\partial^2}{\partial x^2}\left(c(x,\tau)\right)\right\} d\tau \\ &= \frac{1-\alpha}{AB(\alpha)}\left\{-v_x\, {}^{ABC}_{0}D^{\alpha}_{x}\left(c(x,\tau)\right) + D_L \frac{\partial^2}{\partial x^2}\left(c(x,\tau)\right)\right\} \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t \left\{-v_x\, {}^{ABC}_{0}D^{\alpha}_{x}\left(c(x,\tau)\right) + D_L \frac{\partial^2}{\partial x^2}\left(c(x,\tau)\right)\right\} (t-\tau)^{\alpha-1} d\tau \end{aligned} \tag{6-2} $$

Consider a new function $F(x,t,c)$ to simplify:

$$ F(x,t,c) = -v_x\, {}^{ABC}_{0}D^{\alpha}_{x}\left(c(x,t)\right) + D_L \frac{\partial^2}{\partial x^2}\left(c(x,t)\right) \tag{6-3} $$

Thus,

$$ c(x,t) - c(x,0) = \frac{1-\alpha}{AB(\alpha)} F(x,t,c) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t F(x,t,c)(t-\tau)^{\alpha-1} d\tau \tag{6-4} $$

Let

$$ C_{\lambda,\beta} = \overline{I_\lambda(t_0)} \times \overline{B_\beta(x_0)} $$

where,

$$\overline{I_\lambda(t_0)} = [t_0 - \lambda, t_0 + \lambda]$$
$$\overline{\overline{B_\beta(x_0)}} = [x_0 - \beta, x_0 + \beta]$$

The Banach fixed-point theorem is applied by introducing the norm of the supremum (statistical limit of a set) for $I_\lambda$,

$$M = \|\varphi\|_\infty = \begin{matrix} sup|\varphi(t)| \\ t \in I_\lambda(t_0) \end{matrix} \tag{6-5}$$

Considering the practical meaning of $c(x,t)$, it can be assumed that the initial concentration ($c_0$) will always be greater than subsequent concentrations ($c_n$) due to advection, dispersion and diffusion processes which reduce the concentration over time and space,

$$\|c\|_\infty < c_0 \tag{6-6}$$

Considering the max norm for the function $F(x,t,c)$,

$$\|F\|_\infty = \left\| -v_x \frac{AB(\alpha)}{(1-\alpha)} \int_0^x \frac{d}{d\tau} c(\tau,x) E_\alpha \left[ -\frac{\alpha}{1-\alpha} (x-\tau)^\alpha \right] d\tau + D_L \frac{\partial^2}{\partial x^2} \big(c(x,t)\big) \right\|_\infty \tag{6-7}$$

Thus,

$$\|F\|_\infty \le v_x \frac{AB(\alpha)}{(1-\alpha)} \left\| \int_0^x \frac{d}{d\tau} c(\tau,x) E_\alpha \left[ -\frac{\alpha}{1-\alpha} (x-\tau)^\alpha \right] d\tau \right\|_\infty + D_L \left\| \frac{\partial^2}{\partial x^2} \big(c(x,t)\big) \right\|_\infty \tag{6-8}$$

Applying the proven theorem in Section 3.2.2, the second order derivative is bounded ($M_1$), thus

$$\|F\|_\infty \le v_x \frac{AB(\alpha)}{(1-\alpha)} \int_0^x \left\| \frac{d}{d\tau} C(\tau,x) \right\|_\infty \left\| E_\alpha \left[ -\frac{\alpha}{1-\alpha} (x-\tau)^\alpha \right] \right\|_\infty d\tau + D_L M_1 \tag{6-9}$$

The Mittag-Leffler function is bounded because $1 > \alpha > 0$, and the first order derivative is bounded to the physical meaning of the derivative of the spread of a particle in terms of its concentration ($M_2$). Thus, the derivative is considered at the maximum physical time that is applicable to the existence of the concentration ($T_{max}$),

$$\|F\|_\infty \le v_x \frac{AB(\alpha)}{(1-\alpha)} M_2 T_{max} + D_L M_1 < \infty \tag{6-10}$$

Therefore, the solution is bounded because we obtain a positive constant, such that

$$A = \|F\|_\infty = \begin{matrix} sup|F(x,t,c)| \\ t \in C_{\lambda,\beta} \end{matrix} \tag{6-11}$$

Let $C_{\lambda,\beta}$ be a set where, $F: C_{\lambda,\beta} \to C_{\lambda,\beta}$, such that

$$\Gamma\phi(x,t) = c(x,0) + \frac{1-\alpha}{AB(\alpha)} F(x,t,\phi) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t F(x,\tau,\phi)(t-\tau)^{\alpha-1} d\tau \tag{6-12}$$

Thus,

$$\|\Gamma\phi(x,t) - c(x,0)\|_\infty = \left\|\frac{1-\alpha}{AB(\alpha)}F(x,t,\phi) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^t F(x,\tau,\phi)(t-\tau)^{\alpha-1}d\tau\right\|_\infty$$

$$\|\Gamma\phi(x,t) - c(x,0)\|_\infty \le \frac{1-\alpha}{AB(\alpha)}\|F(x,t,\phi)\|_\infty + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^t (t-\tau)^{\alpha-1}\|F(x,\tau,\phi)\|_\infty d\tau \quad (6\text{-}13)$$

The function $F(x,t,c)$ has been shown to be bounded (Equation (6-7) - (6-11)),

$$\|\Gamma\phi(x,t) - c(x,0)\|_\infty \le \frac{1-\alpha}{AB(\alpha)}A + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}A\int_0^t (t-\tau)^{\alpha-1}d\tau$$

The integral is considered at the maximum physical time that is applicable to the existence of the concentration ($T_{max}$),

$$\|\Gamma\phi(x,t) - c(x,0)\|_\infty \le \frac{1-\alpha}{AB(\alpha)}A + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}A\frac{T_{max}^\alpha}{\alpha}$$

$$\le \frac{1-\alpha}{AB(\alpha)}A + \frac{A\,T_{max}^\alpha}{AB(\alpha)\Gamma(\alpha)} < \infty$$

Therefore, $\Gamma$ is well-posed because we obtain a positive constant.

To prove that $\Gamma$ is Lipschitz,

$$\|\Gamma\phi_1 - \Gamma\phi_2\|_\infty = \left\|\frac{1-\alpha}{AB(\alpha)}\big(F(x,t,\phi_1) - F(x,t,\phi_2)\big) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^t \big(F(x,\tau,\phi_1) - F(x,\tau,\phi_2)\big)(t-\tau)^{\alpha-1}d\tau\right\|_\infty$$

$$\|\Gamma\phi_1 - \Gamma\phi_2\|_\infty \le \frac{1-\alpha}{AB(\alpha)}\big\|\big(F(x,t,\phi_1) - F(x,t,\phi_2)\big)\big\|_\infty + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_0^t (t-\tau)^{\alpha-1}\|F(x,\tau,\phi_1) - F(x,\tau,\phi_2)\|_\infty d\tau \quad (6\text{-}14)$$

To achieve this, first evaluate

$$\|F(x,t,\phi_1) - F(x,t,\phi_2)\|_\infty = \left\|-v_x\ {}^{ABC}_{0}D_x^\alpha(\phi_1-\phi_2) + D_L\frac{\partial^2}{\partial x^2}(\phi_1-\phi_2)\right\|_\infty$$

$$\|F(x,t,\phi_1) - F(x,t,\phi_2)\|_\infty \le v_x\left\|{}^{ABC}_{0}D_x^\alpha(\phi_1-\phi_2)\right\|_\infty + D_L\left\|\frac{\partial^2}{\partial x^2}(\phi_1-\phi_2)\right\|_\infty \quad (6\text{-}15)$$

Applying the Atangana-Baleanu fractional derivative, and applying the proven theorem in Section 3.2.2 for the second order derivative is bounded ($\xi_2^2$),

$$\|F(x,t,\phi_1) - F(x,t,\phi_2)\|_\infty \le$$

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\int_0^x \left\|\frac{d}{d\tau}(\phi_1-\phi_2)\right\|_\infty \left\|E_\alpha\left[-\frac{\alpha}{1-\alpha}(x-\tau)^\alpha\right]\right\|_\infty d\tau + D_L\xi^2\|(\phi_1-\phi_2)\|_\infty \quad (6\text{-}16)$$

The Mittag-Leffler function is bounded because $1 > \alpha > 0$, and the first order derivative is bounded to the physical meaning of the derivative of the spread of a particle in terms of its concentration ($\xi_1$).

Thus, the derivative is considered at the maximum physical space that is applicable to the existence of the concentration ($X_{max}$),

$$\|F(x,t,\phi_1) - F(x,t,\phi_2)\|_\infty \leq v_x \frac{AB(\alpha)}{(1-\alpha)} X_{max} \xi_1 \|(\phi_1 - \phi_2)\|_\infty + D_L \xi_2^2 \|(\phi_1 - \phi_2)\|_\infty \tag{6-17}$$

Simplifying,

$$\|F(x,t,\phi_1) - F(x,t,\phi_2)\|_\infty \leq \left( v_x \frac{AB(\alpha)}{(1-\alpha)} X_{max} \xi_1 + D_L \xi_2^2 \right) \|(\phi_1 - \phi_2)\|_\infty < \mathrm{K}_\alpha \|(\phi_1 - \phi_2)\|_\infty \tag{6-18}$$

Applying to Equation (6-14),

$$\|\Gamma\phi_1 - \Gamma\phi_2\|_\infty \leq \frac{1-\alpha}{AB(\alpha)} \mathrm{K}_\alpha \|(\phi_1 - \phi_2)\|_\infty + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \mathrm{K}_\alpha \|(\phi_1 - \phi_2)\|_\infty \int_0^t (t-\tau)^{\alpha-1} d\tau \tag{6-19}$$

Applying a similar process as previously,

$$\begin{aligned} \|\Gamma\phi_1 - \Gamma\phi_2\|_\infty &\leq \frac{1-\alpha}{AB(\alpha)} \mathrm{K}_\alpha \|(\phi_1 - \phi_2)\|_\infty + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \mathrm{K}_\alpha \|(\phi_1 - \phi_2)\|_\infty \frac{T_{max}^\alpha}{\alpha} \\ &\leq \left( \frac{1-\alpha}{AB(\alpha)} \mathrm{K}_\alpha + \frac{T_{max}^\alpha}{AB(\alpha)\Gamma(\alpha)} \mathrm{K}_\alpha \right) \|(\phi_1 - \phi_2)\|_\infty \\ &\leq V \|(\phi_1 - \phi_2)\|_\infty \end{aligned} \tag{6-20}$$

Therefore, $\Gamma$ is a contraction when $V < 1$, which translates to a condition

$$\mathrm{K}_\alpha < \frac{1}{\frac{1-\alpha}{AB(\alpha)} + \frac{T_{max}^\alpha}{AB(\alpha)\Gamma(\alpha)}} \tag{6-21}$$

Then $F(x,t,c)$ has a fixed point using the Banach fixed-point theorem and the fractional advection-dispersion equation with ABC fractional derivative is bounded and has a unique solution under this condition.

### 6.1.2 Semi-discretisation stability

The defined fractional advection-dispersion equation with ABC fractional derivative is discretised in time while the concentration in space is considered constant to evaluate the stability of the equation in time. The forward difference scheme in time is applied to the Atangana-Baleanu in Caputo sense (ABC) fractional derivative, considered for a specific time ($t_n$), and the numerical integration of the Mittag-Leffler function as performed by Alkahtani et al. (2017) is applied,

$${}_0^{ABC}D_t^\alpha\big(c(x,t_n)\big) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-1} \left(c_x^{k+1} - c_x^k\right) \delta_{n,k}^\alpha$$

where,

$$\delta_{n,k}^\alpha = (n-k) E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-k)\right] - (n-k-1) E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-k-1)\right] \tag{6-22}$$

Substituting back into the fractional advection-dispersion equation with the Atangana-Baleanu in Caputo sense (ABC) derivative, and applying the assumption of discretisation in time only

$$\frac{AB(\alpha)}{(1-\alpha)}\sum_{k=0}^{n-1}\left(c_x^{k+1}-c_x^{k}\right)\delta_{n,k}^{\alpha} = -v_x\,{}^{ABC}_{\phantom{A}0}D_x^{\alpha}(c_x^{n}) + D_L\frac{\partial^2}{\partial x^2}(c_x^{n+1}) \tag{6-23}$$

A function $A_{n,k}^{\alpha}$ is applied to simplify,

$$\sum_{k=0}^{n-1}\left(c_x^{k+1}-c_x^{k}\right)A_{n,k}^{\alpha} = -v_x\,{}^{ABC}_{\phantom{A}0}D_x^{\alpha}(c_x^{n}) + D_L\frac{\partial^2}{\partial x^2}(c_x^{n+1}) \tag{6-24}$$

Reformulating to obtain,

$$\left(c_x^{n+1}-c_x^{n}\right)A_n^{\alpha} + \sum_{k=0}^{n-1}\left(c_x^{k+1}-c_x^{k}\right)A_{n,k}^{\alpha} = -v_x\,{}^{ABC}_{\phantom{A}0}D_x^{\alpha}(c_x^{n}) + D_L\frac{\partial^2}{\partial x^2}(c_x^{n+1}) \tag{6-25}$$

Rearranging,

$$c_x^{n+1} = c_x^{n} - \frac{v_x}{A_n^{\alpha}}\,{}^{ABC}_{\phantom{A}0}D_x^{\alpha}(c_x^{n}) + \frac{D_L}{A_n^{\alpha}}\frac{\partial^2}{\partial x^2}(c_x^{n+1}) - \frac{1}{A_n^{\alpha}}\sum_{k=0}^{n-1}\left(c_x^{k+1}-c_x^{k}\right)A_{n,k}^{\alpha} \tag{6-26}$$

Equation (6-26) is the numerical approximation of the fractional advection-equation (ABC) with respect to time. Now, the semi-stability can be evaluated defining the following norms,

$$(f,g) = \int_{\Omega}(f\cdot g)(x)dx$$

where,

$$\|g\|_0 = \sqrt{(g\cdot g)}$$

$$\|g\|_1 = \sqrt{\|g\|_0 + \varepsilon\left\|\frac{d^2}{dx^2}g\right\|_0}$$

When $n=0$, Equation (6-26) becomes

$$c_x^{1} = c_x^{0} - \frac{v_x}{A_n^{\alpha}}\,{}^{ABC}_{\phantom{A}0}D_x^{\alpha}(c_x^{0}) + \frac{D_L}{A_n^{\alpha}}\frac{\partial^2}{\partial x^2}(c_x^{1}) \tag{6-27}$$

Simplifying using functions $\lambda_1$ and $\lambda_2$,

$$c_x^{1} = c_x^{0} - \lambda_1\,{}^{ABC}_{\phantom{A}0}D_x^{\alpha}(c_x^{0}) + \lambda_2\frac{\partial^2}{\partial x^2}(c_x^{1}) \tag{6-28}$$

Applying the norm with respect to $g$,

$$(c_x^{1},g) = (c_x^{0},g) - \lambda_1\left({}^{ABC}_{\phantom{A}0}D_x^{\alpha}c_x^{0},\ {}^{ABC}_{\phantom{A}0}D_x^{\alpha}g\right) + \lambda_2\left(\frac{\partial^2}{\partial x^2}c_x^{1},\frac{\partial^2}{\partial x^2}g\right) \tag{6-29}$$

Let $\forall g\in H^1(\Omega), g = c_x^{1}$

$$(c_x^{1},c_x^{1}) = (c_x^{0},c_x^{1}) - \lambda_1\left({}^{ABC}_{\phantom{A}0}D_x^{\alpha}c_x^{0},\ {}^{ABC}_{\phantom{A}0}D_x^{\alpha}c_x^{1}\right) + \lambda_2\left(\frac{\partial^2}{\partial x^2}c_x^{1},\frac{\partial^2}{\partial x^2}c_x^{1}\right) \tag{6-30}$$

From the defined norms, the following statement is to be proven,

$$\|c_x^{1}\|_1 \le \|c_x^{0}\|_0$$

Reformulating in terms of the defined norms,

$$(c_x^1, c_x^1) - \lambda_2\left(\frac{\partial^2 c_x^1}{\partial x^2}, \frac{\partial^2 c_x^1}{\partial x^2}\right) = (c_x^0, c_x^1) - \lambda_1\left({}^{ABC}_{\ \ 0}D_x^\alpha c_x^0,\ {}^{ABC}_{\ \ 0}D_x^\alpha c_x^1\right)$$
$$\|c_x^1\|_1^2 = \|c_x^0\|_0\|c_x^1\|_0 - \lambda_1\left\|{}^{ABC}_{\ \ 0}D_x^\alpha c_x^0\right\|_0\left\|{}^{ABC}_{\ \ 0}D_x^\alpha c_x^1\right\|_0 \tag{6-31}$$

where,

$$\|{}^{ABC}_{\ \ 0}D_x^\alpha c_x^0\|_0 = \left\|\frac{AB(\alpha)}{(1-\alpha)}\int_0^x \frac{dc_\tau^0}{d\tau} E_\alpha\left[-\frac{\alpha}{1-\alpha}(x-\tau)^\alpha\right] d\tau\right\|_0$$

Thus,

$$\|{}^{ABC}_{\ \ 0}D_x^\alpha c_x^0\|_0 \leq \frac{AB(\alpha)}{(1-\alpha)}\int_0^x \left\|\frac{dc_\tau^0}{d\tau}\right\|_0 \left\|E_\alpha\left[-\frac{\alpha}{1-\alpha}(x-\tau)^\alpha\right]\right\|_0 d\tau \tag{6-32}$$

The Mittag-Leffler function is bounded because $1 > \alpha > 0$, and the first order derivative is bounded to the physical meaning of the derivative of the spread of a particle in terms of its concentration. Thus, the derivative is considered at the maximum physical space that is applicable to the existence of the concentration ($X_{max}$),

$$\begin{aligned}\|{}^{ABC}_{\ \ 0}D_x^\alpha c_x^0\|_0 &\leq \frac{AB(\alpha)}{(1-\alpha)}\int_0^x \left\|\frac{dc_\tau^0}{d\tau}\right\|_0 d\tau \\ &\leq \frac{AB(\alpha)}{(1-\alpha)}\theta\|c_x^0\|_0\int_0^{x_{max}} d\tau \\ &\leq \frac{AB(\alpha)}{(1-\alpha)}\theta\|c_x^0\|_0 X_{max}\end{aligned} \tag{6-33}$$

Substituting back into Equation (6-31),

$$\|c_x^1\|_1^2 < \|c_x^0\|_0\|c_x^1\|_0 - \lambda_1\left\{\frac{AB(\alpha)}{(1-\alpha)}\theta\left\|c_x^0\right\|_0 X_{max}\right\}\left\{\frac{AB(\alpha)}{(1-\alpha)}\theta\left\|c_x^1\right\|_0 X_{max}\right\} \tag{6-34}$$

Rearranging,

$$\begin{aligned}\|c_x^1\|_1^2 &< \|c_x^0\|_0\|c_x^1\|_0 - \lambda_1\left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2\left\|c_x^0\right\|_0\left\|c_x^1\right\|_0 \\ &< \left(1 - \lambda_1\left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2\right)\|c_x^0\|_0\|c_x^1\|_0\end{aligned} \tag{6-35}$$

Applying the assumption that

$$\|c_x^1\|_0 \leq \|c_x^1\|_1$$

Simplifying the stability conditions becomes,

$$\begin{aligned}\|c_x^1\|_1^2 &< \left(1 - \lambda_1\left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2\right)\|c_x^0\|_0\|c_x^1\|_1 \\ \|c_x^1\|_1 &< \left(1 - \lambda_1\left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2\right)\|c_x^0\|_0\end{aligned} \tag{6-36}$$

$$\frac{\|c_x^1\|_1}{\|c_x^0\|_0} < 1 - \lambda_1 \left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2$$

where,

$$1 - \lambda_1 \left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2 < 1$$

$$\lambda_1 \left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2 > 0$$

The first condition is thus upheld and unconditionally stable.

Secondly, Let $\forall g \in H^1(\Omega),\ g = c_x^{n+1}$

$$(c_x^{n+1}, c_x^{n+1}) = (c_x^n, c_x^{n+1}) - \lambda_1 \left({}^{ABC}_{\ 0}D_x^\alpha c_x^n,\ {}^{ABC}_{\ 0}D_x^\alpha c_x^{n+1}\right) + \lambda_2 \left(\frac{\partial^2}{\partial x^2} c_x^{n+1}, \frac{\partial^2}{\partial x^2} c_x^{n+1}\right) - \lambda_3 \sum_{k=0}^{n-1} \left((c_x^{k+1}, c_x^{n+1}) - (c_x^k, c_x^{n+1})\right) \tag{6-37}$$

where,

$$\lambda_3 = \frac{1}{A_n^\alpha} A_{n,k}^\alpha$$

From the defined norms, the following statement is to be proven,

$$\|c_x^{n+1}\|_1 \le \|c_x^0\|_0$$

Reformulating Equation (6-37) in terms of the defined norms,

$$(c_x^{n+1}, c_x^{n+1}) - \lambda_2 \left(\frac{\partial^2 c_x^{n+1}}{\partial x^2}, \frac{\partial^2 c_x^{n+1}}{\partial x^2}\right) = (c_x^n, c_x^{n+1}) - \lambda_1 \left({}^{ABC}_{\ 0}D_x^\alpha c_x^n,\ {}^{ABC}_{\ 0}D_x^\alpha c_x^{n+1}\right) - \lambda_3 \sum_{k=0}^{n-1} \left((c_x^{k+1}, c_x^{n+1}) - (c_x^k, c_x^{n+1})\right) \tag{6-38}$$

$$\|c_x^{n+1}\|_1^2 = \|c_x^n\|_0 \|c_x^{n+1}\|_0 - \lambda_1 \left\|{}^{ABC}_{\ 0}D_x^\alpha c_x^n\right\|_0 \left\|{}^{ABC}_{\ 0}D_x^\alpha c_x^{n+1}\right\|_0 - \lambda_3 \sum_{k=0}^{n-1} \left(\left(\|c_x^{k+1}\|_0 \|c_x^{n+1}\|_0\right) - \left(\|c_x^k\|_0 \|c_x^{n+1}\|_0\right)\right)$$

Applying Equation (6-33),

$$\|c_x^{n+1}\|_1^2 \le \|c_x^n\|_0 \|c_x^{n+1}\|_0 - \lambda_1 A \|c_x^n\|_0 \|c_x^{n+1}\|_0 - \lambda_3 \sum_{k=0}^{n-1} \left(\left(\|c_x^{k+1}\|_0 \|c_x^{n+1}\|_0\right) - \left(\|c_x^k\|_0 \|c_x^{n+1}\|_0\right)\right) \tag{6-39}$$

where,

$$A = \left\{\frac{AB(\alpha)\theta X_{max}}{(1-\alpha)}\right\}^2$$

Using the inductive method for

$$\|c_x^n\|_0 \le \|c_x^0\|_0$$

Equation (6-39) becomes,

$$\|c_x^{n+1}\|_1^2 \leq \|c_x^0\|_0 \|c_x^{n+1}\|_0 - \lambda_1 A \|c_x^0\|_0 \|c_x^{n+1}\|_0 - \lambda_3 \sum_{k=0}^{n-1} \left( \left( \|c_x^0\|_0 \|c_x^{n+1}\|_0 \right) - \left( \|c_x^0\|_0 \|c_x^{n+1}\|_0 \right) \right) \tag{6-40}$$

Reformulating in terms of the defined norms,

$$\|c_x^{n+1}\|_1^2 \leq \|c_x^0\|_0 \|c_x^{n+1}\|_1 - \lambda_1 A \|c_x^0\|_0 \|c_x^{n+1}\|_1 \tag{6-41}$$

Rearranging and simplifying,

$$\|c_x^{n+1}\|_1^2 \leq (1 - \lambda_1 A) \|c_x^0\|_0 \|c_x^{n+1}\|_1 \tag{6-42}$$

$$\|c_x^{n+1}\|_1 \leq (1 - \lambda_1 A) \|c_x^0\|_0$$

where,

$$1 - \lambda_1 A < 1$$

$$\lambda_1 A > 0$$

Thus, the second condition is supported and unconditionally stable. This concludes the semi-discretisation analysis for an evolution equation, and it can be concluded that the advection-dominated fractional transport model with ABC fractional derivative is stable in time.

## 6.2 Upwind numerical approximation schemes

The modified upwind schemes are to be applied to the advection-focused transport model with Atangana-Baleanu in Caputo sense (ABC) derivative for numerical approximation (Equation (4-93)). Applying the Atangana-Baleanu in Caputo sense (ABC) fractional derivative definition to the developed advection-dispersion equation,

$$ {}_{a}^{ABC}D_t^{\alpha} \left( c(x,t) \right) = -v_x \, {}_{a}^{ABC}D_x^{\alpha} \left( c(x,t) \right) + D_L \frac{\partial^2}{\partial x^2} \left( c(x,t) \right) \tag{6-43}$$

where,

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

A forward finite difference scheme in time is applied to the Atangana-Baleanu in Caputo sense (ABC) fractional derivative to investigate the numerical approximation method. The Atangana-Baleanu (ABC) fractional derivative is considered for a specific time, $t_n$:

$$ {}_{a}^{ABC}D_t^{\alpha} f(t_n) = \frac{AB(\alpha)}{(1-\alpha)} \int_0^{t_n} \frac{d}{d\tau} f(\tau) \, E_{\alpha} \left[ -\frac{\alpha}{1-\alpha} (t_n-\tau)^{\alpha} \right] d\tau \tag{6-44}$$

The time integer-order derivative $\tau$ is replaced with the forward finite difference approximation at specific points in time ($t$), and a summation is used to express the integral performed for each time step (time domain discretisation):

$$ {}_{a}^{ABC}D_t^{\alpha} f(t_n) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} \left( \frac{f_i^{k+1} - f_i^k}{\Delta t} \right) E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_n - \tau)^\alpha \right] d\tau \tag{6-45} $$

The approximation of the continuous $\tau$ function, results in two specific points of the function with respect to time ($t$), which allows the approximated derivative to be taken out of the integral:

$$ {}_{a}^{ABC}D_t^{\alpha} f(t_n) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-1} \left( \frac{f_i^{k+1} - f_i^k}{\Delta t} \right) \int_{t_k}^{t_{k+1}} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_n - \tau)^\alpha \right] d\tau \tag{6-46} $$

The numerical approximation by to this point has been similar to the approach followed in the Caputo definition of the fractional derivative, but now a different approach is required to take into account the Mittag-Leffler function ($E_\alpha$). The Mittag-Leffler function is numerically integrated using the known properties of the function (Alkahtani et al., 2017):

$$ \begin{aligned} \int_{t_k}^{t_{k+1}} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_n - \tau)^\alpha \right] d\tau = (t_n - t_k) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (t_n - t_k) \right] \\ -(t_n - t_{k+1}) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (t_n - t_{k+1}) \right] \end{aligned} \tag{6-47} $$

Considering the specific time can be represented as the number of time steps required to reach that time ($t_n = \Delta t \cdot n$) and similarly, $t_k = \Delta t \cdot k$. Thus, the same can be applied to achieve $t_n - t_k = \Delta t(n-k)$ and $t_n - t_{k+1} = \Delta t(n-k-1)$:

$$ \begin{aligned} \int_{t_k}^{t_{k+1}} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_n - \tau)^\alpha \right] d\tau = (\Delta t(n-k)) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (\Delta t(n-k)) \right] \\ -(\Delta t(n-k-1)) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (\Delta t(n-k-1)) \right] \end{aligned} \tag{6-48} $$

Simplifying,

$$ \int_{t_k}^{t_{k+1}} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_n - \tau)^\alpha \right] d\tau = \Delta t \begin{Bmatrix} (n-k) E_{\alpha,2} \left[ -\frac{\alpha\,\Delta t}{1-\alpha} (n-k) \right] \\ -(n-k-1) E_{\alpha,2} \left[ -\frac{\alpha\,\Delta t}{1-\alpha} (n-k-1) \right] \end{Bmatrix} \tag{6-49} $$

Substituting the numerically integrated Mittag-Leffler function into Equation (6-46):

$$ {}_{a}^{ABC}D_t^{\alpha} f(t_n) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-1} \left( f_i^{k+1} - f_i^k \right) \begin{Bmatrix} (n-k) E_{\alpha,2} \left[ -\frac{\alpha\,\Delta t}{1-\alpha} (n-k) \right] \\ -(n-k-1) E_{\alpha,2} \left[ -\frac{\alpha\,\Delta t}{1-\alpha} (n-k-1) \right] \end{Bmatrix} \tag{6-50} $$

Equation (6-50) is the numerically approximated Atangana-Baleanu in Caputo sense (ABC) fractional derivative, where the function is considered at two discrete points in time, and additionally the fractional components of the Mittag-Leffler function are included to account for changes in-between those two discrete points in time.

### 6.2.1 Explicit upwind

The numerical approximation of the Atangana-Baleanu in Caputo sense (ABC) fractional derivative with respect to time has been considered in Equation (6-50), where, a function $\delta_{n,k}^{\alpha}$ is applied to simplify,

$$ {}_{0}^{ABC}D_t^{\alpha}\big(c(x_m, t_k)\big) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-1} \big(c_m^{k+1} - c_m^{k}\big)\delta_{n,k}^{\alpha} \tag{6-51} $$

where,

$$ \delta_{n,k}^{\alpha} = (n-k)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-k)\right] - (n-k-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-k-1)\right] $$

Similarly, the ABC fractional derivative with respect to space (explicit) and the upwind scheme is (Alkahtani et al., 2017),

$$ {}_{0}^{ABC}D_x^{\alpha}\big(c(x_m, t_k)\big) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{i=0}^{m} \big(c_i^{n-1} - c_{i-1}^{n-1}\big) \left\{ \begin{array}{c} (m-i)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-i)\right] \\ -(m-i-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-i-1)\right] \end{array} \right\} \tag{6-52} $$

where, a function $\delta_{m,i}^{\alpha}$ is applied to simplify,

$$ {}_{0}^{ABC}D_x^{\alpha}\big(c(x_m, t_k)\big) = \frac{AB(\alpha)}{(1-\alpha)} \sum_{i=0}^{m} \big(c_i^{n-1} - c_{i-1}^{n-1}\big)\delta_{m,i}^{\alpha} \tag{6-53} $$

Substituting this into the advection-dispersion equation, and using the traditional finite difference approach for the local second order derivative,

$$ \begin{aligned} &\frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-1} \big(c_m^{k+1} - c_m^{k}\big)\delta_{n,k}^{\alpha} + v_x \frac{AB(\alpha)}{(1-\alpha)} \sum_{i=0}^{m} \big(c_i^{n-1} - c_{i-1}^{n-1}\big)\delta_{m,i}^{\alpha} \\ &\qquad - D_L\left(\frac{c_{m+1}^{n-1} - 2c_m^{n-1} + c_{m-1}^{n-1}}{(\Delta x)^2}\right) = 0 \end{aligned} \tag{6-54} $$

Reformulating the following can be obtained,

$$ \begin{aligned} &\frac{AB(\alpha)}{(1-\alpha)}\big(c_m^{n} - c_m^{n-1}\big)\delta_{n,n-1}^{\alpha} + \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-2} \big(c_m^{k+1} - c_m^{k}\big)\delta_{n,k}^{\alpha} + v_x \frac{AB(\alpha)}{(1-\alpha)}\big(c_m^{n-1} - c_{m-1}^{n-1}\big)\delta_{m,i}^{\alpha} \\ &\qquad + v_x \frac{AB(\alpha)}{(1-\alpha)} \sum_{i=0}^{m} \big(c_i^{n-1} - c_{i-1}^{n-1}\big)\delta_{m,i}^{\alpha} - D_L\left(\frac{c_{m+1}^{n-1} - 2c_m^{n-1} + c_{m-1}^{n-1}}{(\Delta x)^2}\right) = 0 \end{aligned} \tag{6-55} $$

Rearranging,

$$ \begin{aligned} c_m^{n}\left(\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right) &= c_m^{n-1}\left(\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} - v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right) \\ &+ c_{m-1}^{n-1}\left(v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right) + c_{m+1}^{n-1}\left(\frac{D_L}{(\Delta x)^2}\right) - \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-2} \big(c_m^{k+1} - c_m^{k}\big)\delta_{n,k}^{\alpha} \\ &- v_x \frac{AB(\alpha)}{(1-\alpha)} \sum_{i=0}^{m} \big(c_i^{n-1} - c_{i-1}^{n-1}\big)\delta_{m,i}^{\alpha} \end{aligned} \tag{6-56} $$

This is the first-order explicit upwind finite difference scheme for the one-dimensional, non-reactive fractional advection-dispersion equation (ABC). The numerical scheme can be simplified as follows,

$$a_4 c_m^n = b_4 c_m^{n-1} + d_4 c_{m-1}^{n-1} + f_4 c_{m+1}^{n-1} - g_4 \sum_{k=0}^{n-2} \left(c_m^{k+1} - c_m^k\right) \delta_{n,k}^{\alpha} - v_x g_4 \sum_{i=0}^{m} \left(c_i^{n-1} - c_{i-1}^{n-1}\right) \delta_{m,i}^{\alpha} \tag{6-57}$$

where,

$$a_4 = \frac{AB(\alpha)}{(1-\alpha)} \delta_{n,n-1}^{\alpha}$$

$$b_4 = \frac{AB(\alpha)}{(1-\alpha)} \delta_{n,n-1}^{\alpha} - v_x \frac{AB(\alpha)}{(1-\alpha)} \delta_{m,i}^{\alpha} - \frac{2D_L}{(\Delta x)^2}$$

$$d_4 = v_x \frac{AB(\alpha)}{(1-\alpha)} \delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2}$$

$$f_4 = \frac{D_L}{(\Delta x)^2}$$

$$g_4 = \frac{AB(\alpha)}{(1-\alpha)}$$

### 6.2.2 Implicit upwind

Applying the same methodology as the explicit upwind numerical approximation, the following is obtained,

$$\frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-1} \left(c_m^{k+1} - c_m^k\right) \delta_{n,k}^{\alpha} + v_x \frac{AB(\alpha)}{(1-\alpha)} \sum_{i=0}^{m} (c_i^n - c_{i-1}^n) \delta_{m,i}^{\alpha} - D_L \left(\frac{c_{m+1}^n - 2c_m^n + c_{m-1}^n}{(\Delta x)^2}\right) = 0 \tag{6-58}$$

Reformulating and rearranging the following can be obtained,

$$\begin{aligned} c_m^n \left(\frac{AB(\alpha)}{(1-\alpha)} \delta_{n,n-1}^{\alpha} + v_x \frac{AB(\alpha)}{(1-\alpha)} \delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right) \\ = c_{m-1}^n \left(v_x \frac{AB(\alpha)}{(1-\alpha)} \delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2}\right) + c_{m+1}^n \left(\frac{D_L}{(\Delta x)^2}\right) \\ - \frac{AB(\alpha)}{(1-\alpha)} \sum_{k=0}^{n-2} \left(c_m^{k+1} - c_m^k\right) \delta_{n,k}^{\alpha} - v_x \frac{AB(\alpha)}{(1-\alpha)} \sum_{i=0}^{m} (c_i^n - c_{i-1}^n) \delta_{m,i}^{\alpha} + c_m^{n-1} \left(\frac{AB(\alpha)}{(1-\alpha)} \delta_{n,n-1}^{\alpha}\right) \end{aligned} \tag{6-59}$$

Equation (6-59) is the implicit upwind finite difference scheme for the one-dimensional fractional advection-dispersion equation (ABC). The numerical scheme can be further simplified by substituting functions,

$$h_4 c_m^n - j_4 c_{m-1}^n - f_4 c_{m+1}^n + g_4 \sum_{k=0}^{n-2} \left(c_m^{k+1} - c_m^k\right) \delta_{n,k}^{\alpha} + v_x g_4 \sum_{i=0}^{m} (c_i^n - c_{i-1}^n) \delta_{m,i}^{\alpha} = a_4 c_m^{n-1} \tag{6-60}$$

where,

$$h_4 = \frac{AB(\alpha)}{(1-\alpha)} \delta_{n,n-1}^{\alpha} + v_x \frac{AB(\alpha)}{(1-\alpha)} \delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}$$

$$j_4 = v_x \frac{AB(\alpha)}{(1-\alpha)} \delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2}$$

### 6.2.3 Upwind advection Crank-Nicolson scheme

For the upwind advection Crank-Nicolson finite difference scheme, the time component remains the same as with the first-order implicit and explicit schemes, and the space components change to,

$$ {}_{0}^{ABC}D_{x}^{\alpha}\big(c(x_m,t_n)\big) = \frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\left[0.5\left(c_i^{n-1}-c_{i-1}^{n-1}\right)+0.5\left(c_i^{n}-c_{i-1}^{n}\right)\right]\delta_{m,i}^{\alpha} \tag{6-61} $$

Substituting this back into the advection-dispersion equation,

$$ \frac{AB(\alpha)}{(1-\alpha)}\sum_{k=0}^{n-1}\left(c_m^{k+1}-c_m^{k}\right)\delta_{n,k}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\left[0.5\left(c_i^{n-1}-c_{i-1}^{n-1}\right)+0.5\left(c_i^{n}-c_{i-1}^{n}\right)\right]\delta_{m,i}^{\alpha} - D_L\left(\frac{c_{m+1}^{n}-2c_m^{n}+c_{m-1}^{n}}{(\Delta x)^2}\right) = 0 $$

Reformulating and rearranging, the following can be obtained

$$ \begin{aligned} c_m^{n}\left(\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}\right) &= c_m^{n-1}\left(\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right) \\ &+c_{m-1}^{n}\left(0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{D_L}{(\Delta x)^2}\right)+c_{m+1}^{n}\left(\frac{D_L}{(\Delta x)^2}\right)+c_{m-1}^{n-1}\left(0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right) \\ &-\frac{AB(\alpha)}{(1-\alpha)}\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^{k}\right)\delta_{n,k}^{\alpha}-v_x\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\left[0.5\left(c_i^{n-1}-c_{i-1}^{n-1}\right)+0.5\left(c_i^{n}-c_{i-1}^{n}\right)\right]\delta_{m,i}^{\alpha} \end{aligned} \tag{6-62} $$

Equation (6-62) is the upwind advection Crank-Nicolson finite difference scheme for the fractional advection-dispersion equation (ABC). The numerical scheme can be simplified with functions,

$$ \begin{aligned} l_4c_m^{n} &= m_4c_m^{n-1}+o_4c_{m-1}^{n}+f_4c_{m+1}^{n}+p_4c_{m-1}^{n-1}-g_4\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^{k}\right)\delta_{n,k}^{\alpha} \\ &-vg_4\sum_{i=0}^{m}\left[0.5\left(c_i^{n-1}-c_{i-1}^{n-1}\right)+0.5\left(c_i^{n}-c_{i-1}^{n}\right)\right]\delta_{m,i}^{\alpha} \end{aligned} \tag{6-63} $$

where,

$$ l_4 = \frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2} $$

$$ m_4 = \frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} $$

$$ o_4 = 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{D_L}{(\Delta x)^2} $$

$$ p_4 = 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} $$

### 6.2.4 Explicit upwind-downwind weighted scheme

The upwind and downwind weighted scheme for the advection term is controlled by a ratio of upwind to downwind ($\theta$), where $0 \le \theta \le 1$. Thus, the space advection component is altered to,

$$ {}_{0}^{ABC}D_{x}^{\alpha}\big(c(x_m,t_n)\big)=\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\big[\theta\big(c_i^{n-1}-c_{i-1}^{n-1}\big)+(1-\theta)\big(c_{i+1}^{n-1}-c_i^{n-1}\big)\big]\,\delta_{m,i}^{\alpha} \tag{6-64} $$

Substituting this back into the advection-dispersion equation,

$$ \frac{AB(\alpha)}{(1-\alpha)}\sum_{k=0}^{n-1}\big(c_m^{k+1}-c_m^{k}\big)\delta_{n,k}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\big[\theta\big(c_i^{n-1}-c_{i-1}^{n-1}\big)+(1-\theta)\big(c_{i+1}^{n-1}-c_i^{n-1}\big)\big]\,\delta_{m,i}^{\alpha} -D_L\left(\frac{c_{m+1}^{n-1}-2c_m^{n-1}+c_{m-1}^{n-1}}{(\Delta x)^2}\right)=0 \tag{6-65} $$

Reformulating and rearranging, the following can be obtained

$$ \begin{aligned} c_m^{n}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}&=c_m^{n-1}\left(\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}-v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{2D_L}{(\Delta x)^2}\right)\\ &+c_{m-1}^{n-1}\left(v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right)-c_{m+1}^{n-1}\left(v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right)\\ &-\frac{AB(\alpha)}{(1-\alpha)}\sum_{k=0}^{n-2}\big(c_m^{k+1}-c_m^{k}\big)\delta_{n,k}^{\alpha}-v_x\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\big[\theta\big(c_i^{n-1}-c_{i-1}^{n-1}\big)+(1-\theta)\big(c_{i+1}^{n-1}-c_i^{n-1}\big)\big]\,\delta_{m,i}^{\alpha} \end{aligned} \tag{6-66} $$

Equation (6-66) is the explicit upwind-downwind weighted finite difference scheme for the one-dimensional, non-reactive fractional advection-dispersion equation (ABC). Simplifying, the following functions as substituted,

$$ \begin{aligned} a_4c_m^{n}&=q_4c_m^{n-1}+r_4c_{m-1}^{n-1}-s_4c_{m+1}^{n-1}\\ &-g_4\sum_{k=0}^{n-2}\big(c_m^{k+1}-c_m^{k}\big)\delta_{n,k}^{\alpha}-v_xg_4\sum_{i=0}^{m}\big[\theta\big(c_i^{n-1}-c_{i-1}^{n-1}\big)+(1-\theta)\big(c_{i+1}^{n-1}-c_i^{n-1}\big)\big]\,\delta_{m,i}^{\alpha} \end{aligned} \tag{6-67} $$

where,

$$ q_4=\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}-v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{2D_L}{(\Delta x)^2} $$

$$ r_4=v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2} $$

$$ s_4=v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2} $$

### 6.2.5 Implicit upwind-downwind weighted scheme

Similarly, considering both the upwind and downwind direction for the advection term for the first-order upwind finite difference scheme approximation (implicit), a ratio of upwind to downwind is applied ($\theta$), where $0 \le \theta \le 1$. Then, the space advection component becomes,

$$ {}_{0}^{ABC}D_{x}^{\alpha}\big(c(x_m,t_n)\big)=\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}[\theta(c_i^{n}-c_{i-1}^{n})+(1-\theta)(c_{i+1}^{n}-c_i^{n})]\,\delta_{m,i}^{\alpha} \tag{6-68} $$

Substituting this back into the advection-dispersion equation,

$$\frac{AB(\alpha)}{(1-\alpha)}\sum_{k=0}^{n-1}\left(c_m^{k+1}-c_m^k\right)\delta_{n,k}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\left[\theta\left(c_i^n-c_{i-1}^n\right)+(1-\theta)\left(c_{i+1}^n-c_i^n\right)\right]\delta_{m,i}^{\alpha} -D_L\left(\frac{c_{m+1}^n-2c_m^n+c_{m-1}^n}{(\Delta x)^2}\right)=0 \quad (6\text{-}69)$$

Reformulating and rearranging, the following can be obtained

$$\begin{aligned} c_m^n&\left(\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}\right)\\ &=c_{m+1}^n\left(\frac{D_L}{(\Delta x)^2}-v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right)+c_{m-1}^n\left(\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right)\\ &+c_m^{n-1}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}-\frac{AB(\alpha)}{(1-\alpha)}\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^k\right)\delta_{n,k}^{\alpha}\\ &-v_x\frac{AB(\alpha)}{(1-\alpha)}\sum_{i=0}^{m}\left[\theta\left(c_i^n-c_{i-1}^n\right)+(1-\theta)\left(c_{i+1}^n-c_i^n\right)\right]\delta_{m,i}^{\alpha} \end{aligned} \quad (6\text{-}70)$$

Equation (6-70) is the implicit upwind-downwind weighted finite difference scheme for the fractional advection-dispersion equation (ABC). The numerical scheme is simplified substituting terms as followings,

$$\begin{aligned} u_4c_m^n&=v_4c_{m+1}^n+r_4c_{m-1}^n+a_4c_m^{n-1}\\ &-g_4\sum_{k=0}^{n-2}\left(c_m^{k+1}-c_m^k\right)\delta_{n,k}^{\alpha}-v_xg_4\sum_{i=0}^{m}\left[\theta\left(c_i^n-c_{i-1}^n\right)+(1-\theta)\left(c_{i+1}^n-c_i^n\right)\right]\delta_{m,i}^{\alpha} \end{aligned} \quad (6\text{-}71)$$

where,

$$u_4=\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}$$

$$v_4=\frac{D_L}{(\Delta x)^2}-v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}$$

This concludes the formulation of the numerical approximations schemes to be investigated for the fractional advection-dispersion equation with ABC fractional derivative. In the following section, the numerical stability of each scheme will be analysed.

## 6.3 Numerical stability analysis

The numerical stability method used in Chapter 2 for the local operator numerical approximation schemes, and Chapter 5 for the fractional advection-dispersion equation with Caputo fractional derivative, will be applied to the developed numerical approximation schemes for the fractional advection-dispersion equation with ABC fractional derivative. The numerical stability for the upwind schemes are evaluated to validate their use in solving the fractional advection-dispersion equation with the ABC fractional definition.

### 6.3.1 Explicit upwind

Substituting the induction method terms for the developed explicit upwind numerical scheme discussed in Section 6.2.1,

$$a_4\hat{c}_n e^{jk_i m} = b_4\hat{c}_{n-1}e^{jk_i m} + d_4\hat{c}_{n-1}e^{jk_i x(m-\Delta m)} + f_4\hat{c}_{n-1}e^{jk_i(m+\Delta m)} \\ -g_4\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_i m} - \hat{c}_k e^{jk_i m}\right)\delta_{n,k}^{\alpha} - v_x g_4\sum_{i=0}^{m}\left(\hat{c}_{n-1}e^{jk_i m} - \hat{c}_{n-1}e^{jk_i(m-\Delta m)}\right)\delta_{m,i}^{\alpha} \tag{6-72}$$

Multiple out and dividing by $e^{jk_i m}$,

$$a_4\hat{c}_n = b_4\hat{c}_{n-1} + d_4\hat{c}_{n-1}e^{-jk_i\Delta m} + f_4\hat{c}_{n-1}e^{jk_i\Delta m} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha} \\ -v_x g_4\sum_{i=0}^{m}\left(\hat{c}_{n-1} - \hat{c}_{n-1}e^{-jk_i\Delta m}\right)\delta_{m,i}^{\alpha} \tag{6-73}$$

The first procedure for the induction numerical stability analysis entails proving for a set $\forall\ n > 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 1$, then

$$a_4\hat{c}_1 = b_4\hat{c}_0 + d_4\hat{c}_0 e^{-jk_i\Delta m} + f_4\hat{c}_0 e^{jk_i\Delta m} - v_x g_4\sum_{i=0}^{m}\left(\hat{c}_0 - \hat{c}_0 e^{-jk_i\Delta m}\right)\delta_{m,i}^{\alpha} \tag{6-74}$$

A subset for $m$ is considered, where $m = 0$,

$$a_4\hat{c}_1 = b_4\hat{c}_0 + d_4\hat{c}_0 e^{-jk_i\Delta m} + f_4\hat{c}_0 e^{jk_i\Delta m} \tag{6-75}$$

Simplifying and rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{b_4 + d_4 e^{-jk_i\Delta m} + f_4 e^{jk_i\Delta m}}{a_4} \tag{6-76}$$

Applying a norm, the condition for the first induction requirement becomes,

$$\frac{|b_4| + |d_4| + |f_4|}{|a_4|} < 1 \tag{6-77}$$

The term is expanded using the simplification terms associated with Equation (6-57),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|} < 1 \tag{6-78}$$

The assumption is made where,

$$\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} < v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \tag{6-79}$$

Then, the condition is

$$\frac{-\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}<1 \tag{6-80}$$

Simplifying,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}<\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} \tag{6-81}$$

Thus, under the assumption in Equation (6-79), the first inductive stability condition for this subset is upheld and conditionally stable.

A subset for $m$ is now considered for all $m \geq 1$,

$$a_4\hat{c}_1=b_4\hat{c}_0+d_4\hat{c}_0e^{-jk_i\Delta m}+f_4\hat{c}_0e^{jk_i\Delta m}-v_xg_4\sum_{i=0}^{m}\left(\hat{c}_0-\hat{c}_0e^{-jk_i\Delta m}\right)\delta_{m,i}^{\alpha} \tag{6-82}$$

Simplifying,

$$a_4\hat{c}_1=\left(b_4+d_4e^{-jk_i\Delta m}+f_4e^{jk_i\Delta m}-v_xg_4\left(1-e^{-jk_i\Delta m}\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha}\right)\hat{c}_0 \tag{6-83}$$

Expanding the summation, and simplifying

$$\begin{aligned}\sum_{i=0}^{m}\delta_{m,i}^{\alpha}&=\sum_{i=0}^{m}(m-i)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-i)\right]-(m-i-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-i-1)\right]\\&=\left\{(m)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m)\right]-(m-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-1)\right]\right\}\\&\quad+\left\{(m-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-1)\right]-(m-2)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-2)\right]\right\}\\&\quad+\left\{(m-2)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-2)\right]-(m-3)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m-3)\right]\right\}+\cdots\\&\quad+\left\{E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}\right]-(-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(-1)\right]\right\}\\&=\left\{(m)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m)\right]\right\}+\left\{E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}\right]-(-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(-1)\right]\right\}\end{aligned} \tag{6-84}$$

Substituting the expanded summation and applying Euler's formula,

$$a_4\hat{c}_1=\left(b_4+d_4e^{-jk_i\Delta m}+f_4e^{jk_i\Delta m}-v_xg_4(1-\cos\phi+i\,sin\,\theta)\beta_{m,E_{\alpha,2}}\right)\hat{c}_0 \tag{6-85}$$

Applying a norm and simplifying,

$$|a_4||\hat{c}|_1=\left(|b_4|+|d_4|+|f_4|+v_x|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)|\hat{c}_0| \tag{6-86}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|}=\frac{|b_4|+|d_4|+|f_4|+v_x|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|a_4|} \tag{6-87}$$

Thus, the condition becomes,

$$\frac{|b_4| + |d_4| + |f_4| + v_x|g_4|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|a_4|} < 1 \tag{6-88}$$

The term is expanded using the simplification terms associated with Equation (6-57),

$$\frac{\left(\begin{array}{c}\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| \\ + \left|\frac{D_L}{(\Delta x)^2}\right| + v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\end{array}\right)}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|} < 1 \tag{6-89}$$

The same assumption is made (Equation (6-79)), then the condition is,

$$\frac{\left(\begin{array}{c}-\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} + v_x\frac{AB(\alpha)}{(1-\alpha)}(2 - 2\cos\phi)\beta_{m,E_{\alpha,2}}\end{array}\right)}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}} < 1 \tag{6-90}$$

Simplifying,

$$2v_x\frac{AB(\alpha)}{(1-\alpha)}\left(\delta_{m,i}^{\alpha} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{4D_L}{(\Delta x)^2} < \frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} \tag{6-91}$$

Therefore, the first inductive stability condition for the second subset of m is conditionally stable under this assumption.

The induction numerical stability analysis has a second process that requires proving for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Rearranging Equation (6-73) for $\hat{c}_n$,

$$a_4\hat{c}_n = \left(b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4\left(1 - e^{-jk_i\Delta m}\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha}\right)\hat{c}_{n-1} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha} \tag{6-92}$$

Following a similar simplification process of applying Euler and expanding the summation as previously performed,

$$a_4\hat{c}_n = \left(b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4(1 - \cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right)\hat{c}_{n-1} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha} \tag{6-93}$$

Taking the norm on both sides,

$$|a_4\hat{c}_n| = \left|\left(b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right)\hat{c}_{n-1} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-94}$$

Therefore,

$$|a_4||\hat{c}_n| < \left|b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_{n-1}| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-95}$$

Remembering that it has been proved that for a set $\forall\, n > 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Thus,

$$\begin{aligned} |a_4||\hat{c}_n| &< \left|b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_{n-1}| \\ &\quad + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \\ &< \left|b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_o| \\ &\quad + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \end{aligned} \tag{6-96}$$

Therefore, it can be inferred that,

$$|a_4||\hat{c}_n| < \left|b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_o| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-97}$$

The remaining summation is considered at the upper limit,

$$\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| < \sum_{k=0}^{n-2}|\hat{c}_{k+1}|\left(\left|1-\frac{\hat{c}_k}{\hat{c}_{k+1}}\right|\right)\delta_{n,k}^{\alpha}$$

Subset $k$ will follow the same assumption made for a set $\forall\, n \geq 1$, where

$$\sum_{k=0}^{n-2}\hat{c}_{k+1}\left(1-\frac{\hat{c}_k}{\hat{c}_{k+1}}\right)\delta_{n,k}^{\alpha} < |\hat{c}_0|\sum_{k=0}^{n-2}\delta_{n,k}^{\alpha}$$

Substituting back into Equation (6-97),

$$|a_4||\hat{c}_n| < \left|b_4 + d_4e^{-jk_i\Delta m} + f_4e^{jk_i\Delta m} - v_xg_4(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_o| + |g_4||\hat{c}_0|\sum_{k=0}^{n-2}\delta_{n,k}^{\alpha} \tag{6-98}$$

Expanding the summation,

$$\sum_{k=0}^{n-2}\delta_{n,k}^{\alpha}=(n-k)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-k)\right]-(n-k-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-k-1)\right]$$

$$=\left\{(n)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n)\right]-(n-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-1)\right]\right\}$$
$$+\left\{(n-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-1)\right]-(n-2)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-2)\right]\right\}$$
$$+\left\{(n-2)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-2)\right]-(n-3)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n-3)\right]\right\}+\cdots$$
$$+\left\{2E_{\alpha,2}\left[-2\frac{\alpha\,\Delta t}{1-\alpha}\right]-E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}\right]\right\}$$

$$=\left\{(n)E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}(n)\right]\right\}+\left\{2E_{\alpha,2}\left[-2\frac{\alpha\,\Delta t}{1-\alpha}\right]-E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}\right]\right\}$$

Substituting the summation and rearranging,

$$|a_4||\hat{c}_n|<\left(\left|b_4+d_4e^{-jk_i\Delta m}+f_4e^{jk_i\Delta m}-v_xg_4(1-\cos\phi+i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right|+|g_4|\left|\beta_{n,E_{\alpha,2}}\right|\right)|\hat{c}_0| \qquad (6\text{-}99)$$

where,

$$\beta_{n,E_{\alpha,2}}=nE_{\alpha,2}\left[-\frac{\alpha\,\Delta t\,n}{1-\alpha}\right]+2E_{\alpha,2}\left[-\frac{2\alpha\,\Delta t}{1-\alpha}\right]-E_{\alpha,2}\left[-\frac{\alpha\,\Delta t}{1-\alpha}\right]$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_0|}<\frac{|b_4|+|d_4|+|f_4|-v_x|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|+|g_4|\left|\beta_{n,E_{\alpha,2}}\right|}{|a_4|} \qquad (6\text{-}100)$$

Thus, the condition becomes,

$$\frac{|b_4|+|d_4|+|f_4|-v_x|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|+|g_4|\left|\beta_{n,E_{\alpha,2}}\right|}{|a_4|}<1 \qquad (6\text{-}101)$$

The condition is expanded using the simplification terms associated with Equation (6-57),

$$\frac{\begin{array}{c}\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{2D_L}{(\Delta x)^2}\right|+\left|v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right|+\left|\frac{D_L}{(\Delta x)^2}\right|\\ -v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|+\left|\frac{AB(\alpha)}{(1-\alpha)}\right|\left|\beta_{n,E_{\alpha,2}}\right|\end{array}}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|}<1 \qquad (6\text{-}102)$$

The assumption in Equation (6-79) is made, and the conditions is

$$\frac{\begin{array}{c}-\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2}\\ -v_x\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}}+\frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}}\end{array}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}<1 \qquad (6\text{-}103)$$

Simplifying,

$$\frac{AB(\alpha)}{(1-\alpha)}\left(2v\delta_{m,i}^{\alpha}-v_x(2-2\cos\phi)\beta_{m,E_{\alpha,2}}+\beta_{n,E_{\alpha,2}}\right)+\frac{4D_L}{(\Delta x)^2}<\frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} \qquad (6\text{-}104)$$

Thus, under the assumption in (6-79), the second inductive stability condition for is sustained and conditionally stable under this condition.

This completes the stability analysis for the explicit upwind scheme for the advection-dispersion equation with ABC fractional derivative, where the scheme is found to be unstable under the assumption not presented, and conditionally stable under the assumption made of,

$$\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} < v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}$$

With the following conditions,

$$2v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{4D_L}{(\Delta x)^2} < \frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha},$$

$$2v_x\frac{AB(\alpha)}{(1-\alpha)}\left(\delta_{m,i}^{\alpha} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{4D_L}{(\Delta x)^2} < \frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha},$$

$$\frac{AB(\alpha)}{(1-\alpha)}\left(2v\delta_{m,i}^{\alpha} - v_x(2-2\cos\phi)\beta_{m,E_{\alpha,2}} + \beta_{n,E_{\alpha,2}}\right) + \frac{4D_L}{(\Delta x)^2} < \frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha},$$

Simplified to,

$$max(\lambda,\mu,\rho) < \frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}$$

where,

$$\lambda = 2v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{4D_L}{(\Delta x)^2}$$

$$\mu = 2v_x\frac{AB(\alpha)}{(1-\alpha)}\left(\delta_{m,i}^{\alpha} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{4D_L}{(\Delta x)^2}$$

$$\rho = \frac{AB(\alpha)}{(1-\alpha)}\left(2v_x\delta_{m,i}^{\alpha} - v_x(2-2\cos\phi)\beta_{m,E_{\alpha,2}} + \beta_{n,E_{\alpha,2}}\right) + \frac{4D_L}{(\Delta x)^2}$$

### 6.3.2 Implicit upwind

Induction stability terms are substituted for the developed finite difference implicit upwind numerical scheme discussed in Section 6.2.2,

$$h_4\hat{c}_n e^{jk_i m} = j_4\hat{c}_n e^{jk_i(m-\Delta m)} + f_4\hat{c}_n e^{jk_i x(m+\Delta m)} - g_4\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_i m} - \hat{c}_k e^{jk_i m}\right)\delta_{n,k}^{\alpha} - v_x g_4\sum_{i=0}^{m}\left(\hat{c}_n e^{jk_i m} - \hat{c}_n e^{jk_i(m-\Delta m)}\right)\delta_{m,i}^{\alpha} + a_4\hat{c}_{n-1}e^{jk_i m} \tag{6-105}$$

Multiple out and simplify,

$$h_4\hat{c}_n = j_4\hat{c}_n e^{-jk_i\Delta m} + f_4\hat{c}_n e^{jk_i\Delta m} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha} - v_x g_4\sum_{i=0}^{m}\left(\hat{c}_n - \hat{c}_n e^{-jk_i\Delta m}\right)\delta_{m,i}^{\alpha} + a_4\hat{c}_{n-1} \tag{6-106}$$

The first procedure for the induction numerical stability analysis requires proving for a set $\forall\, n > 1$, that

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 1$, then

$$h_4\hat{c}_1 = j_4\hat{c}_1 e^{-jk_i\Delta m} + f_4\hat{c}_1 e^{jk_i\Delta m} - v_x g_4 \sum_{i=0}^{m}\left(\hat{c}_1 - \hat{c}_1 e^{-jk_i\Delta m}\right)\delta_{m,i}^{\alpha} + a_4\hat{c}_0 \tag{6-107}$$

A subset for $m$ is now considered, where $m = 0$,

$$h_4\hat{c}_1 = j_4\hat{c}_1 e^{-jk_i\Delta m} + f_4\hat{c}_1 e^{jk_i\Delta m} + a_4\hat{c}_0 \tag{6-108}$$

Simplifying and rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{a_4}{h_4 - j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m}} \tag{6-109}$$

Applying a norm, the condition for the first induction requirement becomes,

$$\frac{|a_4|}{|h_4| + |j_4| + |f_4|} < 1 \tag{6-110}$$

The term is expanded using the simplification terms associated with Equation (6-60),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right| + \left|v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|} < 1 \tag{6-111}$$

The assumption is made where,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} > \frac{D_L}{(\Delta x)^2} \tag{6-112}$$

Then, the condition is

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}} < 1 \tag{6-113}$$

Simplifying,

$$2v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} > 0 \tag{6-114}$$

Therefore, under the assumption in Equation (6-112), the first inductive stability condition for this subset is upheld and unconditionally stable.

The complementary assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}} < 1 \tag{6-115}$$

Simplifying,

$$\frac{4D_L}{(\Delta x)^2} > 0 \tag{6-116}$$

Thus, the first inductive stability condition for this subset is upheld and unconditionally stable under this assumption as well.

A subset for $m$ is now considered for all $m \geq 1$,

$$h_4\hat{c}_1 = j_4\hat{c}_1 e^{-jk_i\Delta m} + f_4\hat{c}_1 e^{jk_i\Delta m} - v_x g_4 \sum_{i=0}^{m} \left(\hat{c}_1 - \hat{c}_1 e^{-jk_i\Delta m}\right)\delta_{m,i}^{\alpha} + a_4\hat{c}_0 \tag{6-117}$$

Simplifying,

$$\left(h_4 - j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4\left(1 - e^{-jk_i\Delta m}\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha}\right)\hat{c}_1 = a_4\hat{c}_0 \tag{6-118}$$

Expanding the summation as presented previously,

$$\left(\begin{array}{c} h_4 - j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4\left(1 - e^{-jk_i\Delta m}\right)\cdot \\ \left((m)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(m)\right] + E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}\right] - (-1)E_{\alpha,2}\left[-\frac{\alpha\,\Delta x}{1-\alpha}(-1)\right]\right) \end{array}\right)\hat{c}_1 = a_4\hat{c}_0 \tag{6-119}$$

where the function $\beta_{m,E_{\alpha,2}}$ is used to simplify as follows,

$$\left(h_4 - j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4\left(1 - e^{-jk_i\Delta m}\right)\beta_{m,E_{\alpha,2}}\right)\hat{c}_1 = a_4\hat{c}_0 \tag{6-120}$$

Let a function simplify to,

$$\phi = k_i\Delta x$$

where,

$$e^{-j\phi} = e^{-jk_i\Delta x}$$

Remembering Euler's formula for complex numbers, and substituting back into Equation (6-120),

$$\left(h_4 - j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}}\right)\hat{c}_1 = a_4\hat{c}_0 \tag{6-121}$$

Applying a norm on both sides and simplifying,

$$\left(|h_4| + |j_4| + |f_4| + v_x|g_4|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)|\hat{c}_1| = |a_4||\hat{c}_0| \tag{6-122}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|a_4|}{\left(|h_4| + |j_4| + |f_4| + v_x|g_4|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)} \tag{6-123}$$

Thus, the condition becomes,

$$\frac{|a_4|}{\left(|h_4| + |j_4| + |f_4| + v_x|g_4|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)} < 1 \tag{6-124}$$

The term is expanded using the simplification terms associated with Equation (6-60),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|}{\left(\begin{array}{c}\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}\right|+\left|v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{D_L}{(\Delta x)^2}\right|+\left|\frac{D_L}{(\Delta x)^2}\right| \\ +v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\end{array}\right)}<1 \tag{6-125}$$

Considering the assumption made in Equation (6-112), the conditions becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\left(\begin{array}{c}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2} \\ +v_x\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}}\end{array}\right)}<1 \tag{6-126}$$

Simplifying,

$$2v_x\left(\delta_{m,i}^{\alpha}+(1-\cos\phi)\beta_{m,E_{\alpha,2}}\right)\frac{AB(\alpha)}{(1-\alpha)}+\frac{2D_L}{(\Delta x)^2}>0 \tag{6-127}$$

Therefore, under the assumption in Equation (6-112), the first inductive stability condition for the second subset of m is upheld and unconditionally stable.

The opposite assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\left(\begin{array}{c}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2} \\ +v_x\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}}\end{array}\right)}<1 \tag{6-128}$$

Simplifying,

$$\frac{4D_L}{(\Delta x)^2}+v_x(2-2\cos\phi)\frac{AB(\alpha)}{(1-\alpha)}\beta_{m,E_{\alpha,2}}>0 \tag{6-129}$$

Therefore, the first inductive stability condition for the second subset of m is upheld and unconditionally stable under this assumption as well.

The second procedure for the induction numerical stability analysis requires proving for a set $\forall\ n\geq 1$,

$$|\hat{c}_n|<|\hat{c}_o|$$

Rearranging Equation (6-106) for $\hat{c}_n$,

$$\begin{aligned}\left(h_4+j_4e^{-jk_i\Delta m}-f_4e^{jk_i\Delta m}+v_xg_4\left(1-e^{-jk_i\Delta m}\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha}\right)\hat{c}_n \\ =a_4\hat{c}_{n-1}-g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\end{aligned} \tag{6-130}$$

Following a similar simplification process as previously performed,

$$\left(h_4 + j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\, sin\, \phi)\beta_{m,E_{\alpha,2}}\right)\hat{c}_n = a_4\hat{c}_{n-1} - g_4 \sum_{k=0}^{n-2} (\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha} \quad (6\text{-}131)$$

Applying a norm on both sides,

$$\left|\left(h_4 + j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\, sin\, \phi)\beta_{m,E_{\alpha,2}}\right)\hat{c}_n\right| = \left|a_4\hat{c}_{n-1} - g_4 \sum_{k=0}^{n-2} (\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \quad (6\text{-}132)$$

Therefore,

$$\left|h_4 + j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\, sin\, \phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_n| < |a_4||\hat{c}_{n-1}| + |g_4|\left|\sum_{k=0}^{n-2} (\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \quad (6\text{-}133)$$

Remembering that it has been proved that for a set $\forall\, n > 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Thus,

$$\begin{aligned}\left|h_4 + j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\, sin\, \phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_n| &< |a_4||\hat{c}_{n-1}| + |g_4|\left|\sum_{k=0}^{n-2} (\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \\ &< |a_4||\hat{c}_o| + |g_4|\left|\sum_{k=0}^{n-2} (\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right|\end{aligned} \quad (6\text{-}134)$$

Therefore, it can be inferred that,

$$\left|h_4 + j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\, sin\, \phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_n| < |a_4||\hat{c}_o| + |g_4|\left|\sum_{k=0}^{n-2} (\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \quad (6\text{-}135)$$

The remaining summation is considered at the upper limit as previously,

$$\left|h_4 + j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_n| < |a_4||\hat{c}_o| + |g_4||\hat{c}_0| \sum_{k=0}^{n-2} \delta_{n,k}^{\alpha} \quad (6\text{-}136)$$

Expanding the summation and simplifying as previously outlined,

$$\left|h_4 + j_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4(1 - \cos\phi + i\, sin\, \phi)\beta_{m,E_{\alpha,2}}\right||\hat{c}_n| < |a_4||\hat{c}_o| + |g_4||\hat{c}_0|\beta_{n,E_{\alpha,2}} \quad (6\text{-}137)$$

Rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_o|} < \frac{|a_4| + |g_4|\beta_{n,E_{\alpha,2}}}{\left||h_4| + |j_4| + |f_4| + v_x|g_4|(|1 - \cos\phi| + i\,|sin\,\phi|)\beta_{m,E_{\alpha,2}}\right|} \quad (6\text{-}138)$$

Thus, the condition becomes,

$$\frac{|a_4| + |g_4|\beta_{n,E_{\alpha,2}}}{|h_4| + |j_4| + |f_4| + v_x|g_4|(|1-\cos\phi| + i\,|sin\,\phi|)|\beta_{m,E_{\alpha,2}}|} < 1 \tag{6-139}$$

The condition is expanded using the simplification terms associated with Equation (6-60),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right| + \left|\frac{AB(\alpha)}{(1-\alpha)}\right|\beta_{n,E_{\alpha,2}}}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right| + \left|v\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right| \\ +v\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2-2\cos\phi)|\beta_{m,E_{\alpha,2}}|} < 1 \tag{6-140}$$

The assumption in Equation (6-112) is applied, and the condition develops,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + \frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} \\ +v_x\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}}} < 1 \tag{6-141}$$

Simplifying,

$$2v_x\left(\delta_{m,i}^{\alpha} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{2D_L}{(\Delta x)^2} > \beta_{n,E_{\alpha,2}} \tag{6-142}$$

Thus, under the assumption (Equation (6-112)), the second inductive stability condition for is upheld and conditionally stable, under this condition.

The opposite assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + \frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} \\ +v_x\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}}} < 1 \tag{6-143}$$

Simplifying,

$$2v_x(1-\cos\phi)\beta_{m,E_{\alpha,2}} + \frac{4D_L}{(\Delta x)^2} > \beta_{n,E_{\alpha,2}} \tag{6-144}$$

Thus, under this assumption, the second inductive stability condition for is also upheld and conditionally stable, under this condition.

The stability analysis for the implicit upwind scheme for the advection-dispersion equation with ABC fractional derivative found the scheme to be unconditionally stable for the first section of the induction method analysis, and conditionally stable under the following conditions,

$$2v_x\left(\delta_{m,i}^{\alpha} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{2D_L}{(\Delta x)^2} > \beta_{n,E_{\alpha,2}},$$

and

$$2v_x(1-\cos\phi)\beta_{m,E_{\alpha,2}} + \frac{4D_L}{(\Delta x)^2} > \beta_{n,E_{\alpha,2}}$$

This can be simplified to an overall condition,

$$min(\gamma,\eta) > \beta_{n,E_{\alpha,2}}$$

where,

$$\gamma = 2v_x\left(\delta_{m,i}^{\alpha} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{2D_L}{(\Delta x)^2}$$
$$\eta = 2v_x(1-\cos\phi)\beta_{m,E_{\alpha,2}} + \frac{4D_L}{(\Delta x)^2}$$

The error of the approximation is thus reduced throughout the solution and decreases with each time step, under these conditions, where for all values of n, $|\hat{c}_{n+1}| < |\hat{c}_o|$.

### 6.3.3 Upwind advection Crank-Nicolson scheme

Substituting the induction method terms for the developed upwind advection Crank-Nicolson numerical scheme discussed in Section 6.2.3,

$$l_4\hat{c}_n e^{jk_im} = m_4\hat{c}_{n-1}e^{jk_im} + o_4\hat{c}_n e^{jk_i(m-\Delta m)} + f_4\hat{c}_n e^{jk_ix(m+\Delta m)} + p_4\hat{c}_{n-1}e^{jk_i(m-\Delta m)}$$
$$-g_4\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_im} - \hat{c}_k e^{jk_im}\right)\delta_{n,k}^{\alpha} - v_xg_4\sum_{i=0}^{m}\begin{bmatrix}0.5\left(\hat{c}_{n-1}e^{jk_im} - \hat{c}_{n-1}e^{jk_i(m-\Delta m)}\right)\\ +0.5\left(\hat{c}_n e^{jk_im} - \hat{c}_n e^{jk_i(m-\Delta m)}\right)\end{bmatrix}\delta_{m,i}^{\alpha} \quad (6\text{-}145)$$

Multiple out and simplify,

$$l_4\hat{c}_n = m_4\hat{c}_{n-1} + o_4\hat{c}_n e^{-jk_i\Delta m} + f_4\hat{c}_n e^{jk_i\Delta m} + p_4\hat{c}_{n-1}e^{-jk_i\Delta m} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}$$
$$-v_xg_4\sum_{i=0}^{m}\left[0.5\left(\hat{c}_{n-1} - \hat{c}_{n-1}e^{-jk_i\Delta m}\right) + 0.5\left(\hat{c}_n - \hat{c}_n e^{-jk_i\Delta m}\right)\right]\delta_{m,i}^{\alpha} \quad (6\text{-}146)$$

The first procedure for the induction numerical stability analysis requires proving for a set $\forall\, n > 1$, that

$$|\hat{c}_n| < |\hat{c}_o|$$

If $n = 1$, then

$$l_4\hat{c}_1 = m_4\hat{c}_0 + o_4\hat{c}_1 e^{-jk_i\Delta m} + f_4\hat{c}_1 e^{jk_i\Delta m} + p_4\hat{c}_0 e^{-jk_i\Delta m}$$
$$-v_xg_4\sum_{i=0}^{m}\left[0.5\left(\hat{c}_0 - \hat{c}_0 e^{-jk_i\Delta m}\right) + 0.5\left(\hat{c}_1 - \hat{c}_1 e^{-jk_i\Delta m}\right)\right]\delta_{m,i}^{\alpha} \quad (6\text{-}147)$$

A subset for $m$ is now considered, where $m = 0$,

$$l_4\hat{c}_1 = m_4\hat{c}_0 + o_4\hat{c}_1 e^{-jk_i\Delta m} + f_4\hat{c}_1 e^{jk_i\Delta m} + p_4\hat{c}_0 e^{-jk_i\Delta m} \quad (6\text{-}148)$$

Simplifying and rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0} = \frac{m_4 + p_4 e^{-jk_i\Delta m}}{l_4 - o_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m}} \quad (6\text{-}149)$$

Applying a norm, the condition for the first induction requirement becomes,

$$\frac{|m_4| + |p_4|}{|l_4| + |o_4| + |f_4|} < 1 \tag{6-150}$$

The term is expanded using the simplification terms associated with Equation (6-63),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| + \left|0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right|}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right|} < 1 \tag{6-151}$$

The assumption is made where,

$$0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} > \frac{D_L}{(\Delta x)^2} \tag{6-152}$$

Then, the condition is

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}} < 1 \tag{6-153}$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2} > 0 \tag{6-154}$$

Therefore, under the assumption made in Equation (6-152), the first inductive stability condition for this subset is upheld and unconditionally stable.

The complementary assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} - 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2}} < 1 \tag{6-155}$$

Simplifying,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} < \frac{4D_L}{(\Delta x)^2} \tag{6-156}$$

Thus, the first inductive stability condition for this subset is upheld and conditionally stable under this assumption.

A subset for $m$ is now considered for all $m \geq 1$,

$$\begin{aligned} l_4\hat{c}_1 = {} & m_4\hat{c}_0 + o_4\hat{c}_1 e^{-jk_i\Delta m} + f_4\hat{c}_1 e^{jk_i\Delta m} + p_4\hat{c}_0 e^{-jk_i\Delta m} \\ & - v_x g_4 \sum_{i=0}^{m}\left[0.5\left(\hat{c}_0 - \hat{c}_0 e^{-jk_i\Delta m}\right) + 0.5\left(\hat{c}_1 - \hat{c}_1 e^{-jk_i\Delta m}\right)\right]\delta_{m,i}^{\alpha} \end{aligned} \tag{6-157}$$

Simplifying,

$$\left(l_4 - o_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} - 0.5\left(1 - e^{-jk_i\Delta m}\right) v_x g_4 \sum_{i=0}^{m} \delta_{m,i}^{\alpha}\right)\hat{c}_1 = \left(m_4 + p_4 e^{-jk_i\Delta m} - 0.5\left(1 - e^{-jk_i\Delta m}\right) v_x g_4 \sum_{i=0}^{m} \delta_{m,i}^{\alpha}\right)\hat{c}_0 \tag{6-158}$$

Expanding the summation, and simplifying as previously,

$$\left(l_4 - o_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} - 0.5 v_x g_4 (1 - \cos\phi + i\, sin\, \phi)\, \beta_{m,E_{\alpha,2}}\right)\hat{c}_1 = \left(m_4 + p_4 e^{-jk_i\Delta m} - 0.5 v_x g_4 (1 - \cos\phi + i\, sin\, \phi)\beta_{m,E_{\alpha,2}}\right)\hat{c}_0 \tag{6-159}$$

Taking a norm on both sides and simplifying,

$$\left(|l_4| + |o_4| + |f_4| + 0.5 v_x |g_4| (2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)|\hat{c}_1| = \left(|m_4| + |p_4| + 0.5 v_x |g_4| (2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)|\hat{c}_0| \tag{6-160}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|m_4| + |p_4| + v_x |g_4| (1 - \cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|l_4| + |o_4| + |f_4| - v_x |g_4| (1 - \cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} \tag{6-161}$$

Thus, the condition becomes,

$$\frac{|m_4| + |p_4| + v_x |g_4| (1 - \cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|l_4| + |o_4| + |f_4| - v_x |g_4| (1 - \cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} < 1 \tag{6-162}$$

The term is expanded using the simplification terms associated with Equation (6-63),

$$\frac{\left(\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| + \left|0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| + v_x \left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1 - \cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)}{\left(\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right| + v_x \left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1 - \cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)} < 1 \tag{6-163}$$

The same assumption is made as in Equation (6-152), then the conditions is,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + 0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x \frac{AB(\alpha)}{(1-\alpha)}(1 - \cos\phi)\beta_{m,E_{\alpha,2}}}{\left(\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} + 0.5 v_x \frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2} + \frac{D_L}{(\Delta x)^2} + v_x \frac{AB(\alpha)}{(1-\alpha)}(1 - \cos\phi)\beta_{m,E_{\alpha,2}}\right)} < 1 \tag{6-164}$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2} > 0 \tag{6-165}$$

Therefore, under the assumption made in Equation (6-152), the first inductive stability condition for the second subset of m is upheld and unconditionally stable.

The opposite assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\cos\phi)\beta_{m,E_{\alpha,2}}}{\left(\begin{array}{c}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}-0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}+\frac{D_L}{(\Delta x)^2}\\+v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\cos\phi)\beta_{m,E_{\alpha,2}}\end{array}\right)}<1 \tag{6-166}$$

Simplifying,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}<\frac{4D_L}{(\Delta x)^2} \tag{6-167}$$

Therefore, the first inductive stability condition for the second subset of m is upheld and conditionally stable under this assumption.

The second procedure for the induction numerical stability analysis requires proving for a set $\forall\ n\geq 1$,

$$|\hat{c}_n|<|\hat{c}_o|$$

Rearranging Equation (6-146) for $\hat{c}_n$,

$$\begin{aligned}&\left(l_4-o_4e^{-jk_i\Delta m}-f_4e^{jk_i\Delta m}+v_xg_4\left(0.5\left(1-e^{-jk_i\Delta x}\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha}\right)\right)\hat{c}_n\\&\quad=\left(m_4+p_4e^{-jk_i\Delta m}-v_xg_4\left(0.5\left(1-e^{-jk_i\Delta x}\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha}\right)\right)\hat{c}_{n-1}-g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\end{aligned} \tag{6-168}$$

Following a similar simplification process as previously performed,

$$\begin{aligned}&\left(l_4-o_4e^{-jk_i\Delta m}-f_4e^{jk_i\Delta m}+v_xg_4\left(0.5(1-\cos\phi+i\sin\phi)\beta_{m,E_{\alpha,2}}\right)\right)\hat{c}_n\\&\quad=\left(m_4+p_4e^{-jk_i\Delta m}-v_xg_4\left(0.5(1-\cos\phi+i\sin\phi)\beta_{m,E_{\alpha,2}}\right)\right)\hat{c}_{n-1}-g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\end{aligned} \tag{6-169}$$

Applying a norm,

$$\begin{aligned}&\left|\left(l_4-o_4e^{-jk_i\Delta m}-f_4e^{jk_i\Delta m}+v_xg_4\left(0.5(1-\cos\phi+i\sin\phi)\beta_{m,E_{\alpha,2}}\right)\right)\hat{c}_n\right|\\&\quad=\left|\left(m_4+p_4e^{-jk_i\Delta m}-v_xg_4\left(0.5(1-\cos\phi+i\sin\phi)\beta_{m,E_{\alpha,2}}\right)\right)\hat{c}_{n-1}-g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right|\end{aligned} \tag{6-170}$$

Therefore,

$$\begin{aligned}&\left|\left(l_4-o_4e^{-jk_i\Delta m}-f_4e^{jk_i\Delta m}+v_xg_4\left(0.5(1-\cos\phi+i\sin\phi)\beta_{m,E_{\alpha,2}}\right)\right)\right||\hat{c}_n|\\&\qquad<\left|\left(m_4+p_4e^{-jk_i\Delta m}-v_xg_4\left(0.5(1-\cos\phi+i\sin\phi)\beta_{m,E_{\alpha,2}}\right)\right)\right||\hat{c}_{n-1}|\\&\qquad\qquad+|g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right|\end{aligned} \tag{6-171}$$

Remembering that it has been proved that for a set $\forall\ n>1$,

$$|\hat{c}_{n-1}|<|\hat{c}_o|$$

Thus,

$$\left|\left(l_4 - o_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_n| < \left|\left(m_4 + p_4 e^{-jk_i\Delta m} - v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_{n-1}| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| < \left|\left(m_4 + p_4 e^{-jk_i\Delta m} - v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_o| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-172}$$

Therefore, it can be inferred that,

$$\left|\left(l_4 - o_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_n| < \left|\left(m + p_4 e^{-jk_i\Delta m} - v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_o| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1} - \hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-173}$$

The remaining summation is considered at the upper limit as previously,

$$\left|\left(l_4 - o_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_n| < \left|\left(m_4 + p_4 e^{-jk_i\Delta m} - v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_o| + |g_4||\hat{c}_0|\sum_{k=0}^{n-2}\delta_{n,k}^{\alpha} \tag{6-174}$$

Expanding the summation,

$$\left|\left(l_4 - o_4 e^{-jk_i\Delta m} - f_4 e^{jk_i\Delta m} + v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_n| < \left|\left(m_4 + p_4 e^{-jk_i\Delta m} - v_x g_4\big(0.5(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}}\big)\right)\right||\hat{c}_o| + |g_4||\hat{c}_0|\beta_{n,E_{\alpha,2}} \tag{6-175}$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_o|} < \frac{|m_4| + |p_4| + v_x|g_4|(1-\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|l_4| + |o_4| - |f_4| + v_x|g_4|(1-\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} \tag{6-176}$$

Thus, the condition becomes,

$$\frac{|m_4| + |p_4| + v_x|g_4|(1-\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|l_4| + |o_4| - |f_4| + v_x|g_4|(1-\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} < 1 \tag{6-177}$$

The condition is expanded using the simplification terms associated with Equation (6-63),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| + \left|0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| + v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1-\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{\left(\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right| + \left|0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2}\right| + \left|\frac{D_L}{(\Delta x)^2}\right| + v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1-\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)} < 1 \tag{6-178}$$

The same assumption is made as in Equation (6-152), and the condition then becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\cos\phi)\beta_{m,E_{\alpha,2}}}{\left(\begin{array}{c}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{D_L}{(\Delta x)^2}\\+\frac{D_L}{(\Delta x)^2}+v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\cos\phi)\beta_{m,E_{\alpha,2}}\end{array}\right)}<1 \tag{6-179}$$

Simplifying,

$$\frac{2D_L}{(\Delta x)^2}>0 \tag{6-180}$$

Thus, under this assumption, the second inductive stability condition for is upheld and unconditionally stable under this condition.

The opposite assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\cos\phi)\beta_{m,E_{\alpha,2}}}{\left(\begin{array}{c}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}-0.5v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}\\+\frac{D_L}{(\Delta x)^2}+v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\cos\phi)\beta_{m,E_{\alpha,2}}\end{array}\right)}<1 \tag{6-181}$$

Simplifying,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}<\frac{4D_L}{(\Delta x)^2} \tag{6-182}$$

Under this condition and this assumption, the second inductive stability condition for is supported and conditionally stable.

This completes the stability analysis for the upwind advection Crank-Nicolson scheme for the advection-dispersion equation with ABC fractional derivative, where the scheme is unconditionally stable for assumption made in Equation (6-152), and conditionally stable under the complementary assumption. The determined conditions stated are given in Equation (6-156), (6-167), and (6-182).

### 6.3.4 Explicit upwind-downwind weighted scheme

Replacing the induction method terms in the developed explicit upwind-downwind weighted numerical scheme discussed in Section 6.2.4,

$$\begin{aligned}&a_4\hat{c}_n e^{jk_i m}=q_4\hat{c}_{n-1}e^{jk_i m}+r_4\hat{c}_{n-1}e^{jk_i(m-\Delta m)}-s_4\hat{c}_{n-1}e^{jk_i(m+\Delta m)}\\&-g_4\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_i m}-\hat{c}_k e^{jk_i m}\right)\delta_{n,k}^{\alpha}-v_x g_4\sum_{i=0}^{m}\left[\begin{array}{c}\theta\left(\hat{c}_{n-1}e^{jk_i m}-\hat{c}_{n-1}e^{jk_i(m-\Delta m)}\right)\\+(1-\theta)\left(\hat{c}_{n-1}e^{jk_i x(m+\Delta m)}-\hat{c}_{n-1}e^{jk_i m}\right)\end{array}\right]\delta_{m,i}^{\alpha}\end{aligned} \tag{6-183}$$

Multiple out and dividing by $e^{jk_i m}$,

$$a_4\hat{c}_n=q_4\hat{c}_{n-1}+r_4\hat{c}_{n-1}e^{-jk_i\Delta m}-s_4\hat{c}_{n-1}e^{jk_i\Delta m} \tag{6-184}$$

$$-g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}-v_x g_4\sum_{i=0}^{m}\begin{bmatrix}\theta\left(\hat{c}_{n-1}-\hat{c}_{n-1}e^{-jk_i\Delta m}\right)\\+(1-\theta)\left(\hat{c}_{n-1}e^{jk_i\Delta m}-\hat{c}_{n-1}\right)\end{bmatrix}\delta_{m,i}^{\alpha}$$

The first procedure for the induction numerical stability analysis requires proving for a set $\forall\ n>1$, that

$$|\hat{c}_n|<|\hat{c}_o|$$

If $n=1$, then

$$a_4\hat{c}_n=q_4\hat{c}_{n-1}+r_4\hat{c}_{n-1}e^{-jk_i\Delta m}-s_4\hat{c}_{n-1}e^{jk_i\Delta m}-v_x g_4\sum_{i=0}^{m}\begin{bmatrix}\theta\left(\hat{c}_{n-1}-\hat{c}_{n-1}e^{-jk_i\Delta m}\right)\\+(1-\theta)\left(\hat{c}_{n-1}e^{jk_i\Delta m}-\hat{c}_{n-1}\right)\end{bmatrix}\delta_{m,i}^{\alpha}\quad(6\text{-}185)$$

A subset for $m$ is now considered, where $m=0$,

$$a_4\hat{c}_1=q_4\hat{c}_0+r_4\hat{c}_0e^{-jk_i\Delta m}-s_4\hat{c}_0e^{jk_i\Delta m}\quad(6\text{-}186)$$

Simplifying and rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0}=\frac{a_4}{q_4+r_4e^{-jk_i\Delta m}-s_4e^{jk_i\Delta m}}\quad(6\text{-}187)$$

Applying the norm, the condition for the first induction requirement becomes,

$$\frac{|a_4|}{|q_4|+|r_4|+|s_4|}<1\quad(6\text{-}188)$$

The term is expanded using the simplification terms associated with Equation (6-67),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}-2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{2D_L}{(\Delta x)^2}\right|+\left|v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right|+\left|v_x(1-\theta)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}\right|}<1\quad(6\text{-}189)$$

The assumption is made where,

$$\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}<2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}\quad(6\text{-}190)$$

Under the assumption (Equation (6-190), the condition is

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{-\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{D_L}{(\Delta x)^2}}<1\quad(6\text{-}191)$$

Simplifying,

$$2v_x(\theta-1)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}>\frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\quad(6\text{-}192)$$

Thus, the first inductive stability condition for this subset is upheld and conditionally stable under this assumption.

A subset for $m$ is now considered for all $m \geq 1$,

$$a_4\hat{c}_1 = q_4\hat{c}_0 + r_4\hat{c}_0 e^{-jk_i\Delta m} - s_4\hat{c}_0 e^{jk_i\Delta m} - v_x g_4 \sum_{i=0}^{m} \begin{bmatrix} \theta\left(\hat{c}_0 - \hat{c}_0 e^{-jk_i\Delta m}\right) \\ +(1-\theta)\left(\hat{c}_0 e^{jk_i\Delta m} - \hat{c}_0\right) \end{bmatrix} \delta_{m,i}^{\alpha} \tag{6-193}$$

Simplifying,

$$a_4\hat{c}_1 = \begin{pmatrix} q_4 e^{jk_i\Delta m} + r_4 e^{-jk_i\Delta m} - s_4 e^{jk_i\Delta m} - v_x g_4 \theta\left(1 - e^{-jk_i\Delta m}\right) \sum_{i=0}^{m} \delta_{m,i}^{\alpha} \\ -v g_4 (1-\theta)\left(e^{jk_i\Delta m} - 1\right) \sum_{i=0}^{m} \delta_{m,i}^{\alpha} \end{pmatrix} \hat{c}_0 \tag{6-194}$$

Expanding the summation, and applying a norm as previously,

$$|a_4||\hat{c}_1| = \begin{pmatrix} |q_4| + |r_4| + |s_4| + v_x\theta|g_4|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \\ +v_x|g_4|(1-\theta)(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \end{pmatrix} |\hat{c}_0| \tag{6-195}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|q_4| + |r_4| + |s_4| + v_x\theta|g_4|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x|g_4|(1-\theta)(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|a_4|} \tag{6-196}$$

Thus, the condition becomes,

$$\frac{|q_4| + |r_4| + |s_4| + v_x\theta|g_4|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x|g_4|(1-\theta)(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|}{|a_4|} < 1 \tag{6-197}$$

The term is expanded using the simplification terms associated with Equation (6-71),

$$\frac{\begin{pmatrix} \left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} - v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{2D_L}{(\Delta x)^2}\right| \\ +\left|v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| + \left|v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2}\right| \\ +v_x\theta\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1-\theta)(2 - 2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \end{pmatrix}}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|} < 1 \tag{6-198}$$

The same assumption is made as in Equation (6-190), and then the conditions is

$$\frac{\begin{pmatrix} -\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \\ +v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{D_L}{(\Delta x)^2} \\ +v_x\theta\frac{AB(\alpha)}{(1-\alpha)}(2 - 2\cos\phi)\beta_{m,E_{\alpha,2}} + v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\theta)(2 - 2\cos\phi)\beta_{m,E_{\alpha,2}} \end{pmatrix}}{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}} < 1 \tag{6-199}$$

Simplifying,

$$\frac{2AB(\alpha)}{(1-\alpha)}\left(\delta_{n,n-1}^{\alpha}+v_x\delta_{m,i}^{\alpha}+v_x\cos\phi\,\beta_{m,E_{\alpha,2}}\right)>\frac{2AB(\alpha)}{(1-\alpha)}\left(2v_x\theta\delta_{m,i}^{\alpha}+v_x\beta_{m,E_{\alpha,2}}\right)+\frac{4D_L}{(\Delta x)^2} \tag{6-200}$$

Therefore, the first inductive stability condition for the second subset of m is upheld and conditionally stable under this assumption.

The second procedure for the induction numerical stability analysis requires proving for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Rearranging Equation (6-184),

$$a_4\hat{c}_n=\begin{pmatrix} q_4+r_4e^{-jk_i\Delta m}-s_4e^{jk_i\Delta m} \\ -v_xg_4\left(\theta(1-e^{-jk_i\Delta m})+(1-\theta)(e^{jk_i\Delta m}-1)\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha}\end{pmatrix}\hat{c}_{n-1}-g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha} \tag{6-201}$$

Following a similar simplification process as previously performed,

$$a_4\hat{c}_n=\begin{pmatrix} q_4+r_4e^{-jk_i\Delta m}-s_4e^{jk_i\Delta m} \\ -v_xg_4\left(\theta(1-\cos\phi+i\sin\phi)+(1-\theta)\big((\cos\phi+i\sin\phi)-1\big)\right)\beta_{m,E_{\alpha,2}}\end{pmatrix}\hat{c}_{n-1} -g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha} \tag{6-202}$$

Taking the norm on both sides,

$$|a_4\hat{c}_n|=\left|\begin{pmatrix} q_4+r_4e^{-jk_i\Delta m}-s_4e^{jk_i\Delta m} \\ -v_xg_4\left(\theta(1-\cos\phi+i\sin\phi)+(1-\theta)\big((\cos\phi+i\sin\phi)-1\big)\right)\beta_{m,E_{\alpha,2}}\end{pmatrix}\hat{c}_{n-1} -g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-203}$$

Therefore,

$$|a_4||\hat{c}_n|<\left|\begin{pmatrix} q_4+r_4e^{-jk_i\Delta m}-s_4e^{jk_i\Delta m} \\ -v_xg_4\left(\theta(1-\cos\phi+i\sin\phi)+(1-\theta)\big((\cos\phi+i\sin\phi)-1\big)\right)\beta_{m,E_{\alpha,2}}\end{pmatrix}\right||\hat{c}_{n-1}| +|g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-204}$$

Remembering that it has been proved that for a set $\forall\, n > 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Therefore, it can be inferred that,

$$|a_4||\hat{c}_n|<\left|\begin{pmatrix} q_4+r_4e^{-jk_i\Delta m}-s_4e^{jk_i\Delta m} \\ -v_xg_4\left(\theta(1-\cos\phi+i\sin\phi)+(1-\theta)\big((\cos\phi+i\sin\phi)-1\big)\right)\beta_{m,E_{\alpha,2}}\end{pmatrix}\right||\hat{c}_{o}| +|g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-205}$$

The remaining summation is considered at the upper limit and expanded as previously,

$$|a_4||\hat{c}_n| < \left(\left|\begin{matrix} q_4 + r_4 e^{-jk_i\Delta m} - s_4 e^{jk_i\Delta m} \\ -v_x g_4\left(\theta(1-\cos\phi + i\sin\phi) + (1-\theta)\left((\cos\phi + i\sin\phi) - 1\right)\right)\beta_{m,E_{\alpha,2}} \end{matrix}\right| + |g_4|\left|\beta_{n,E_{\alpha,2}}\right|\right)|\hat{c}_o| \tag{6-206}$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_o|} < \frac{\begin{pmatrix} |q_4| + |r_4| + |s_4| + v_x\theta|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \\ +v_x|g_4|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + |g|\left|\beta_{n,E_{\alpha,2}}\right| \end{pmatrix}}{|a_4|} \tag{6-207}$$

Thus, the condition becomes,

$$\frac{\begin{pmatrix} |q_4| + |r_4| + |s_4| + v_x\theta|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \\ +v_x|g_4|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + |g|\left|\beta_{n,E_{\alpha,2}}\right| \end{pmatrix}}{|a_4|} < 1 \tag{6-208}$$

The condition is expanded using the simplification terms associated with Equation (6-67),

$$\frac{\begin{matrix} \left|\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1} - 2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} - \frac{2D_L}{(\Delta x)^2}\right| \\ + \left|v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{D_L}{(\Delta x)^2}\right| \\ + \left|v_x\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} - v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{D_L}{(\Delta x)^2}\right| + v_x\theta\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \\ +v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + \left|\frac{AB(\alpha)}{(1-\alpha)}\right|\left|\beta_{n,E_{\alpha,2}}\right| \end{matrix}}{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1}\right|} < 1 \tag{6-209}$$

The same assumption is made again (Equation (6-190)), and under this assumption the condition is,

$$\frac{\begin{matrix} -\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1} + 2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{2D_L}{(\Delta x)^2} \\ +v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{D_L}{(\Delta x)^2} \\ -v_x\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} - \frac{D_L}{(\Delta x)^2} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \\ +v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\theta)(2-2\cos\phi)\beta_{m,E_{\alpha,2}} + \frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}} \end{matrix}}{\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1}} < 1 \tag{6-210}$$

Simplifying,

$$\frac{2AB(\alpha)}{(1-\alpha)}\left(\delta^{\alpha}_{n,n-1} + v_x\delta^{\alpha}_{m,i} + v_x\cos\phi\,\beta_{m,E_{\alpha,2}}\right) > \frac{AB(\alpha)}{(1-\alpha)}\left(2v_x\beta_{m,E_{\alpha,2}} + 4v_x\theta\delta^{\alpha}_{m,i} + \beta_{n,E_{\alpha,2}}\right) + \frac{4D_L}{(\Delta x)^2} \tag{6-211}$$

Thus, under this assumption, the second inductive stability condition for is upheld and conditionally stable under this condition.

This concludes the stability analysis for the explicit upwind-downwind weighted scheme for the advection-dispersion equation with ABC fractional derivative, where the scheme is found to be unstable under the assumption not presented and is conditionally stable under the assumption (Equation (6-190)), with the following stability conditions,

$$2v_x(\theta-1)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}>\frac{2AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha},$$

$$\frac{2AB(\alpha)}{(1-\alpha)}\left(\delta_{n,n-1}^{\alpha}+v_x\delta_{m,i}^{\alpha}+v_x\cos\phi\,\beta_{m,E_{\alpha,2}}\right)>\frac{2AB(\alpha)}{(1-\alpha)}\left(2v_x\theta\delta_{m,i}^{\alpha}+v_x\beta_{m,E_{\alpha,2}}\right)+\frac{4D_L}{(\Delta x)^2},$$

$$\frac{2AB(\alpha)}{(1-\alpha)}\left(\delta_{n,n-1}^{\alpha}+v_x\delta_{m,i}^{\alpha}+v_x\cos\phi\,\beta_{m,E_{\alpha,2}}\right)>\frac{AB(\alpha)}{(1-\alpha)}\left(4v_x\theta\delta_{m,i}^{\alpha}+2v_x\beta_{m,E_{\alpha,2}}+\beta_{n,E_{\alpha,2}}\right)+\frac{4D_L}{(\Delta x)^2}$$

### 6.3.5 Implicit upwind-downwind weighted scheme

Substituting the induction method terms for the implicit upwind-downwind weighted numerical scheme discussed in Section 6.2.5,

$$\begin{aligned}u_4\hat{c}_n e^{jk_i m} &= v_4\hat{c}_n e^{jk_i x(m+\Delta m)}+r_4\hat{c}_n e^{jk_i(m-\Delta m)}+a_4\hat{c}_{n-1}e^{jk_i m}\\&-g_4\sum_{k=0}^{n-2}\left(\hat{c}_{k+1}e^{jk_i m}-\hat{c}_k e^{jk_i m}\right)\delta_{n,k}^{\alpha}\\&-v_x g_4\sum_{i=0}^{m}\left[\theta\left(\hat{c}_n e^{jk_i m}-\hat{c}_n e^{jk_i(m-\Delta m)}\right)+(1-\theta)\left(\hat{c}_n e^{jk_i x(m+\Delta m)}-\hat{c}_n e^{jk_i m}\right)\right]\delta_{m,i}^{\alpha}\end{aligned} \quad (6\text{-}212)$$

Multiple out and dividing by $e^{jk_i m}$,

$$\begin{aligned}u_4\hat{c}_n &= v_4\hat{c}_n e^{jk_i\Delta m}+r_4\hat{c}_n e^{-jk_i\Delta m}+a_4\hat{c}_{n-1}-g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\\&-v_x g_4\sum_{i=0}^{m}\left[\theta\left(\hat{c}_n-\hat{c}_n e^{-jk_i\Delta m}\right)+(1-\theta)\left(\hat{c}_n e^{jk_i\Delta m}-\hat{c}_n\right)\right]\delta_{m,i}^{\alpha}\end{aligned} \quad (6\text{-}213)$$

As stated previously, the first procedure for the induction numerical stability analysis requires proving for a set $\forall\, n>1$, that

$$|\hat{c}_n|<|\hat{c}_o|$$

If $n=1$, then

$$u_4\hat{c}_1=v_4\hat{c}_1 e^{jk_i\Delta m}+r_4\hat{c}_1 e^{-jk_i\Delta m}+a_4\hat{c}_0-v_x g_4\sum_{i=0}^{m}\begin{bmatrix}\theta\left(\hat{c}_1-\hat{c}_1 e^{-jk_i\Delta m}\right)\\+(1-\theta)\left(\hat{c}_1 e^{jk_i\Delta m}-\hat{c}_1\right)\end{bmatrix}\delta_{m,i}^{\alpha} \quad (6\text{-}214)$$

A subset for $m$ is now considered, where $m=0$,

$$u_4\hat{c}_1=v_4\hat{c}_1 e^{jk_i\Delta m}+r_4\hat{c}_1 e^{-jk_i\Delta m}+a_4\hat{c}_0 \quad (6\text{-}215)$$

Simplifying and rearranging,

$$\frac{\hat{c}_1}{\hat{c}_0}=\frac{a_4}{u_4-v_4 e^{jk_i\Delta m}-r_4 e^{-jk_i\Delta m}} \quad (6\text{-}216)$$

Applying a norm, the condition for the first induction requirement becomes,

$$\frac{|a_4|}{|u_4|+|v_4|+|r_4|}<1 \tag{6-217}$$

The term is expanded using the simplification terms associated with Equation (6-63),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|}{\left(\begin{gathered}\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}\right|\\+\left|\frac{D_L}{(\Delta x)^2}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right|+\left|\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right|\end{gathered}\right)}<1 \tag{6-218}$$

The assumption is made where,

$$\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}>v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} \tag{6-219}$$

Under the assumption (Equation (6-219)), the condition is

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\left(\begin{gathered}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}\\+\frac{D_L}{(\Delta x)^2}-v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\end{gathered}\right)}<1 \tag{6-220}$$

Simplifying,

$$(2\theta-1)v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}>0 \tag{6-221}$$

Remembering the weighting factor $\theta$, the condition for this subset of $m$ is unconditionally stable when $0.5 \le \theta \le 1$, but conditionally stable when $0 \le \theta < 0.5$.

The opposed assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\left(\begin{gathered}-\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}-2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{2D_L}{(\Delta x)^2}\\-\frac{D_L}{(\Delta x)^2}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\end{gathered}\right)}<1 \tag{6-222}$$

Simplifying,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}>\left(\delta_{n,n-1}^{\alpha}+v_x\theta\delta_{m,i}^{\alpha}\right)\frac{AB(\alpha)}{(1-\alpha)}+\frac{D_L}{(\Delta x)^2} \tag{6-223}$$

Hence, the first inductive stability condition for this subset is sustained and conditionally stable under the complementary assumption.

A subset for $m$ is now considered for all $m \ge 1$,

$$u_4\hat{c}_1=v_4\hat{c}_1e^{jk_i\Delta m}+r_4\hat{c}_1e^{-jk_i\Delta m}+a_4\hat{c}_0-v_xg_4\sum_{i=0}^{m}\left[\begin{gathered}\theta\left(\hat{c}_1-\hat{c}_1e^{-jk_i\Delta m}\right)\\+(1-\theta)\left(\hat{c}_1e^{jk_i\Delta m}-\hat{c}_1\right)\end{gathered}\right]\delta_{m,i}^{\alpha} \tag{6-224}$$

Simplifying,

$$\begin{pmatrix} u_4 - v_4 e^{jk_i\Delta m} - r_4 e^{-jk_i\Delta m} + v_x g_4 \theta\left(1 - e^{-jk_i\Delta m}\right) \sum_{i=0}^{m} \delta_{m,i}^{\alpha} \\ +v_x g_4 (1-\theta)\left(e^{jk_i\Delta m} - 1\right) \sum_{i=0}^{m} \delta_{m,i}^{\alpha} \end{pmatrix} \hat{c}_1 = a_4 \hat{c}_0 \tag{6-225}$$

Expanding the summation, and applying a norm on both sides as previously,

$$\begin{aligned}\left(|u| + |v_4| + |r_4| + v_x\theta|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x|g_4|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\right)|\hat{c}_1| \\ = |a_4||\hat{c}_0|\end{aligned} \tag{6-226}$$

Rearranging,

$$\frac{|\hat{c}_1|}{|\hat{c}_0|} = \frac{|a_4|}{|u_4| + |v_4| + |r_4| + v_x\theta|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x|g_4|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} \tag{6-227}$$

Thus, the condition becomes,

$$\frac{|a_4|}{|u_4| + |v_4| + |r_4| + v_x\theta|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x|g_4|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} < 1 \tag{6-228}$$

The term is expanded using the simplification terms associated with Equation (6-71),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right|}{\begin{pmatrix} \left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right| \\ + \left|\frac{D_L}{(\Delta x)^2} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| + \left|\frac{D_L}{(\Delta x)^2} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| \\ +v_x\theta\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| \end{pmatrix}} < 1 \tag{6-229}$$

The assumption in Equation (6-219) is made, and the resulting stability condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\begin{pmatrix} \frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} \\ +v_x\theta\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}} + v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\theta)(2-2\cos\phi)\beta_{m,E_{\alpha,2}} \end{pmatrix}} < 1 \tag{6-230}$$

Simplifying,

$$v_x(2\theta-1)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x(1-\cos\phi)\frac{AB(\alpha)}{(1-\alpha)}\beta_{m,E_{\alpha,2}} + \frac{2D_L}{(\Delta x)^2} > 0 \tag{6-231}$$

Therefore, under the assumption (Equation (6-219)), the first inductive stability condition for the second subset of m is defended and unconditionally stable when $0.5 \leq \theta \leq 1$; and conditionally stable when $0 \leq \theta < 0.5$.

The complementary assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}}{\begin{pmatrix} -\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} - 2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - \frac{2D_L}{(\Delta x)^2} \\ -\frac{D_L}{(\Delta x)^2} + v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} \\ +v_x\theta\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}} + v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\theta)(2-2\cos\phi)\beta_{m,E_{\alpha,2}} \end{pmatrix}} < 1 \tag{6-232}$$

Simplifying,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\left(\beta_{m,E_{\alpha,2}} + \delta_{m,i}^{\alpha}\right) > \frac{AB(\alpha)}{(1-\alpha)}\left(\delta_{n,n-1}^{\alpha} + v_x\theta\delta_{m,i}^{\alpha} + v_x\cos\phi\,\beta_{m,E_{\alpha,2}}\right) + \frac{D_L}{(\Delta x)^2} \tag{6-233}$$

Therefore, under this assumption the first inductive stability condition for the second subset of m is upheld and conditionally stable.

The second procedure for the induction numerical stability analysis requires proving for a set $\forall\, n \geq 1$,

$$|\hat{c}_n| < |\hat{c}_o|$$

Rearranging Equation (6-213) for $\hat{c}_n$,

$$\begin{pmatrix} u_4 - v_4e^{jk_i\Delta m} - r_4e^{-jk_i\Delta m} + v_xg_4\theta\left(1-e^{-jk_i\Delta m}\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha} \\ + v_xg_4(1-\theta)\left(e^{jk_i\Delta m}-1\right)\sum_{i=0}^{m}\delta_{m,i}^{\alpha} \end{pmatrix}\hat{c}_n = a_4\hat{c}_{n-1} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha} \tag{6-234}$$

Following a similar simplification process as previously performed,

$$\begin{pmatrix} u_4 - v_4e^{jk_i\Delta m} - r_4e^{-jk_i\Delta m} + v_xg_4\theta(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}} \\ +v_xg_4(1-\theta)\left((\cos\phi + i\sin\phi)-1\right)\beta_{m,E_{\alpha,2}} \end{pmatrix}\hat{c}_n = a_4\hat{c}_{n-1} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha} \tag{6-235}$$

Applying a norm,

$$\left|\begin{pmatrix} u_4 - v_4e^{jk_i\Delta m} - r_4e^{-jk_i\Delta m} + v_xg_4\theta(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}} \\ +v_xg_4(1-\theta)\left((\cos\phi + i\sin\phi)-1\right)\beta_{m,E_{\alpha,2}} \end{pmatrix}\hat{c}_n\right| = \left|a_4\hat{c}_{n-1} - g_4\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-236}$$

Therefore,

$$\left|\begin{pmatrix} u_4 - v_4e^{jk_i\Delta m} - r_4e^{-jk_i\Delta m} + v_xg_4\theta(1-\cos\phi + i\sin\phi)\beta_{m,E_{\alpha,2}} \\ +v_xg_4(1-\theta)\left((\cos\phi + i\sin\phi)-1\right)\beta_{m,E_{\alpha,2}} \end{pmatrix}\right||\hat{c}_n| < |a_4||\hat{c}_{n-1}| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-237}$$

Remembering that it has been proved that for a set $\forall\, n > 1$,

$$|\hat{c}_{n-1}| < |\hat{c}_o|$$

Thus,

$$\left|\begin{pmatrix} u_4 - v_4 e^{jk_i\Delta m} - r_4 e^{-jk_i\Delta m} + v_x g_4 \theta(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}} \\ +v_x g_4(1-\theta)\big((\cos\phi + i\,sin\,\phi) - 1\big)\beta_{m,E_{\alpha,2}} \end{pmatrix}\right| |\hat{c}_n| < |a_4||\hat{c}_{n-1}| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| < |a_4||\hat{c}_o| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-238}$$

Therefore, it can be inferred that,

$$\left|\begin{pmatrix} u_4 - v_4 e^{jk_i\Delta m} - r_4 e^{-jk_i\Delta m} + v_x g_4 \theta(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}} \\ +v_x g_4(1-\theta)\big((\cos\phi + i\,sin\,\phi) - 1\big)\beta_{m,E_{\alpha,2}} \end{pmatrix}\right| |\hat{c}_n| < |a_4||\hat{c}_o| + |g_4|\left|\sum_{k=0}^{n-2}(\hat{c}_{k+1}-\hat{c}_k)\delta_{n,k}^{\alpha}\right| \tag{6-239}$$

The remaining summation is considered at the upper limit and expanded as previously performed,

$$\left|\begin{pmatrix} u_4 - v_4 e^{jk_i\Delta m} - r_4 e^{-jk_i\Delta m} + v_x g_4 \theta(1-\cos\phi + i\,sin\,\phi)\beta_{m,E_{\alpha,2}} \\ +v_x g_4(1-\theta)\big((\cos\phi + i\,sin\,\phi) - 1\big)\beta_{m,E_{\alpha,2}} \end{pmatrix}\right| |\hat{c}_n| < \big(|a_4| + |g_4|\left|\beta_{n,E_{\alpha,2}}\right|\big)|\hat{c}_o| \tag{6-240}$$

Simplifying and rearranging,

$$\frac{|\hat{c}_n|}{|\hat{c}_o|} < \frac{|a_4| + |g_4|\left|\beta_{n,E_{\alpha,2}}\right|}{|u_4| + |v_4| + |r_4| + v_x\theta|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x|g_4|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} \tag{6-241}$$

Thus, the condition becomes,

$$\frac{|a_4| + |g_4|\left|\beta_{n,E_{\alpha,2}}\right|}{|u_4| + |v_4| + |r_4| + v_x\theta|g_4|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x|g_4|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|} < 1 \tag{6-242}$$

The condition is expanded using the simplification terms associated with Equation (6-71),

$$\frac{\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}\right| + \left|\frac{AB(\alpha)}{(1-\alpha)}\right|\left|\beta_{n,E_{\alpha,2}}\right|}{\begin{gathered}\left|\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2}\right| \\ + \left|\frac{D_L}{(\Delta x)^2} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| + \left|\frac{D_L}{(\Delta x)^2} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\right| \\ +v_x\theta\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right| + v_x\left|\frac{AB(\alpha)}{(1-\alpha)}\right|(1-\theta)(2-2\cos\phi)\left|\beta_{m,E_{\alpha,2}}\right|\end{gathered}} < 1 \tag{6-243}$$

Similarly, the assumption in Equation (6-219) is made, and hence the conditions is,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + \frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}}}{\begin{gathered}\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha} + 2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{2D_L}{(\Delta x)^2} \\ + \frac{D_L}{(\Delta x)^2} - v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} + \frac{D_L}{(\Delta x)^2} + v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha} \\ +v_x\theta\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}} + v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\theta)(2-2\cos\phi)\beta_{m,E_{\alpha,2}}\end{gathered}} < 1 \tag{6-244}$$

Simplifying,

$$2v_x \frac{AB(\alpha)}{(1-\alpha)}\left(\delta_{m,i}^{\alpha}(2\theta-1)+(1\ -\cos\phi)\beta_{m,E_{\alpha,2}}\right)+\frac{4D_L}{(\Delta x)^2}>\frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}} \tag{6-245}$$

According to the assumption in Equation (6-219) and stability condition, the second inductive stability condition for is upheld and unconditionally stable when $0.5 \le \theta \le 1$, and conditionally stable when $0 \le \theta < 0.5$. The complementary assumption is made, and the condition becomes,

$$\frac{\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}+\frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}}}{\begin{array}{c}-\frac{AB(\alpha)}{(1-\alpha)}\delta_{n,n-1}^{\alpha}-2v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-\frac{2D_L}{(\Delta x)^2}\\ -\frac{D_L}{(\Delta x)^2}+v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}-v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{D_L}{(\Delta x)^2}+v_x\theta\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}\\ +v_x\theta\frac{AB(\alpha)}{(1-\alpha)}(2-2\cos\phi)\beta_{m,E_{\alpha,2}}+v_x\frac{AB(\alpha)}{(1-\alpha)}(1-\theta)(2-2\cos\phi)\beta_{m,E_{\alpha,2}}\end{array}}<1 \tag{6-246}$$

Simplifying,

$$2v_x \frac{AB(\alpha)}{(1-\alpha)}\left((1-\theta)\delta_{m,i}^{\alpha}+(1\ -\cos\phi)\beta_{m,E_{\alpha,2}}\right)-\frac{2D_L}{(\Delta x)^2}>\frac{AB(\alpha)}{(1-\alpha)}\left(2\delta_{n,n-1}^{\alpha}+\beta_{n,E_{\alpha,2}}\right) \tag{6-247}$$

Under the complementary assumption and condition, the second inductive stability condition for is supported and the numerical scheme is conditionally stable.

This completes the stability analysis for the implicit upwind-downwind weighted scheme for the advection-dispersion equation with ABC fractional derivative, where the scheme is stable under the following condition,

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}>\left(\delta_{n,n-1}^{\alpha}+v_x\theta\delta_{m,i}^{\alpha}\right)\frac{AB(\alpha)}{(1-\alpha)}+\frac{D_L}{(\Delta x)^2},$$

$$v_x\frac{AB(\alpha)}{(1-\alpha)}\left(\beta_{m,E_{\alpha,2}}+\delta_{m,i}^{\alpha}\right)>\frac{AB(\alpha)}{(1-\alpha)}\left(\delta_{n,n-1}^{\alpha}+v_x\theta\delta_{m,i}^{\alpha}+v_x\cos\phi\,\beta_{m,E_{\alpha,2}}\right)+\frac{D_L}{(\Delta x)^2},$$

$$2v_x \frac{AB(\alpha)}{(1-\alpha)}\left(\delta_{m,i}^{\alpha}(2\theta-1)+(1\ -\cos\phi)\beta_{m,E_{\alpha,2}}\right)+\frac{4D_L}{(\Delta x)^2}>\frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}}$$

$$2v_x \frac{AB(\alpha)}{(1-\alpha)}\left((1-\theta)\delta_{m,i}^{\alpha}+(1\ -\cos\phi)\beta_{m,E_{\alpha,2}}\right)-\frac{2D_L}{(\Delta x)^2}>\frac{AB(\alpha)}{(1-\alpha)}\left(2\delta_{n,n-1}^{\alpha}+\beta_{n,E_{\alpha,2}}\right)$$

Additional conditions are activated when the weighting factor is $0 \le \theta < 0.5$,

$$(2\theta-1)v_x\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+\frac{2D_L}{(\Delta x)^2}>0,$$

$$v_x(2\theta-1)\frac{AB(\alpha)}{(1-\alpha)}\delta_{m,i}^{\alpha}+v_x(1-\cos\phi)\frac{AB(\alpha)}{(1-\alpha)}\beta_{m,E_{\alpha,2}}+\frac{2D_L}{(\Delta x)^2}>0$$

Only under these conditions, the error of the approximation made by the implicit upwind-downwind weighted numerical scheme is not propagated throughout the solution.

### 6.3.6 Evaluation of numerical stability results

The stability conditions for the traditional upwind (implicit/explicit), upwind advection Crank-Nicolson and weighted upwind-downwind (implicit/explicit) numerical schemes are summarised in Table 6-1. The traditional implicit upwind scheme applied to the fractional advection-dispersion equation with ABC fractional derivative is conditionally stable under both assumptions made with a single condition for each assumption. There is only one practically applicable assumption for the customary explicit upwind scheme, which has three sub-conditions. The upwind advection Crank-Nicolson numerical scheme applied to the fractional advection-dispersion equation with ABC fractional derivative is unconditionally stable under the first assumption, and has a single condition under the second assumption made. The implicit upwind-downwind weighted numerical scheme is conditionally stable under both assumptions made, but unconditionally stable for the first assumption when the weighting factor is $0.5 \leq \theta \leq 1$. Similar to the explicit upwind scheme, the explicit upwind-downwind weighted numerical scheme has one practically applicable assumption, which has three conditions for stability.

Of the numerical schemes analysed, the upwind advection Crank-Nicolson is the most stable numerical scheme, and would be suggested for use with the fractional advection-dispersion equation (ABC). The implicit upwind formulations are found to be more stable than the comparable explicit formulations. The proposed weighted implicit upwind-downwind scheme is more stable than the traditional upwind scheme when the weighting factor is $0.5 \leq \theta \leq 1$, which denotes at least half upwind weighted or more, with the downwind influence less than half.

## 6.4 Chapter summary

To improve the governing equation for groundwater transport modelling, the Atangana-Baleanu in Caputo sense (ABC) fractional derivative is applied to the advection-dispersion equation with a focus on the advection term to account for *anomalous advection*. Boundedness, existence and uniqueness for the developed advection-focused transport equation is presented. In addition, a semi-discretisation analysis is performed to demonstrate the equation stability in time. The augmented upwind schemes are developed to facilitate the solution of the complex equation, and stability analysis conducted. The numerical stability analysis found the upwind Crank-Nicolson to be the most stable, and is thus recommended for use with the fractional advection-dispersion equation with ABC fractional derivative.

**Table 6-1 Summary of the stability conditions for the upwind-based numerical schemes for the fractional advection-dispersion equation with ABC derivative**

| Scheme | Assumption | Stability conditions |
|---|---|---|
| **Implicit upwind** | $v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} > \frac{D_L}{(\Delta x)^2}$ | $2v\left(\delta^{\alpha}_{m,i} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{2D_L}{(\Delta x)^2} > \beta_{n,E_{\alpha,2}}$ |
| | $v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} < \frac{D_L}{(\Delta x)^2}$ | $2v(1-\cos\phi)\beta_{m,E_{\alpha,2}} + \frac{4D_L}{(\Delta x)^2} > \beta_{n,E_{\alpha,2}}$ |
| **Explicit upwind** | Assumption not made | Unstable |
| | $\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1} < v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{2D_L}{(\Delta x)^2}$ | $max(\lambda,\mu,\rho) < \frac{2AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1}$ |
| **Upwind advection Crank-Nicolson** | $0.5v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} > \frac{D_L}{(\Delta x)^2}$ | Unconditionally stable |
| | $0.5v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} < \frac{D_L}{(\Delta x)^2}$ | $v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} < \frac{4D_L}{(\Delta x)^2}$ |
| **Implicit upwind-downwind weighted scheme** | $\frac{D_L}{(\Delta x)^2} + v\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} > v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i}$ | $(2\theta-1)v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{2D_L}{(\Delta x)^2} > 0$<br>$(2\theta-1)\frac{AB(\alpha)v}{(1-\alpha)}\delta^{\alpha}_{m,i} + (1-\cos\phi)\frac{AB(\alpha)v}{(1-\alpha)}\beta_{m,E_{\alpha,2}} + \frac{2D_L}{(\Delta x)^2} > 0$<br>$2v\frac{AB(\alpha)}{(1-\alpha)}\left(\delta^{\alpha}_{m,i}(2\theta-1) + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right) + \frac{4D_L}{(\Delta x)^2} > \frac{AB(\alpha)}{(1-\alpha)}\beta_{n,E_{\alpha,2}}$<br>*Unconditionally stable when $0.5 \le \theta \le 1$, or conditionally stable when $0 \le \theta < 0.5$ |
| | $\frac{D_L}{(\Delta x)^2} + v\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} < v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i}$ | $v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} > \left(\delta^{\alpha}_{n,n-1} + v\theta\delta^{\alpha}_{m,i}\right)\frac{AB(\alpha)}{(1-\alpha)} + \frac{D_L}{(\Delta x)^2}$<br>$v\left(\beta_{m,E_{\alpha,2}} + \delta^{\alpha}_{m,i}\right)\frac{AB(\alpha)}{(1-\alpha)} > \left(\delta^{\alpha}_{n,n-1} + v\theta\delta^{\alpha}_{m,i} + v\cos\phi\,\beta_{m,E_{\alpha,2}}\right)\frac{AB(\alpha)}{(1-\alpha)} + \frac{D_L}{(\Delta x)^2}$<br>$2v\left((1-\theta)\delta^{\alpha}_{m,i} + (1-\cos\phi)\beta_{m,E_{\alpha,2}}\right)\frac{AB(\alpha)}{(1-\alpha)} - \frac{2D_L}{(\Delta x)^2} > \left(2\delta^{\alpha}_{n,n-1} + \beta_{n,E_{\alpha,2}}\right)\frac{AB(\alpha)}{(1-\alpha)}$ |
| **Explicit upwind-downwind weighted scheme** | Assumption not made | Unstable |
| | $\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1} + v\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} < 2v\theta\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{2D_L}{(\Delta x)^2}$ | $2v(\theta-1)\frac{AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{m,i} + \frac{2D_L}{(\Delta x)^2} > \frac{2AB(\alpha)}{(1-\alpha)}\delta^{\alpha}_{n,n-1}$<br>$\left(\delta^{\alpha}_{n,n-1} + v\delta^{\alpha}_{m,i} + v\cos\phi\,\beta_{m,E_{\alpha,2}}\right)\frac{2AB(\alpha)}{(1-\alpha)} > \left(2v\theta\delta^{\alpha}_{m,i} + v\beta_{m,E_{\alpha,2}}\right)\frac{2AB(\alpha)}{(1-\alpha)} + \frac{4D_L}{(\Delta x)^2}$<br>$\left(\delta^{\alpha}_{n,n-1} + v\delta^{\alpha}_{m,i} + v\cos\phi\,\beta_{m,E_{\alpha,2}}\right)\frac{2AB(\alpha)}{(1-\alpha)} > \left(2v\beta_{m,E_{\alpha,2}} + 4v\theta\delta^{\alpha}_{m,i} + \beta_{n,E_{\alpha,2}}\right)\frac{AB(\alpha)}{(1-\alpha)} + \frac{4D_L}{(\Delta x)^2}$ |

# 7 Fractional-fractal Advection-dispersion Equation

A fractal advection-dispersion equation and a fractional space-time advection-dispersion equation has been developed thus far to improve the simulation of groundwater transport specifically in fractured aquifers. However, the practicality of simulating a space-time fractional advection-dispersion equation is limited due to the computational power required and complexity of the required algorithms. On the other hand, the fractal advection-dispersion equation only considered fractal derivatives in space, and not time. Considering these two observations, it is theorised that combining these two approaches, fractional derivative in time and fractal derivative in space, could be the most efficient way of incorporating non-locality into both time and space components.

Fractional and fractal derivatives have been considered together by many authors, but mostly separately for comparison and not fully combined in a single model (Nyikos and Pajkossy, 1985; Berry and Klein, 1996; Hilfer and Anton, 1995; El-Nabulsi, 2010; Chen et al., 2010a; Chen et al., 2010b; Sun et al., 2013; Chen and Liang, 2017; Sun et al., 2017b). Chen et al. (2010a) compared a fractal and fractional diffusion model, and found that both models can characterise the power law phenomena of anomalous diffusion, yet represent different processes from a statistical perspective. Namely, a stretch Gaussian process for the fractal model, and a Levy process for the fractional model. An important difference defined in terms of practical simulation, was that the fractal model is a local operator and can be solved with local approximation techniques more efficiently than the fractional model.

More recently, a few authors have combined the fractional and fractal derivative in a model or description (Feng, 2000; Jiang et al., 2010; Chen et al., 2012; Wang et al., 2015; Fan et al., 2016; Atangana, 2017; Yadav and Agarwal, 2019). Fan et al. (2016) develop a fractional-fractal diffusion model based on work done by Jiang et al. (2010), using Riemann-Liouville and Caputo fractional derivatives. The fractional-fractal model is applied to the diffusion process of methane gas in coal beds, and was found to capture anomalous diffusion in porous media. Additionally, a Bayesian method was applied to determine the fractional order and fractal dimension automatically, which did correspond with experimental data. Atangana (2017) developed new fractal-fractional differential and integral operators, and concludes with the new operators will provide tools for future investigations. Furthermore, superdiffusion and subdiffusion in heterogeneous aquifers were suggested as a specific application. A space-time fractional-fractal Boussinesq equation was developed Yadav and Agarwal (2019) to improve the simulation of groundwater flow in unconfined systems, where a Caputo fractional derivative was applied in time and the fractal derivative developed in this thesis applied to space.

The application of a fractional-fractal advection-dispersion equation for transport in fractured aquifers is thus validated considering the application of the fractional-fractal diffusion models applied to anomalous gas diffusion and unconfined groundwater flow.

## 7.1 Fractional-fractal advection-dispersion equation

The fractional-fractal advection-dispersion equation is developed by applying the Caputo fractional derivative in time, and the fractal derivative as described in Section 3.2.1 in space for both the advection and dispersion terms. There are two non-local parameters, namely the fractional order ($\alpha$) and the fractal dimension, now denoted as $\beta$. The fractional-fractal equation can thus be defined as:

$$ {}_0^C D_t^{\alpha}\left(c(x,t)\right) = V_F^{\beta}(x)\frac{\partial}{\partial x}c(x,t) + D_F^{\beta}(x)\frac{\partial^2}{\partial x^2}c(x,t) \tag{7-1} $$

Where,

${}_0^C D_t^{\alpha}$ denotes the Caputo fractional derivative

$V_F^{\beta}$ denotes the fractal velocity in the x-direction

$D_F^{\beta}$ denotes the fractal dispersivity in the x-direction

## 7.2 Numerical approximation

The typical numerical approximation is applied to the Caputo fractional derivative in time, as described in Section 5.1. A finite difference method is applied to approximate the advective term (central difference) and the dispersion term (standard second-order difference), resulting in:

$$\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{k=0}^{n-1}\left(c_m^{k+1}-c_m^{k}\right)\delta_{n,k}^{\alpha}\right]=V_F^{\beta}\left(\frac{c_{m+1}^{n-1}-c_{m-1}^{n-1}}{2\Delta x}\right)+\ D_F^{\beta}\left(\frac{c_{m+1}^{n-1}-2c_m^{n-1}+c_{m-1}^{n-1}}{(\Delta x)^2}\right) \tag{7-2}$$

where,

$$\delta_{n,k}^{\alpha}=(n-k)^{1-\alpha}-(n-k-1)^{1-\alpha}$$

$$V_F^{\beta}=-v\left(\frac{x^{1-\alpha}}{\alpha}\right)+D_L\left(\frac{(1-\alpha)}{\alpha}\right)x^{1-2\alpha}$$

$$D_F^{\beta}=D_L\left(\frac{x^{2-2\alpha}}{\alpha^2}\right)$$

An algorithm is developed in *Maple* to solve the fractional-fractal equation using the numerical approximation scheme as described. The first step where $n=1$ is defined as:

$$c[m,1]=\frac{\Gamma(2-\alpha)}{(\Delta t)^{-\alpha}}\left(\begin{array}{c}V_F^{\beta}\left(\dfrac{c[m+1,0]-c[m-1,0]}{2\Delta x}\right)\\+D_F^{\beta}\left(\dfrac{c[m+1,0]-2c[m,0]+c[m-1,0]}{(\Delta x)^2}\right)\end{array}\right)+c[m,0] \tag{7-3}$$

And, the recursive step where $k\ =\ n-1$ is defined as:

$$\begin{aligned}c[m,n]=\frac{1}{(n-1)^{1-\alpha}}&\left[\frac{\Gamma(2-\alpha)}{(\Delta t)^{-\alpha}}\left(\begin{array}{c}V_F^{\beta}\left(\dfrac{c[m+1,n-1]-c[m-1,n-1]}{2\Delta x}\right)\\+D_F^{\beta}\left(\dfrac{c[m+1,n-1]-2c[m,0]+c[m-1,0]}{(\Delta x)^2}\right)\end{array}\right)\right.\\&\left.-\sum_{k=0}^{n-1}(c[m,k+1]-c[m,k])(n-k)^{1-\alpha}-(n-k-1)^{1-\alpha}\right]+c[m,n-1]\end{aligned} \tag{7-4}$$

## 7.3 Relationship between fractional and fractal dimensions

A fractional in time and fractal in space formulation of the advection-dispersion equation has two parameters to consider, namely the fractional order ($\alpha$) and the fractal dimension ($\beta$). An investigation of the fractal velocity/dispersivity was conducted in Section 3.6, and found an exponential increase in the fractal velocity and dispersivity as the fractal dimension decreases. From this initial evaluation, it was suggested to use fractal dimensions below 0.5 with caution as the increase becomes ultra-advection. A similar trend in the fractal dimension influence on the fractional-fractal velocity/dispersivity is expected, but the additional influence of the fractional order requires exploration. To achieve this, variable fractal dimensions are plot for a series of fractional orders, i.e. $\alpha, \beta: \{0.9, 0.7, 0.5, 0.3, 0.1\}$. To facilitate this analysis, a fractional-fractal velocity/dispersivity ($V_{FF}^{\alpha};\ D_{FF}^{\alpha}$) is represented by applying the numerical approximation in Equation (7-4),

$$\frac{\Gamma(2-\alpha)}{(\Delta t)^{-\alpha}}\left(\left(-v\left(\frac{x^{(1-\beta)}}{\beta}\right)+D_L\left(\frac{1-\beta}{\beta}\right)x^{(1-2\beta)}\right)+D_L\left(\frac{x^{(2-2\beta)}}{\beta^2}\right)\right) \tag{7-5}$$

where,

$\Delta t$ is the time step size
$\alpha$ is the fractional order
$\beta$ is the fractal dimension
$v$ is the groundwater velocity
$D_L$ is the longitudinal hydrodynamic dispersivity

For the analysis, a constant groundwater velocity ($v$) is defined at 0.05 m/d, dispersivity ($D_L$) of 0.3 m$^2$/d, and a fractional time step ($\Delta t$) of 0.01 d. The first plot of $\alpha = 1;\ \beta = 1$, forms the comparison base because this represents the traditional advection-dispersion model with no fractional order or fractal dimension (Figure 7-1). Initially the fractional-fractal velocity over space for a fractional order $\alpha = 1$ (simplifying back to the local equation) and varying fractal dimensions ($0.1 \leq \beta \leq 1$) is plot on a variable scale. These plots only assess the influence of the fractal derivative in space as the fractional order simplifies to the classical advection-dispersion equation in time, and as expected the influence of the fractal dimension follows the same trend as in Section 3.6 for the fractal advection-dispersion equation. However, the exponential increase is subdued due to the small fractional time step and discretisation (Figure 3-6 and Figure 7-1). In the subsequent plots (Figure 7-2 to Figure 7-6), the variable fractal dimension is evaluated at a series of fractional orders, $\alpha = 0.9, 0.7, 0.5, 0.3, 0.1$. Again, varying the fractal dimension produces the same trend at each fractional order, but a growth factor (on average 3) is found between each decrement of the fractional order. Thus, the fractional-fractal velocity/dispersivity increases not only exponentially with a decrease in the fractal order, but also with a decrease in the fractional order.

The established relationship between the fractional order and fractal dimension with the fractional-fractal velocity/dispersivity highlights the importance of selecting appropriate combinations. Considering the suggestion of using fractal dimensions of greater than 0.5 in Section 3.6, the range of appropriate fractional orders and fractal dimensions for the combined fractional-fractal model should be stricter due to the cumulative increase in velocity/dispersion. Thus, a recommendation of fractional order above 0.5, and a fractal dimension above 0.7 would be suggested for practical applications.

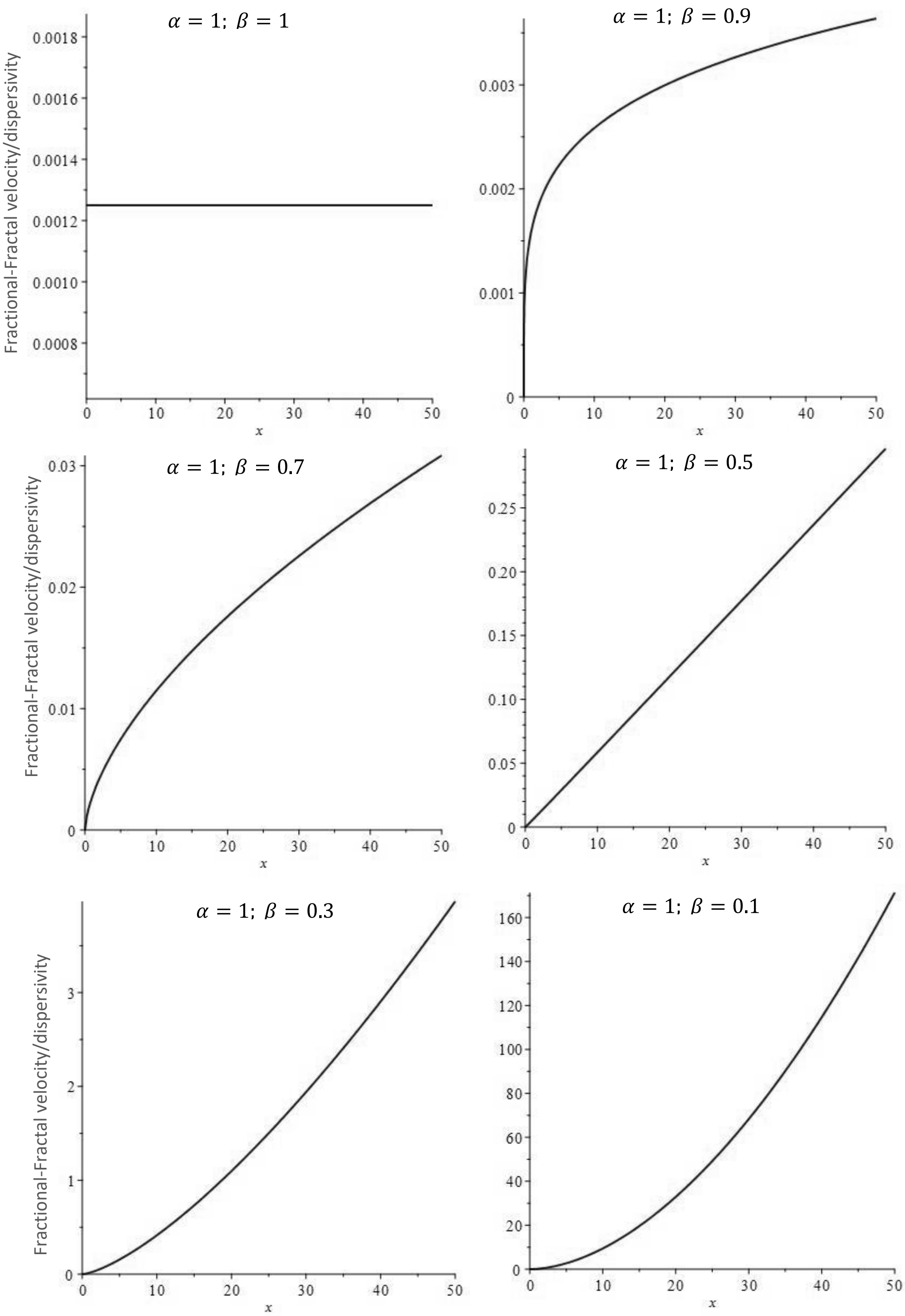


**Figure 7-1 Fractional-fractal velocity over space for a fractional order $\alpha = 1$ (simplifying back to the local equation in time) and varying fractal dimensions ($0.1 \leq \beta \leq 1$) on a variable plot scale. These plots solely evaluate the influence of the fractal derivative in space, and thus form a base of comparison, and the plot of $\alpha = 1$ ; $\beta = 1$ represents the traditional-local model in both time and space.**

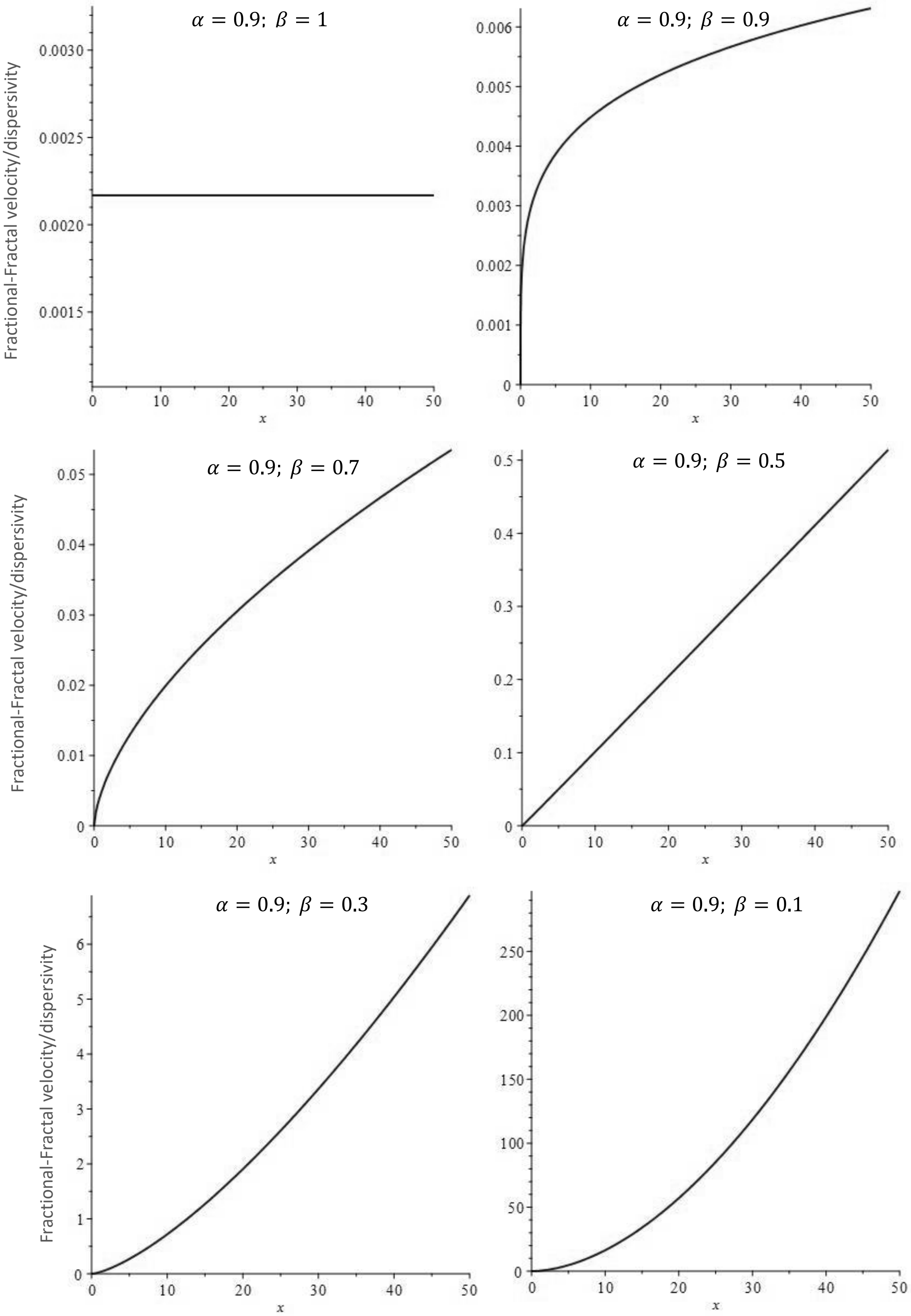


**Figure 7-2 Fractional-fractal velocity over space for a fractional order $\alpha = 0.9$ and varying fractal dimensions ($0.1 \le \beta \le 1$) on a variable plot scale.**

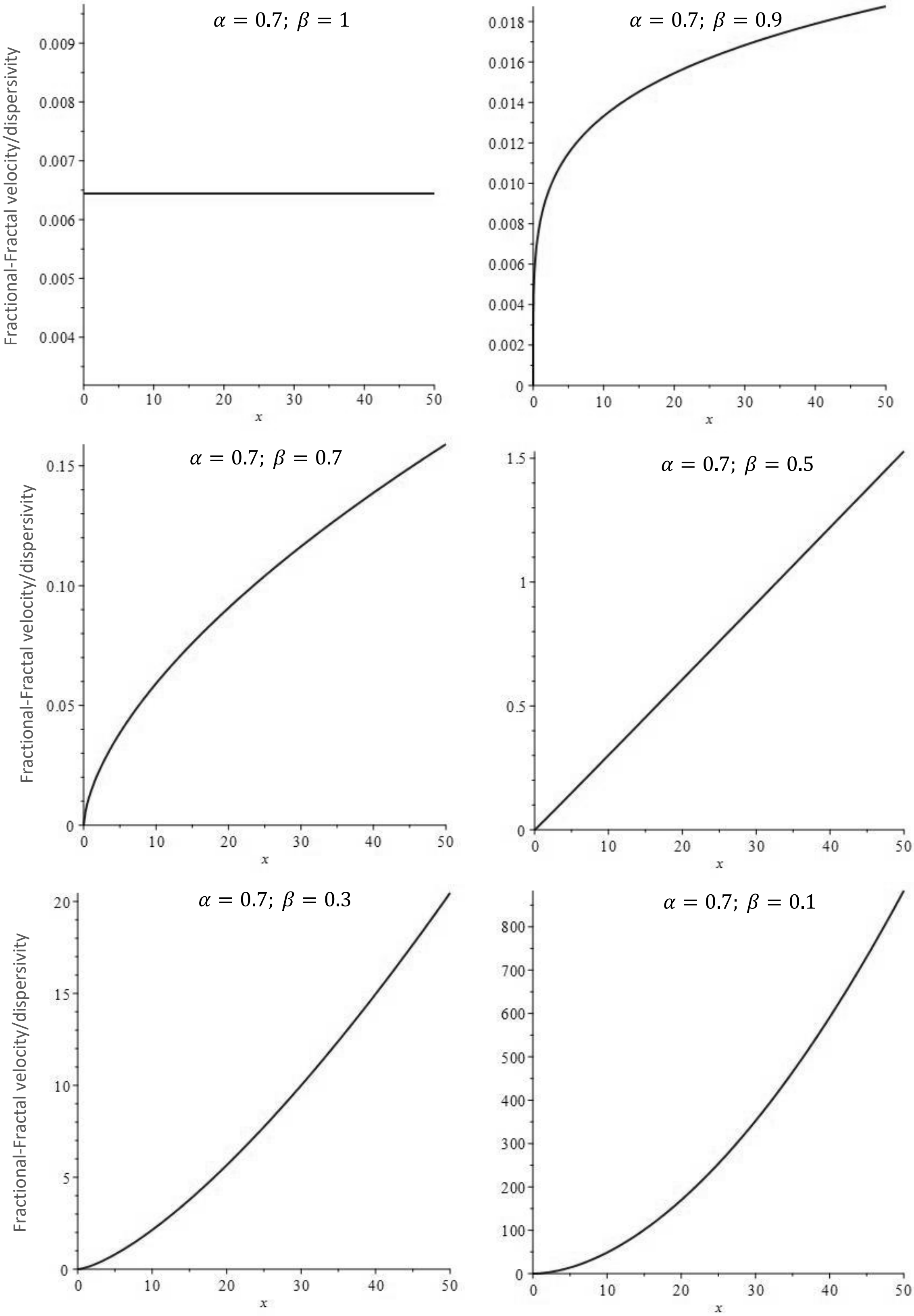


**Figure 7-3 Fractional-fractal velocity over space for a fractional order $\alpha = 0.7$ and varying fractal dimensions ($0.1 \leq \beta \leq 1$) on a variable plot scale.**

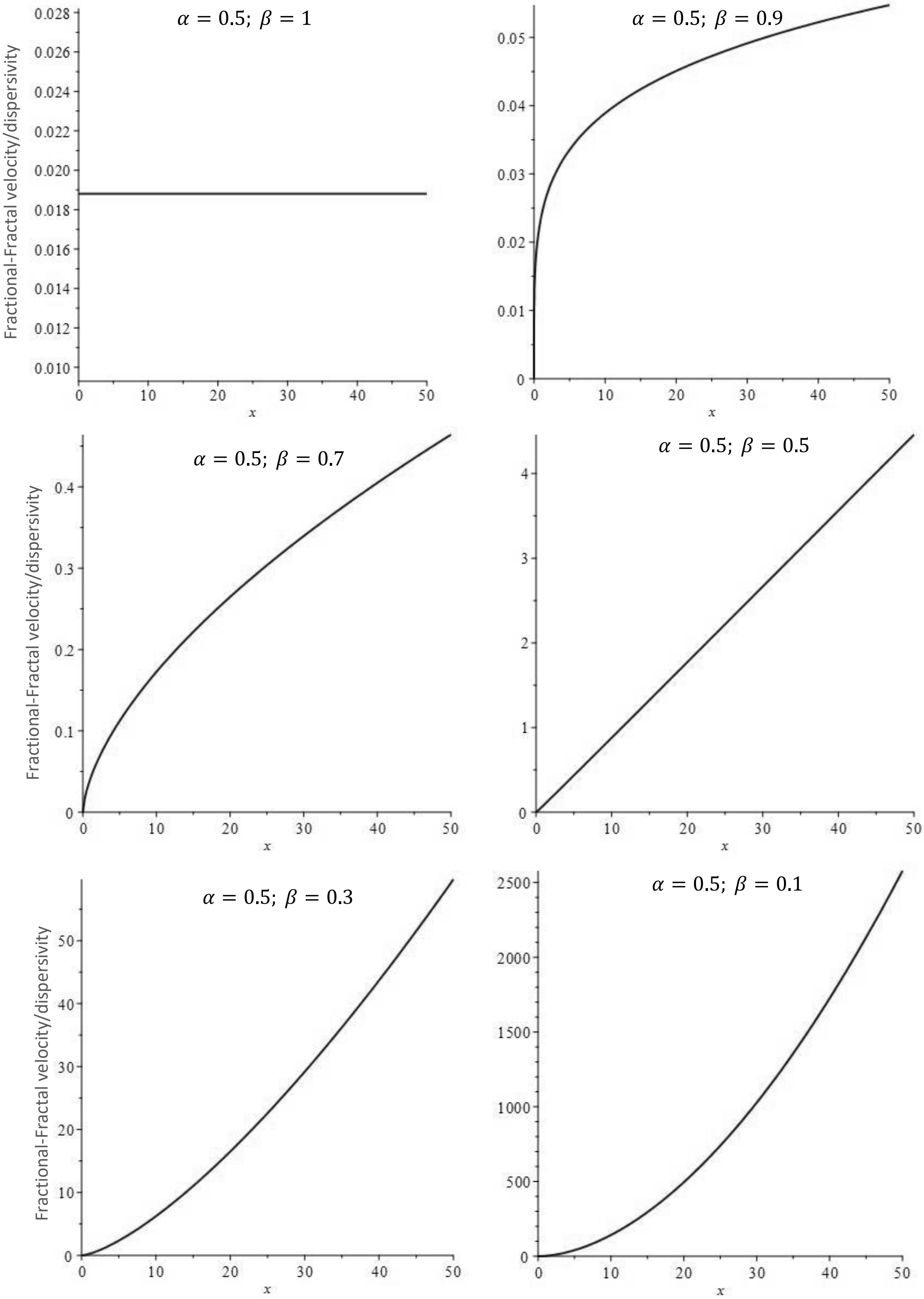


**Figure 7-4 Fractional-fractal velocity over space for a fractional order $\alpha = 0.5$ and varying fractal dimensions ($0.1 \leq \beta \leq 1$) on a variable plot scale.**

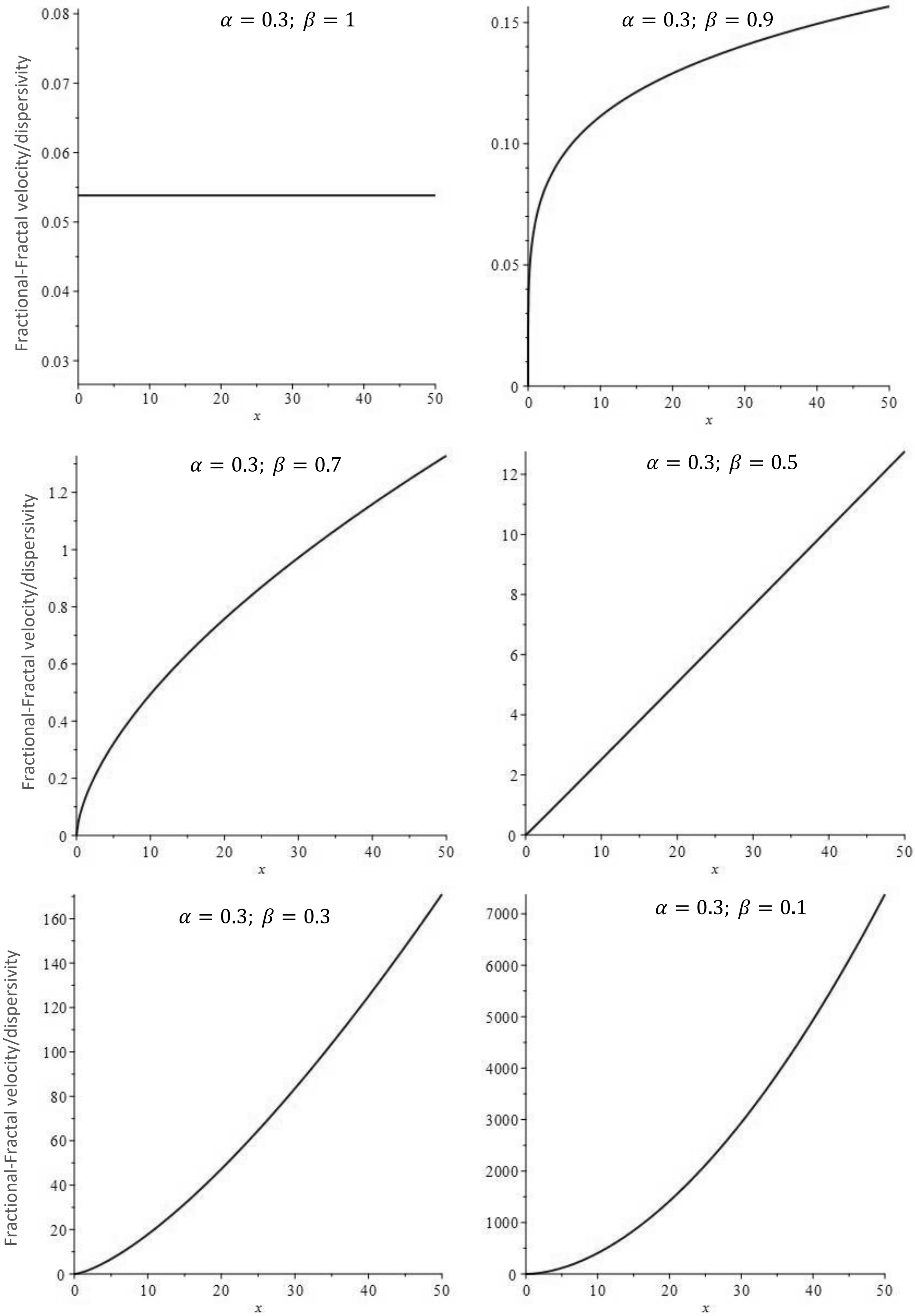


**Figure 7-5 Fractional-fractal velocity over space for a fractional order $\alpha = 0.3$ and varying fractal dimensions ($0.1 \leq \beta \leq 1$) on a variable plot scale.**

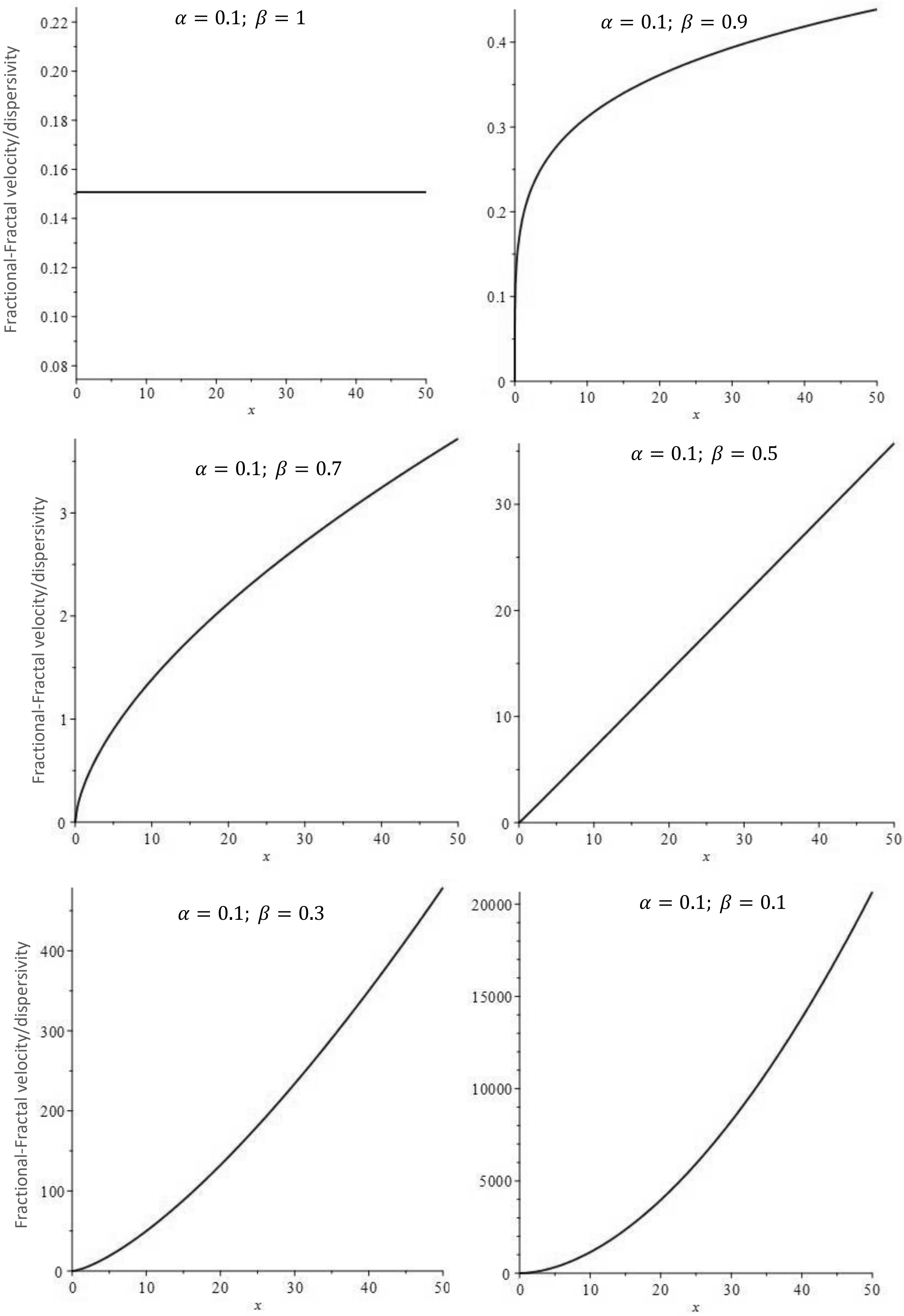


**Figure 7-6 Fractional-fractal velocity over space for a fractional order $\alpha = 0.1$ and varying fractal dimensions ($0.1 \leq \beta \leq 1$) on a variable plot scale.**

## 7.4 Simulation

To test the recommendations made for the fractional order and fractal dimension, a fractional-fractal model is simulated for a simple transport problem in the software programme *Maple* (Appendix B). The simple one-dimensional transport problem used in Section 3.5 is applied again, and simulated in the software programme *Maple* (Figure 2-1). The parameters include a constant velocity within the aquifer at 0.5 m/d, longitudinal hydrodynamic dispersivity is 0.3 $m^2/d$, and the initial contaminant concentration ($C_0$) is 10 mg/l. The initial condition and boundary conditions for the defined problem are

$$\left.\begin{array}{ll} c(x,0) = C_0 & x \geq 0 \\ c(0,t) = C_0 \cdot \exp(\lambda t) & t \geq 0 \\ c(L,t) = 0 & t \geq 0 \end{array}\right.$$

The presence of two fractional-fractal parameters ($\alpha$ and $\beta$) increases the number of combinations which are possible as seen in Section 7.3. The fractional-fractal velocity/dispersivity is highly sensitive to these parameters and a simulation of the potential combinations is simulated to investigate this relationship. The fractional-fractal model is applied to the simple transport model for fractional orders, $\alpha = 0.9, 0.8, 0.7, 0.6, 0.5$ and for each, the fractal dimension is varied from 0.9 to where the simulation becomes unstable or unrealistic. Graphical illustrations of the simulations are presented in Figure 7-7 to Figure 7-11, and the suitable $\alpha, \beta$ combinations tabulated in Table 7-1. When the fractional order and fractal dimension are 1, the solution represents the classical advection-dispersion model, where the movement of contaminants form a symmetrical breakthrough curve along the x-direction (Figure 7-7). When the fractional order is at $\alpha = 1$, and the derivative in time becomes an integer-order, the fractal dimension is appropriate from $0.5 \leq \beta \leq 0.9$, after which the solution becomes unstable. Varying the fractal dimension changes the shape of the breakthrough curve, changing from a Gaussian distribution, to a skewed distribution with a progressively heavier tail. In Figure 7-8, the fractional order is $\alpha = 0.9$, and the fractal dimension is appropriate from $0.5 \leq \beta \leq 0.9$. The same trend is seen as the fractal dimension is decreased, yet the peak concentration in the breakthrough curve is more pronounced. It appears that the additional influence of a fractional order in time on a fractal dimension in space advection-dispersion model is a control on the breakthrough curve peak, while the fractal dimension controls the degree of tailing of the curve. These two controls could provide the tools to better represent measured anomalous breakthrough curves that cannot be fit to the classical model. The same trend is seen in Figure 7-9 for fractional order $\alpha = 0.8$, and in Figure 7-10 for fractional order $\alpha = 0.7$.

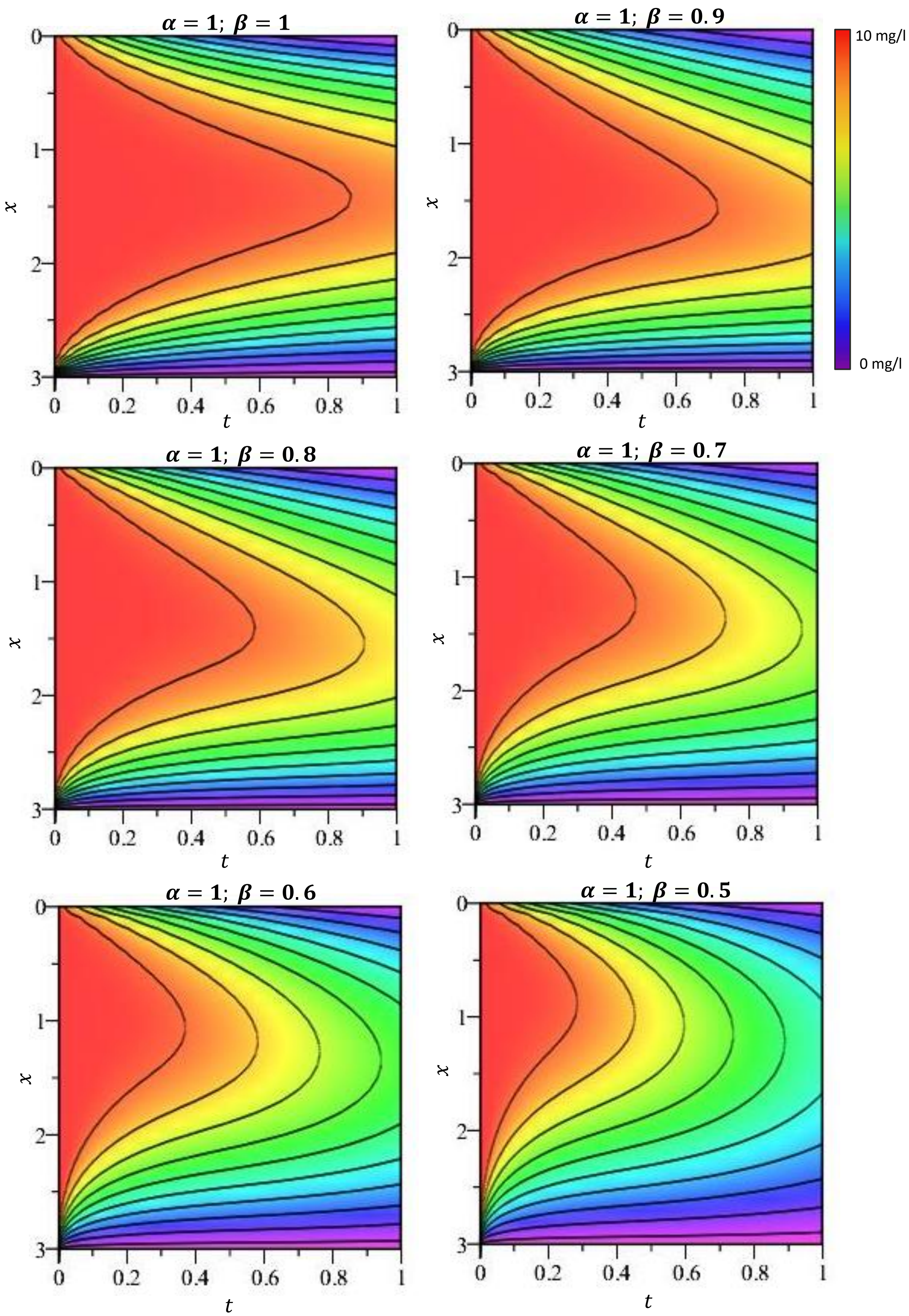


**Figure 7-7 Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order $\alpha = 1$ (simplifies to a local order), and varying fractal dimensions ($0.5 \leq \beta \leq 1$)**

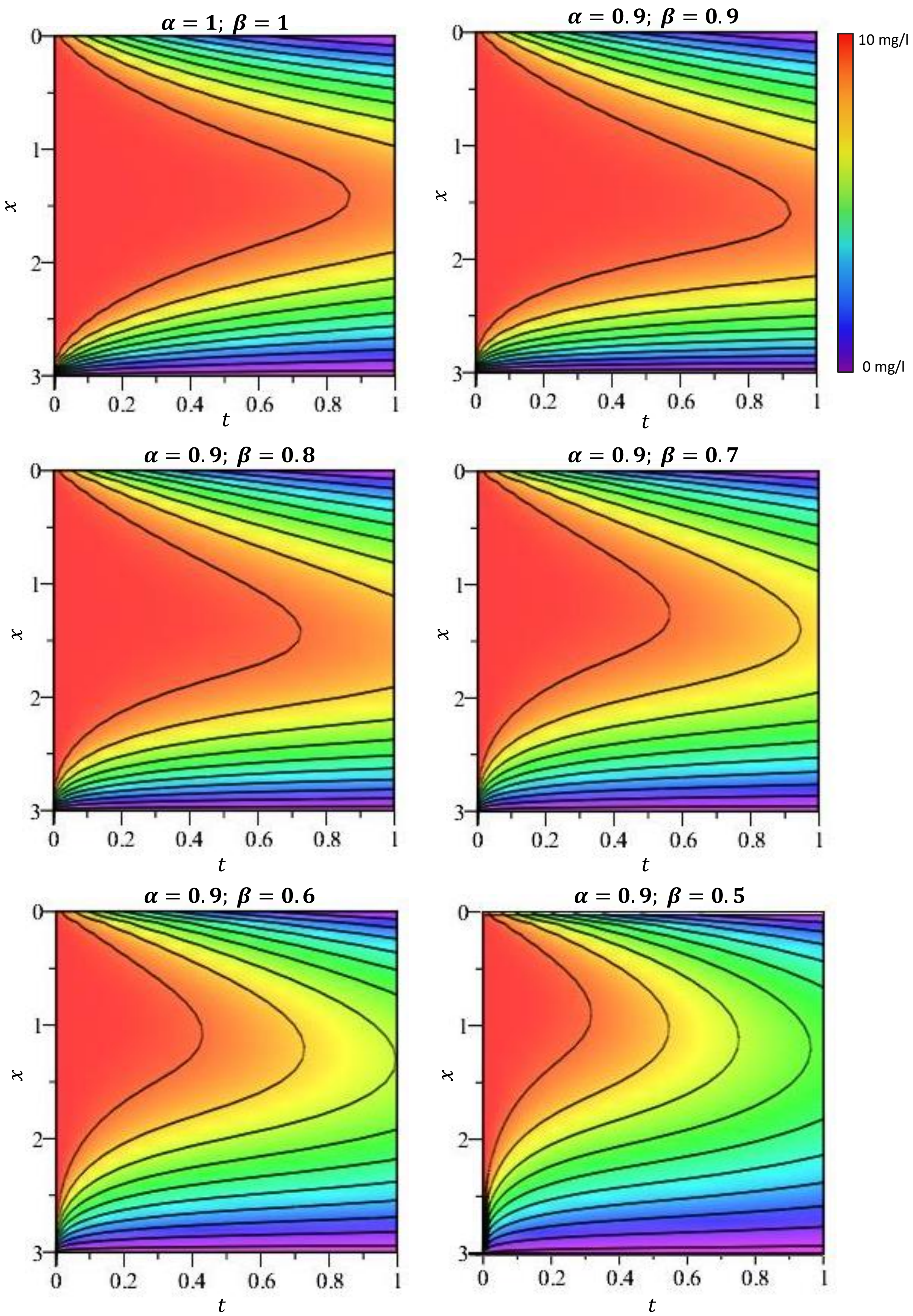


**Figure 7-8 Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order $\alpha = 0.9$, and varying fractal dimensions ($0.5 \leq \beta \leq 1$)**

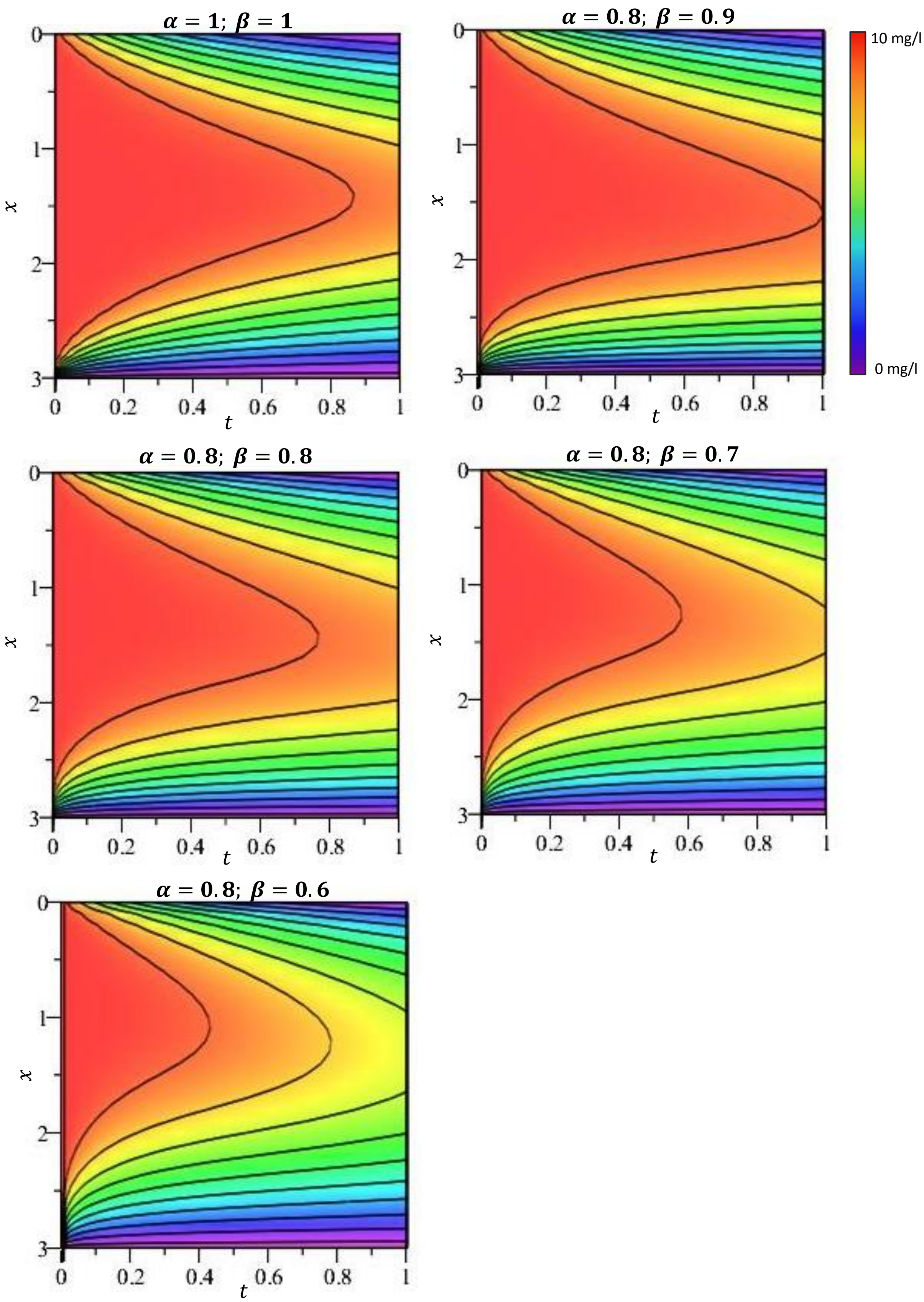


**Figure 7-9 Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order $\alpha = 0.8$, and varying fractal dimensions ($0.6 \leq \beta \leq 1$)**

However, the range of appropriate fractal dimensions decreases systematically. For simulations $\alpha = 0.9, \beta = 0.5$; $\alpha = 0.8, \beta = 0.6$; and $\alpha = 0.7, \beta = 0.7$ the influence of the exponential distribution of the fractional-fractal velocity/dispersivity becomes evident, where near the end of the x-directional line the velocity and dispersivity increase exponentially and the concentrations are preferentially peaked at this location at the beginning of the simulator time. This eventually causes instabilities as this rapid movement along the line becomes unrealistic. The result of this are clearly seen in simulations $\alpha = 0.6, \beta = 0.8$ and $\alpha = 0.5, \beta = 0.9$ where all the contaminants accumulate at the end of the x-direction line at the beginning of the simulation time (Figure 7-11).

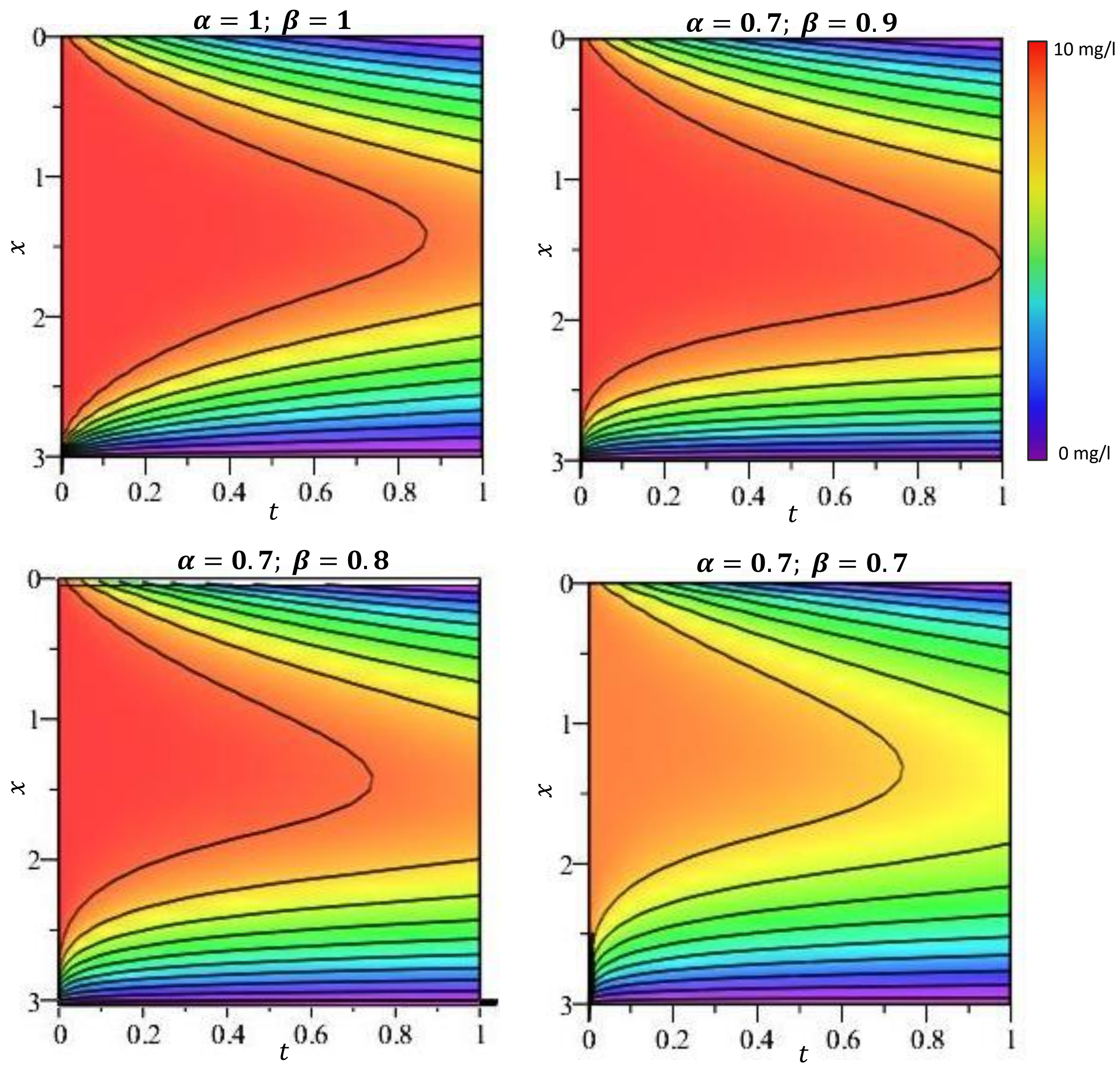


**Figure 7-10 Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order $\alpha = 0.7$, and varying fractal dimensions ($0.7 \leq \beta \leq 1$)**

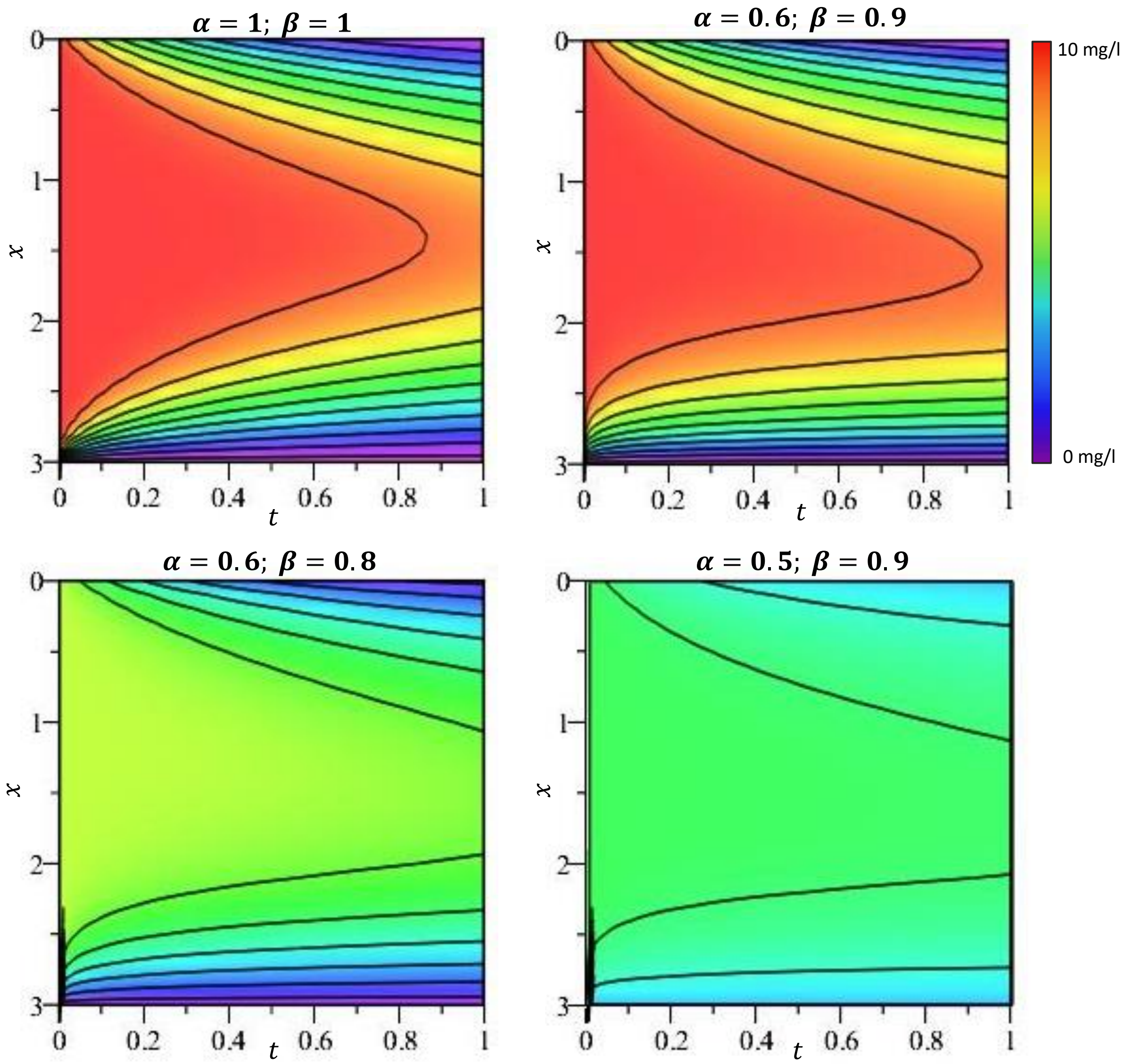


**Figure 7-11 Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order $\alpha = 0.6, 0.5$, and varying fractal dimensions ($0.8 \leq \beta \leq 1$)**

**Table 7-1 Tabulation of the fractional order (α) and fractal dimension (β) valid combination options for the fractional-fractal advection-dispersion equation. Valid combinations (x), Non-valid combinations (grey), recommended combinations (green).**

| | **$\beta$ = 1** | **$\beta$ = 0.9** | **$\beta$ = 0.8** | **$\beta$ = 0.7** | **$\beta$ = 0.6** | **$\beta$ = 0.5** | **$\beta$ = 0.4** |
|---|---|---|---|---|---|---|---|
| **α = 1** | x | x | x | x | x | x | |
| **α = 0.9** | x | x | x | x | x | x | |
| **α = 0.8** | x | x | x | x | x | | |
| **α = 0.7** | x | x | x | x | | | |
| **α = 0.6** | x | x | x | | | | |
| **α = 0.5** | x | x | | | | | |
| **α = 0.4** | | | | | | | |

Thus, the recommendations made based on the relationship of the fractional-fractal parameters to the fractional-fractal velocity/dispersivity are validated, where fractional order above 0.5, and a fractal dimension above 0.7 would be suggested for practical applications. Yet, this recommendation is refined based on the simulations to a fractional order and fractal dimension of $0.7 \leq \alpha, \beta \leq 1$.

## 7.5 Chapter summary

A fractional-fractal advection-dispersion model is developed from the fractional and fractal advection-dispersion equations already considered, producing an efficient tool to model anomalous diffusion with the same non-local advantages. However, the fractional-fractal model has two parameters to consider, the fractional order ($\alpha$) and the fractal dimension ($\beta$), and this increases the number of combinations available for simulation. An investigation on the influence of the fractional-fractal parameters on the fractional-fractal velocity/dispersivity found the fractional-fractal velocity/dispersivity increases not only exponentially with a decrease in the fractal order, but also with a decrease in the fractional order. A recommendation to use a fractional order above 0.5, and a fractal dimension above 0.7 was made based on the evaluation. The established relationship highlighted the importance of selecting appropriate combinations, and validated simulating the combinations for a simple transport problem. From the simulations, it is found that the fractional order controls the breakthrough curve peak, and the fractal dimension controls the position of the peak and tailing effect. These two controls potentially provide the tools to better represent measured anomalous breakthrough curves that cannot be fit to the classical model. The range of valid combinations decrease with decreasing fractional order and fractal dimension, and a final recommendation is made for a fractional order and fractal dimension of $0.7 \leq \alpha, \beta \leq 1$.

# 8 DISCUSSION

The endeavour to improve the representation of natural systems, to increase comprehension and management of those systems will be continued perpetually beyond this research because the complexity of natural phenomena is endless with many more facets to explore. Yet, each step made in progress improves the collective understanding and furthers the cause. Research conducted in this thesis is but a small step forward, but a step forward now the less. The numerical schemes and reformulated advection-dispersion equations will improve how groundwater transport, and potentially other systems, are simulated. Yet, it is important to understand the assumptions and limitations associated with these improvements.

The numerical schemes developed to improve the classical advection-dispersion model are evaluated for numerical stability and application to a simple transport problem of limited extent and time. While this is appropriate from a research perspective, it should be noted that a full-scale application with measured observations has not been tested. For further applications, the augmented upwind numerical schemes should be extended to three-dimensions and tested on a large-scale testing facility for contaminant transport.

The fractal advection-dispersion equation developed has the ability to model superdiffusion for fractal dimension less than 1, as well as subdiffusion for fractal dimensions greater than 1, without explicitly defining fractures or preferential pathways. The fractal advection-dispersion model is simulated on a slightly larger scale of 200 m and 200 days due to local numerical methods being used. Yet, this is still limited and has not been applied with measured anomalous transport data. Similarly, for further applications, the fractal advection-dispersion model should be extended to three-dimensions and tested on a large-scale testing facility for contaminant transport.

Fractional advection-dispersion equations are developed for fractured groundwater systems using the Caputo and Atangana-Baleanu fractional derivatives. The improvement from previous fractional advection-dispersion equations is the incorporation of the fractional derivative in time and space with the advection term in space as opposed to the typical application to the diffusion/dispersion term. The upwind schemes developed for the classical advection-dispersion equation are tested for the fractional advection-dispersion models in terms of numerical stability. Proving the numerical stability is important, but the simulation of these equations to a practical problem is restricted due to computational limitations, where a memory component in both space and time requires greater computational effort. For future analysis, the numerical schemes should be simulated for a transport problem to provide a complete evaluation. This particular limitation motivated the development of the fractional-fractal advection-dispersion model because the fractional in time and fractal in space provides similar advantages with less computational effort.

The fractional-fractal advection-dispersion equation facilitates simulation on a simple transport problem to evaluate the combinations of the fractional order and fractal dimension. However, the computational effort is larger than that of the classical approach and the extent and time of the transport problem is limited, and only in one physical dimension ($x$). The fractional-fractal is the most appropriate tool in terms of generally available computing power and in future research should be applied in three-dimensions to a field-scale transport modelling application.

In general, a wide spread use of non-local approaches to solve practical problems remains hindered by the lack of a physical definition and the computational power required to simulate the intrinsic memory of fractional derivatives and integrals at large-scales. When our understand of fractional calculus becomes sufficiently tangible and computer processors advance, the use of fractional derivatives will change the way we model our world. Until then, small advancing steps, such as the research done here, will strive forward until this objective is reached.

# 9 CONCLUSIONS

The complexity of real world systems inspire scientists to continually advance the methods used to represent these systems as understanding and technology advance. This fundamental principle is applied to groundwater transport, a real world problem where the current understanding often cannot describe what is observed. To improve the simulation of groundwater transport there are two approaches, 1) improve the physical characterisation of the heterogeneous system, or 2) improve the formulation of the governing equations used to simulate the system. The latter approach is followed by investigating numerical approximation schemes for the classical advection-dispersion equation, incorporating fractal and fractional derivatives into the formulation, and combining fractional and fractal derivatives.

## 9.1 Local advection-dispersion equation

The solution of the classical advection-dispersion equation for fractured groundwater systems is improved by developing augmented upwind finite difference numerical approximation schemes, which are better suited for advection-dominated systems. A numerical scheme combining the traditional upwind and Crank-Nicolson schemes is developed, along with a novel advection upwind Crank-Nicolson combination, and weighted upwind-downwind schemes. A stability analysis on the developed numerical schemes found the implicit formulations to be more stable and practically viable, and the new advection upwind Crank-Nicolson and weighted upwind-downwind schemes are improvements from the traditional approaches. In conclusion, the augmented upwind schemes improve the simulation of the local advection-dispersion equation for fractured systems.

## 9.2 Fractal advection-dispersion equation

The simulation of anomalous transport in fractured aquifer systems is improved by providing a fractal advection-dispersion equation with numerical integration and approximation methods for solution. The fractal advection-dispersion model is applied to a simple transport problem; illustrating that the fractal formulation of the advection-dispersion equation can model superdiffusion for fractal dimension less than 1, and subdiffusion for fractal dimensions greater than 1, without explicitly defining fractures or preferential pathways. In this way, anomalous transport in fractured systems can be modelled without explicit locations and details of the fractures, especially where limited information is available on the preferential pathway causing the discrepancy. The relationship between the fractal velocity and dispersivity with the fractal dimension indicated that fractal dimensions $\alpha \geq 0.5$ are the most appropriate for practical use, due to the exponential increase in velocity and dispersivity for fractal dimensions $0.1 \leq \alpha \leq 0.5$.

## 9.3 Fractional advection-dispersion equation

To improve the governing equation for groundwater transport modelling, the Caputo and Atangana-Baleanu in Caputo sense (ABC) fractional derivatives are applied to the advection-dispersion equation with a focus on the advection term to account for *anomalous advection*. The new advection-dispersion equation with ABC fractional derivative is proven to be bound, exist, unique and stable in time. The augmented upwind numerical schemes developed are applied to numerically approximate the solutions. A recursive method stability analysis, for the advection-dispersion model with Caputo fractional derivative, indicated the implicit weighted scheme to be an improvement on the traditional implicit upwind scheme, where the inclusion of the weighting factor (θ) provides a means to improve the likelihood of upholding the stability condition. Thus, the upwind advection Crank-Nicolson and implicit weighted upwind-downwind schemes are applicable for solution of the space-time fractional advection-dispersion equation (Caputo), when the stability criterion are upheld. The upwind Crank-Nicolson scheme is recommended for use with the fractional advection-dispersion equation (ABC), as it was the most stable according to the recursive method stability analysis.

## 9.4 Fractional-fractal advection-dispersion equation

The fractional-fractal advection-dispersion equation is developed to provide an efficient non-local, in both space and time, modelling tool. The fractional-fractal model has two parameters, fractional order

($\alpha$) and fractal dimension ($\beta$), where simulations are valid for specific combinations. The range of valid combinations decrease with decreasing fractional order and fractal dimension, and a final recommendation is a fractional order and fractal dimension of $0.7 \leq \alpha, \beta \leq 1$. The fractional-fractal model provides a flexible tool to model anomalous diffusion, where the fractional order controls the breakthrough curve peak, and the fractal dimension controls the position of the peak and tailing effect. These two controls potentially provide the tools to improve the representation of anomalous breakthrough curves that cannot be described by the classical model.

In conclusion, the main aim of the research has been achieved by providing:

- ✓ Improved numerical approximation schemes for the classical advection-dispersion model for fractured groundwater systems
- ✓ Fractal advection-dispersion equation proven to simulate superdiffusion and subdiffusion by varying the fractal dimension, without explicit characterisation of fractures or preferential pathways
- ✓ Fractional advection-dispersion equations for advection-dominated systems with the Caputo and Atangana-Baleanu fractional derivatives, and appropriate numerical approximation methods
- ✓ Fractional-fractal advection-dispersion equation, which forms an efficient non-local modelling tool for practical applications, and provides a flexible, two-parameter system for representing anomalous diffusion in fractured groundwater systems without explicit characterisation of fractures or preferential pathways

A modest step forward made, in the bigger scheme of progress, toward the collective mission of resolving the difference between modelled and observed to increase the comprehension and management of natural systems.

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# APPENDIX A – SCILAB CODES

**First-order upwind explicit scheme**

```
timer()
dx=2*10^(-1);dt=4*10^(-2);T=10;Vx=0.5;DL=0.3;lambda=0.5;
a=1-((dt*Vx)/dx)-((2*dt*DL)/(dx^2));
b=((dt*Vx)/dx)+(dt*DL)/(dx^2);
c=(dt*DL)/(dx^2);
L=30;N=L/dx;C0=10;

B=a*diag(ones(N-1,1))+b*diag(ones(N-2,1),-1)+c*diag(ones(N-2,1),1);
Vect=zeros(N-1,1);
for i=1:N-1
   U(i)=0;
end
k=T/dt;
for m=1:k
  Vect(1)=b*C0;
   U=B*(U+Vect);
end
V(1)=C0;
V(N+1)=0;
for j=2:N
   V(j)=U(j-1);
end
timer();

X=0:dx:L;
plot2d(X,V,9)
//tt=linspace(0,1,100);
//uex=sin(%pi*tt)*exp(-1);
//plot2d(tt,uex)
//wex=sin(%pi*X)*exp(-1);
//err=norm(wex'-V,'inf')
```

**First-order upwind implicit scheme**

```
timer()
dx=2*10^(-1);dt=4*10^(-2);T=10;Vx=0.5;DL=0.3;lambda=0.5;
a=1+((dt*Vx)/dx)+((2*dt*DL)/(dx^2));
b=-((dt*Vx)/dx)-((dt*DL)/(dx^2));
c=-((dt*DL)/(dx^2));
L=30;N=L/dx;C0=10;

B=a*diag(ones(N-1,1))+b*diag(ones(N-2,1),-1)+c*diag(ones(N-2,1),1);
Vect=zeros(N-1,1);
for i=1:N-1
   U(i)=0;
end
k=T/dt;
for m=1:k
```

```
  Vect(1)=-b*C0;
   U=inv(B)*(U+Vect);
end
V(1)=C0;
V(N+1)=0;
for j=2:N
   V(j)=U(j-1);
end
timer();

X=0:dx:L;
plot2d(X,V,3)
//tt=linspace(0,1,100);
//uex=sin(%pi*tt)*exp(-1);
//plot2d(tt,uex)
//wex=sin(%pi*X)*exp(-1);
//err=norm(wex'-V,'inf')
```

**First-order upwind Crank-Nicolson scheme**

```
timer();
dx=2*10^(-1);dt=4*10^(-2);T=10;Vx=0.5;DL=0.3;lambda=0.5;
L=30;N=L/dx;C0=10;
a=1+(0.5*Vx*dt)/dx+(dt*DL)/(dx^2);
b=-((0.5*Vx*dt)/dx)-((0.5*dt*DL)/(dx^2));
c=-(0.5*dt*DL)/(dx^2);
d=1-(0.5*Vx*dt)/dx-((dt*DL)/(dx^2));
e=((0.5*Vx*dt)/dx)+((0.5*dt*DL)/(dx^2));
f=(0.5*dt*DL)/(dx^2);

B=a*diag(ones(N-1,1))+b*diag(ones(N-2,1),-1)+c*diag(ones(N-2,1),1);
A=d*diag(ones(N-1,1))+e*diag(ones(N-2,1),-1)+f*diag(ones(N-2,1),1);
Vect=zeros(N-1,1);
for i=1:N-1
   U(i)=0;
end
k=T/dt;
for m=1:k
  Vect(1)=(e-b)*C0;
  U=inv(B)*(A*(U+Vect));
end
V(1)=C0;
V(N+1)=0;
for j=2:N
   V(j)=U(j-1);
end
timer()

X=0:dx:L;
plot2d(X,V,2)
//tt=linspace(0,1,100);
//uex=sin(%pi*tt)*exp(-1);
//plot2d(tt,uex)
//wex=sin(%pi*X)*exp(-1);
//err=norm(wex'-V,'inf')
```

**First-order upwind advection Crank-Nicolson scheme (explicit)**

```
timer()
dx=2*10^(-1);dt=4*10^(-2);T=10;Vx=0.5;DL=0.3;lambda=0.5;
L=30;N=L/dx;C0=10;
a=1+(0.5*Vx*dt)/dx;
b=-(0.5*Vx*dt)/dx;
c=1-((0.5*Vx*dt)/dx)-((2*dt*DL)/(dx^2));
d=(dt*DL)/(dx^2);
f=(dt*DL)/(dx^2)+(0.5*Vx*dt)/dx;

B=a*diag(ones(N-1,1))+b*diag(ones(N-2,1),-1);
A=c*diag(ones(N-1,1))+f*diag(ones(N-2,1),-1)+d*diag(ones(N-2,1),1)
Vect=zeros(N-1,1);
for i=1:N-1
    U(i)=0;
end
k=T/dt;
for m=1:k
   Vect(1)=(f-b)*C0;
   U=inv(B)*(A*(U+Vect));
end
V(1)=C0;
V(N+1)=0;
for j=2:N
    V(j)=U(j-1);
end
timer();

X=0:dx:L;
plot2d(X,V,1)
//tt=linspace(0,1,100);
//uex=sin(%pi*tt)*exp(-1);
//plot2d(tt,uex)
//wex=sin(%pi*X)*exp(-1);
//err=norm(wex'-V,'inf')
```

**First-order upwind advection Crank-Nicolson scheme (implicit)**

```
timer();
dx=2*10^(-1);dt=4*10^(-2);T=10;Vx=0.5;DL=0.3;lambda=0.5;
L=30;N=L/dx;C0=10;

a=1+(0.5*Vx*dt)/dx+(2*dt*DL)/(dx^2);
b=-((0.5*Vx*dt)/dx)-((dt*DL)/(dx^2))
c=-(dt*DL)/(dx^2)
d=1-(0.5*Vx*dt)/dx
e=(0.5*Vx*dt)/dx

B=a*diag(ones(N-1,1))+b*diag(ones(N-2,1),-1)+c*diag(ones(N-2,1),1);
A=d*diag(ones(N-1,1))+e*diag(ones(N-2,1),-1)
Vect=zeros(N-1,1);
for i=1:N-1
    U(i)=0;
end
```

```
k=T/dt;
for m=1:k
   Vect(1)=(e-b)*C0;
   U=inv(B)*(A*(U+Vect));
end
V(1)=C0;
V(N+1)=0;
for j=2:N
    V(j)=U(j-1);
end
timer()

X=0:dx:L;
plot2d(X,V,1)
//tt=linspace(0,1,100);
//uex=sin(%pi*tt)*exp(-1);
//plot2d(tt,uex)
//wex=sin(%pi*X)*exp(-1);
//err=norm(wex'-V,'inf')
```

**First-order weighted upwind-downwind scheme (explicit)**

```
timer()
    dx=2*10^(-1);dt=4*10^(-2);T=10;Vx=0.5;DL=0.3;theta=0.9;lambda=0.5;
    a=1+(2*dt*DL)/(dx^2)+(theta*dt*Vx)/dx-((1-theta)*dt*Vx)/dx;
    b=-((theta*dt*Vx)/dx)-((dt*DL)/(dx^2));
    c=(((1-theta)*dt*Vx)/dx)-((dt*DL)/(dx^2));
    L=30;N=L/dx;C0=10;
    B=a*diag(ones(N-1,1))+b*diag(ones(N-2,1),-1)+c*diag(ones(N-2,1),1);
    Vect=zeros(N-1,1);
    for i=1:N-1
        U(i)=0;
    end
    k=T/dt;
    for m=1:k
       Vect(1)=-b*C0;
        U=inv(B)*(U+Vect);
    end
    V(1)=C0;
    V(N+1)=0;
    for j=2:N
        V(j)=U(j-1);
    end
    timer();

    X=0:dx:L;
    plot2d(X,V,13)
    //tt=linspace(0,1,100);
    //uex=sin(%pi*tt)*exp(-1);
    //plot2d(tt,uex)
    //wex=sin(%pi*X)*exp(-1);
    //err=norm(wex'-V,'inf')
```

**First-order weighted upwind-downwind scheme (implicit)**

```
timer();
dx=2*10^(-1);dt=4*10^(-2);T=10;Vx=0.5;DL=0.3;theta=0.5;lambda=0.5;
a=1-(theta*((dt*Vx)/dx))-(1-theta)*((dt*Vx)/dx)-((2*dt*DL)/(dx^2));
b=theta*((dt*Vx)/dx)+(dt*DL)/(dx^2);
c=-(1-theta)*((dt*Vx)/dx)+(dt*DL)/(dx^2);
L=30;N=L/dx;C0=10;

B=a*diag(ones(N-1,1))+b*diag(ones(N-2,1),-1)+c*diag(ones(N-2,1),1);
Vect=zeros(N-1,1);
for i=1:N-1
    U(i)=0;
end
k=T/dt;
for m=1:k
   Vect(1)=b*C0;
    U=B*(U+Vect);
end
V(1)=C0;
V(N+1)=0;
for j=2:N
    V(j)=U(j-1);
end
timer()

X=0:dx:L;
plot2d(X,V,2)
//tt=linspace(0,1,100);
//uex=sin(%pi*tt)*exp(-1);
//plot2d(tt,uex)
//wex=sin(%pi*X)*exp(-1);
//err=norm(wex'-V,'inf')
```

# APPENDIX B – MAPLE CODES

## Fractal advection-dispersion model

$with \cdot (PDEtools, solve)$

$$with\,(PDEtools, solve) \quad (1)$$

$\alpha := 1$

$$\alpha := 1 \quad (2)$$

$V := 0.05$

$$V := 0.05 \quad (3)$$

$DL := 0.3$

$$DL := 0.3 \quad (4)$$

$VF := -V \cdot \left(\frac{x^{(1-\alpha)}}{\alpha}\right) + DL \cdot \left(\frac{1-\alpha}{\alpha}\right) \cdot x^{(1-2\cdot\alpha)}$

$$VF := -0.05 \quad (5)$$

$DF := DL \cdot \left(\frac{x^{2-2\alpha}}{\alpha^2}\right)$

$$DF := 0.3 \quad (6)$$

$C0 := 10$

$$C0 := 10 \quad (7)$$

$eq := [diff(c(x,t),t) - VF \cdot diff(c(x,t),x) - DF \cdot diff(c(x,t),x,x) = 0, c(x,0) = C0, c(0,t) = C0 \cdot \exp(-3 \cdot t), D[1](c)(200,t) = 0]$

$$eq := \left[\frac{\partial}{\partial t} c(x,t) + 0.05 \frac{\partial}{\partial x} c(x,t) - 0.3 \frac{\partial^2}{\partial x^2} c(x,t) = 0, c(x,0) = 10, c(0,t) = 10\,e^{-3\,t}, D_1(c)(200,t) = 0\right] \quad (8)$$

$sol1 := PDEtools{:}\text{-}Solve(eq, numeric)$

$$sol1 := \textbf{module}(\,)\ \ldots\ \textbf{end module} \quad (9)$$

## Fractional-fractal advection-dispersion model

$\alpha := 1:$
$\beta := 1:$
$C0 := 10:$
$DL := 0.3:$
$V := 0.5:$
$\lambda := 3:$
$h := 0.1:$
$dt := 0.001:$

**for** $n$ **from** 0 **to** 1000**do**
$u[0,n] := C0 \cdot \exp(-\lambda \cdot n \cdot dt):$
**end do**
**for** $m$ **from** 0 **to** 30 **do**
$u[m,0] := C0:$
**end do**
**for** $m$ **from** 1 **to** 29 **do**

$$u[m,1] := \frac{\Gamma(2-\alpha)}{dt^{(-\alpha)}} \cdot \left(\left(-V \cdot \frac{(m \cdot h)^{(1-\beta)}}{\beta} + \frac{DL \cdot (1-\beta)}{\beta} \cdot (m \cdot h)^{(1-2\cdot\beta)}\right) \cdot \frac{u[m+1,0] - u[m-1,0]}{2 \cdot h} + \left(\frac{DL \cdot (m \cdot h)^{(2-2\cdot\beta)}}{\beta^2}\right) \cdot \frac{u[m+1,0] - 2 \cdot u[m,0] + u[m-1,0]}{h^2}\right) + u[m,0]:$$

**end do**

$u[30,1] := 0$

$$u_{30,1} := 0 \quad (1)$$

**for** $n$ **from** 2 **to** 1000 **do**
**for** $m$ **from** 1 **to** 29 **do**
$val := 0:$
**for** $l$ **from** 0 **to**$(n-2)$ **do**
$val := val + \left((u[m,l+1] - u[m,l]) \cdot \left((n-l)^{(1-\alpha)} - (n-l-1)^{(1-\alpha)}\right)\right):$
**end do**

$$u[m, n] := \frac{1}{(n-1)^{(1-\alpha)}} \cdot \left( \frac{\Gamma(2-\alpha)}{dt^{(-\alpha)}} \cdot \left( \left( -V \cdot \frac{(m \cdot h)^{(1-\beta)}}{\beta} + \frac{DL \cdot (1-\beta)}{\beta} \cdot (m \cdot h)^{1-2\cdot\beta} \right) \cdot \frac{u[m+1, n-1] - u[m-1, n-1]}{2 \cdot h} + \left( \frac{DL \cdot (m \cdot h)^{(2-2\cdot\beta)}}{\beta^2} \right) \cdot \frac{u[m+1, n-1] - 2 \cdot u[m, n-1] + u[m-1, n-1]}{h^2} \right) - val \right) + u[m, n-1] :$$

**end do**:
$u[30, n] := 0$ :
**end do**:
$u[20, 580]$

$$9.633725867 \quad (3)$$

*with*(*plots*) :

$B := [seq([seq([i \cdot h, j \cdot dt, u[i, j]], i = 0 ..30)], j = 0 ..1000)]$ :
*surfdata*(*B*)