FRACTIONAL AND FRACTAL ADVECTION-DISPERSION MODEL

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Abstract. A fractal advection-dispersion equation and a fractional space-time advection-dispersion equation have been developed to improve the simulation of groundwater transport in fractured aquifers. The space-time fractional advection-dispersion simulation is limited due to complex algorithms and the computational power required; conversely, the fractal advection-dispersion equation can be solved simply, yet only considers the fractal derivative in space. These limitations lead to combining these methods, creating a fractional and fractal advection-dispersion equation to provide an efficient non-local, in both space and time, modeling tool. The fractional and fractal model has two parameters, fractional order ($\alpha$) and fractal dimension ($\beta$), where simulations are valid for specific combinations. The range of valid combinations reduces with decreasing fractional order and fractal dimension, and a final recommendation of $0.7 \leq \alpha, \beta \leq 1$ is made. The fractional and 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 tools to improve the representation of anomalous breakthrough curves that cannot be described by the classical model.

1. Introduction. Groundwater is a vital source of fresh water to many people across the globe, yet it is susceptible to contamination by various 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 modeled and observed [42, 55, 18, 21, 10, 43, 34].

2020 Mathematics Subject Classification. Primary: 58F15, 58F17; Secondary: 53C35.
Key words and phrases. Fractional and Fractal, Advection-dispersion Equation, Anomalous Transport, Fractured groundwater transport, Breakthrough curves, Tailing effect.
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A progressive approach to improve the simulation of groundwater transport is to redefine the governing equations with non-local derivatives, i.e. fractal and fractional derivatives. Fractal geometries describe irregular objects in nature with 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, and display fractal geometries [1, 44].

On the other hand, fractional derivatives have been incorporated into many applications to improve simulations by adding non-local properties to governing partial differential equations. There are many examples of fractional derivative applications, but a few recent developments of importance are [5, 6, 27, 28, 29]. A fractional derivative was first applied to the advection-dispersion equation specifically by [8]. [7] demonstrated the inadequacy of the Fickian or traditional equation to model the measured concentrations in an anomalous diffusion system, and by incorporating the fractional derivative and adjusting the fractional order ($\alpha$) a model can be developed to improve the representation.

Many authors have considered fractional and fractal derivatives, but mostly separately for comparison and not fully combined in a single model [35, 9, 23, 15, 13, 14, 47, 12, 46],[13] compared a fractal and fractional diffusion model, and found that both models can characterize 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. Recently, a fractal advection-dispersion equation, and a fractional space-time advection-dispersion equation have been developed to improve the simulation of groundwater transport specifically in fractured aquifers [2, 3].

For groundwater transport simulations, 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. With currently available and common computer processors, only small 2D model domains with simple geometry can be simulated for space-time fractional models. This is a limitation because groundwater models need to encompass large-scale groundwater flow systems on a regional scale. Thus, developing an efficient non-local modelling tool that could potentially be applied on a larger scale would add practical value to this discipline.

Furthermore, the fractal advection-dispersion equation only considers fractal derivatives in space, and not time. Considering these two observations, it is theorized 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 for groundwater transport modeling. The incorporation of non-local parameters in both space and time for the groundwater transport equation would improve the ability to capture non-local process such as anomalous diffusion and preferential pathway flow. Being able to better capture these processes, the accuracy of groundwater transport modelling improves and with it the remediation and mitigation procedures the models test, with the end goal to better protect the environment and groundwater resource.
In this paper, the combination of a fractional-time and fractal-space advection-dispersion equation is investigated, starting with a motivation for the use of fractional-fractal derivatives in general as well as specifically in groundwater transport modelling. A qualitative analysis for the fractional and fractal advection-dispersion equation is performed, proving the boundedness, existence and uniqueness. The relationship between the physical parameters of velocity/dispersion and fractal dimensions is explored before presenting the relationship between the numerical simulation results. The simulated simple transport problem using the developed fractional and fractal advection-dispersion equation shows that the fractional order in time controls the breakthrough-curve peak location and the fractal dimension in space controls the degree of tailing in the simulated breakthrough curve. Having these additional controls on a groundwater transport model would allow the modeller to better represent a heterogeneous, anomalous system without having to resort to unrealistic groundwater parameters.

2. Motivation for fractal and fractional derivatives.

2.1. Fractal geometry and derivative. It has been established that simulating groundwater transport within a fractured aquifer with the classical Fickian advection-dispersion transport equation is not able to capture the fractal nature of the fracture network [2]. This limitation is related to both lack of detailed characterization of the fracture network and heterogeneity of the system, and subdiffusion and/or superdiffusion. Often the information required to characterize a fracture system fully is not available, and the formulation of the traditional advection-dispersion equation cannot account for anomalous diffusion [2].

This leads to the use of non-local approaches to simulate anomalous diffusion systems. Numerous methods have been applied, including the application of fractional derivatives in time and space [54, 48]. While, the fractional advection-dispersion equation formulations have proven successful in describing non-Fickian transport, some three-dimensional applications have been found to show scale-dependent dispersivity problems [33, 26].

The fractal nature of fractures naturally lead to the application of a fractal derivative. [47] developed a fractal Richard’s equation to model unsaturated flow in heterogeneous soils that exhibit anomalous Boltzmann scaling. Anomalous behaviour recorded in unsaturated flow systems 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) [19, 22]. 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 [39, 51].

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 characterization of the heterogeneity of the system. A fractal advection-dispersion equation applying the fractal derivative in space was developed by [2] and will be used here as the base for the fractal component of the fractional and fractal advection-dispersion equation.
2.2. Fractional derivative. The application of fractional derivatives is not a new idea, as first applied by [8] and since has been applied by many authors with numerous fractional derivative definitions [5, 6, 27, 28, 29]. The usual approach incorporates a fractional derivative either in time [32, 37, 40], in space (but only for the diffusion/dispersion term) [8, 7, 45, 52], or in time and space (diffusion-dispersion term) [25, 38, 30]. [49] found that new fractional derivatives could change the way anomalous diffusion is modeled by incorporating different memory effects. The Caputo-Liouville [36] and Atangana-Baleanu [20, 24, 41] fractional derivatives are non-local and have memory because the fractional order exponent is present in the kernel and associated with time \( t \).

It was conceptualized by [2] 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. 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. Thus, the application of a fractional derivative to the advection-dispersion equation allows for anomalous advection and dispersion to be captured in the governing equation. Specifically, applying the fractional derivative in time, where the waiting time distribution is associated. Incorporating the fractional derivative for time, allows these features to be activated in the advection-dispersion equation solution, i.e. for the Caputo-Liousville derivative a power law distribution.

2.3. Fractional and fractal derivatives. A few authors have combined the fractional and fractal derivative in a model or description [17, 31, 11, 52]. [16] develop a fractional-fractal diffusion model based on work done by [31], using Riemann-Liouville and Caputo-Liousville 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. [4] developed new fractal-fractional differential and integral operators, and concluded that those new operators would provide tools for future investigations. Furthermore, superdiffusion and subdiffusion in heterogeneous aquifers were suggested as a specific application by [4]. A space-time fractional-fractal Boussinesq equation was developed by [53] to improve the simulation of groundwater flow in unconfined systems, where a Caputo-Liousville fractional derivative was applied in time and the fractal derivative developed by [2] applied in space. An application of a fractional and 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.

3. Fractional and fractal advection-dispersion equation. The fractional and fractal advection-dispersion equation was developed by applying the Caputo-Liousville fractional derivative in time, and the fractal derivative in space for both the advection and dispersion terms as originally described in [2]. There are two non-local parameters, namely the fractional order \( \alpha \) and fractal dimension \( \beta \). The fractional-fractal equation can thus be defined as:

\[
\frac{C}{0}D^{\alpha}_t (c(x,t)) = V_F^\beta (x) \frac{\partial}{\partial x} c(x,t) + D_F^\beta (x) \frac{\partial^2}{\partial x^2} c(x,t)
\] (1)
Where,

c(x, t) is the simulated concentration of a contaminant in groundwater with respect to the x-direction and time.

\( C^0_D^\alpha_t (c(x, t)) \) denotes the left Caputo-Liouville fractional derivative

\[
C^0_D^\alpha_t c(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d\tau}{\tau^{\alpha}} c(t-\tau)^{-\alpha} d\tau
\]

\( V_F^\beta(x) \) denotes the fractal velocity in the x-direction

\[
V_F^\beta(x) = -v \left( \frac{x^{1-\alpha}}{\alpha} \right) + D_L \left( \frac{(1-\alpha)}{\alpha} \right) x^{1-2\alpha}
\]

where, \( v \) is the groundwater velocity and \( D_L \) is the longitudinal dispersivity parameter of the aquifer through which groundwater is moving.

\( D_F^\beta(x) \) denotes the fractal dispersivity in the x-direction

\[
D_F^\beta(x) = D_L \left( \frac{x^{2-2\alpha}}{\alpha^2} \right)
\]

The development of the fractal model is discussed in detail in [2]. The use of the Caputo-Liouville fractional derivative in time is commonly applied for its ease of use. These fractional and fractal components are investigated as an efficient means of incorporating non-locality into both time and space components for groundwater transport modeling using the advection-dispersion equation.

4. **Qualitative analysis for the fractional and fractal advection-dispersion equation.** Firstly, the boundedness, existence and uniqueness of the fractional (time) and fractal (space) transport model is determined by applying the Picard-Lindelöf theorem.

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

Considering the fractional and fractal advection-dispersion equation defined in Eq. (1), let

\[
C^0_D^\alpha_t (c(x, t)) = F(x, t, c(x, t))
\]

Applying the Riemann-Liouville integral to both sides of Eq. (2), we obtain

\[
c(x, t) - c(x, 0) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} F(x, \tau, c(x, \tau)) d\tau
\]

It is imposed that \( V_F^\beta \) and \( D_F^\beta \) are bounded. Thus, \( M_1 \) and \( M_2 \) can be defined by introducing the norm of the supremum (statistical limit of a set),

\[
\|V_F^\beta\|_\infty = \sup_{x \in [0, x]} |V_F^\beta| < M_1
\]

and,

\[
\|D_F^\beta\|_\infty = \sup_{x \in [0, x]} |D_F^\beta| < M_2
\]

Therefore,

\[
c(x, t) - c(x, 0) \leq C_0
\]

where, \( C_0 \) is the initial concentration, which by the nature of contaminant transport
will be the highest concentration in a single-source system. Considering this requirement,
\[
c(x,t) - c(x,0) \leq \frac{1}{\Gamma(\alpha)} \int_0^t \| F(x,t,c(x,\tau)) \| (t-\tau)^{\alpha-1} d\tau
\]
\[
\leq \frac{M\| F(x,t,c(\tau)) \|}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} d\tau
\]
\[
\leq \frac{M\| F(x,t,c(\tau)) \|}{\Gamma(\alpha+1)} t^\alpha
\]

Thus,
\[
\frac{M\| F \|}{\Gamma(\alpha+1)} t_{max}^\alpha < C_0
\]

Rearranging,
\[
t_{max}^\alpha < \left( \frac{C_0 M \| F \|}{\Gamma(\alpha+1)} \right)^{\frac{1}{\alpha}}
\]

This is the condition for the fractional (time) and fractal (space) advection dispersion equation.

Now, a mapping is defined, where Λ is Picard’s operator
\[
\Lambda v(x,t) = c(x,0) + \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} F(x,\tau,v(x,\tau)) d\tau
\]
\[
\Lambda u(x,t) = c(x,0) + \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} F(x,\tau,u(x,\tau)) d\tau
\]

Thus,
\[
\Lambda v(x,t) - \Lambda u(x,t)
\]
\[
= \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} [F(x,\tau,v(x,\tau)) - F(x,\tau,u(x,\tau))] d\tau
\]

The required Lipschitz condition is,
\[
\| \Lambda v(x,t) - \Lambda u(x,t) \| < K\| v(x,t) - u(x,t) \|
\]

Eq. (12) shows the operator is Lipchitz continuous with Lipchitz constant K. Applying a norm to both sides of Eq. (11), we obtain the following relationship,
\[
\| \Lambda v(x,t) - \Lambda u(x,t) \|
\]
\[
= \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} \| F(x,\tau,v(x,\tau)) - F(x,\tau,u(x,\tau)) \| d\tau
\]

where,
\[
F(x,t,v(x,t)) - F(x,t,u(x,t))
\]
\[
= V^\beta(x) \frac{\partial}{\partial x} [v(x,t) - u(x,t)] + D^\beta(x) \frac{\partial^2}{\partial x^2} [v(x,t) - u(x,t)]
\]
Applying a norm to both sides of Eq. (14),
\[ \| F(x, t, v(x, t)) - F(x, t, u(x, t)) \| \leq \| V_\beta F(x) \| \left| \frac{\partial}{\partial x} [v(x, t) - u(x, t)] \right| + \| D_\beta F(x) \| \left| \frac{\partial^2}{\partial x^2} [v(x, t) - u(x, t)] \right| \]

Applying the proven theorem by [2],
\[ \| F(x, t, v(x, t)) - F(x, t, u(x, t)) \| < M_1 \theta_1 \| v(x, t) - u(x, t) \| + M_2 \theta_2 \| v(x, t) - u(x, t) \| \]

where, this can be expressed in the form,
\[ \| F(x, t, v(x, t)) - F(x, t, u(x, t)) \| < K \| v(x, t) - u(x, t) \| \]

Thus, \( \Lambda \) is Lipschitz mapping, and \( \Lambda \) is a contraction if and only if \( K < 1 \). \( \Lambda \) has a unique solution if \( K < 1 \), and the first condition is upheld (Eq. 9).

The Picard’s operator is a contraction, thus using the Banach fixed Theorem, we conclude the existence and the uniqueness.

This completes the proof, and confirms the fractional-time and fractal-space advection-dispersion equation is stable and has a unique solution.

5. Relationship between velocity/dispersion and fractal dimensions. Simulations of variable fractal dimension have validated the use of the model for fractured groundwater systems lacking detailed characterization of heterogeneity [2]. 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 \( (V_\beta F) \) and fractal dispersivity \( (D_\beta F) \) with respect to the fractal dimension are evaluated. For the analysis, a constant groundwater velocity \( (v) \) is defined at 0.05 m/d, dispersivity \( (D_L) \) of 0.3 m²/d, and a time step \( (\Delta t) \) of 0.01 days.

The first plot of \( \beta = 1 \), forms the base for comparison, representing the traditional advection-dispersion model with no fractional order or fractal dimension (Figure 1 and Figure 2). For a fractal dimension of 1 \( (\beta = 1) \), the fractal velocity equals a constant velocity of 0.25 m/d (Figure 1). The introduction of the fractal order at \( \beta = 0.8 \), increases the constant velocity from 0.25 m/d to 2.1 m/d at 50 m. A steadily increasing trend of exponential distributions are seen from \( \beta = 0.8 \) to \( \beta = 0.6 \), until a linear relationship over distance is found at \( \beta = 0.5 \). From a fractal order of 0.5, an exponential trend is seen up to \( \beta = 0.1 \), but an increased rate of increase. At a fractal dimension of \( \beta = 0.2 \), the fractal velocity ranges from 0.25 m/d to 3 800 m/d at 50 m.

A plot of the fractal dispersivity illustrates the same trends, where for a fractal dimension of 1 \( (\beta = 0.8) \), the fractal dispersivity equals the defined constant dispersivity of 0.3 m²/d (Figure 2). Similar to the fractal velocity trend, the introduction of the fractal order at \( \beta = 0.8 \) results in dispersivity values ranging from 0.3 m²/d to 2.2 m²/d at 50 m. The same trend of increasing exponential distributions is seen from \( \beta = 0.8 \) to \( \beta = 0.6 \), until a linear relationship over distance is found at \( \beta = 0.5 \). Decreasing the fractal dimension below \( \beta = 0.5 \) shows a faster exponential increase.
from $\beta = 0.4$ to $\beta = 0.1$, where at $\beta = 0.2$ the fractal dispersivity has increased to 3800 m$^2$/d at 50 m.

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, and can be considered ultra-advection/dispersivity. From a practical interpretation, the use of a fractal dimensions below $\alpha = 0.5$ should be used with caution because of the exponential increase in velocity and hydrodynamic dispersivity.

![Figure 1. Fractal velocity ($V_{F\beta}$) over space for varying fractal dimensions $\beta = 1, 0.8, 0.5, 0.2$](image)

6. **Numerical approximation.** Two numerical approaches are applied to the fractional and fractal advection-dispersion equation, a common numerical approximation method and an alternative approach developed by [50].

The typical numerical approximation method is applied to the Caputo-Liouville fractional derivative in time, as described in [3]. A commonly used finite difference method is applied to approximate the advective term (central difference) and the
dispersion term (standard second-order difference) in space, and a backward implicit
scheme in time, resulting in:

\[
\frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \left[ \sum_{k=0}^{n-1} (c_{m+1}^{k+1} - c_{m}^{k}) \delta_{n,k}^{\alpha} \right] = V_{F}^{\beta}(x_{i}) \left( \frac{c_{m+1}^{n-1} - c_{m-1}^{n-1}}{2\Delta x} \right) + D_{F}^{\beta}(x_{i}) \left( \frac{c_{m+1}^{n-1} - 2c_{m}^{n-1} + c_{m-1}^{n-1}}{(\Delta x)^{2}} \right)
\]

where,

\[
\delta_{n,k}^{\alpha} = (n-k)^{1-\alpha} - (n-k-1)^{1-\alpha}
\]

An algorithm is developed in Maple to solve the fractional and fractal equation
using the numerical approximation scheme as described. The first step where \( n = 1 \)
is defined as:
\[
c[m, 1] = \frac{\Gamma (2 - \alpha)}{(\Delta t)^{-\alpha}} \left( V_F^\beta \left( \frac{c[m+1,0] - c[m-1,0]}{2\Delta x} + D_F^\beta \left( \frac{c[m+1,0] - 2c[m,0] + c[m-1,0]}{(\Delta x)^2} \right) \right) + c[m, 0]
\]
(18)
and, the recursive step where \( k = n - 1 \) is defined as:
\[
c[m, n] = \frac{1}{(n-1)^{1-\alpha}} \left[ \frac{\Gamma (2 - \alpha)}{\Delta t)^{-\alpha}} \left( V_F^\beta \left( \frac{c[m+1,n-1] - c[m-1,n-1]}{2\Delta x} + D_F^\beta \left( \frac{c[m+1,n-1] - 2c[m,n-1] + c[m-1,n-1]}{(\Delta x)^2} \right) \right) \right]

- \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]
\]
(19)

An alternative numerical approximation method developed by [50] is also considered. Information related to the stability, error analysis and convergence of this numerical approximation is provided in [50]. This method involves defining the function first \( f(x, t, c(x, t)) \),
\[
F(x, t, c(x, t)) = V_F^\beta (x) \frac{\partial}{\partial x} c(x, t) + D_F^\beta (x) \frac{\partial^2}{\partial x^2} c(x, t)
\]
(20)
Thus,
\[
\beta^\alpha D_t^\alpha (c(x, t)) = F(x, t, c(x, t))
\]
(21)
Integrating on both sides,
\[
c(x, t) - c(x, 0) = \frac{1}{\Gamma (\alpha)} \int_0^t (t - \tau)^{\alpha-1} F(x, \tau, c(x, \tau)) d\tau
\]
(22)
At a specific point in space and time \( (c(x_i, t_{n+1})) \),
\[
c(x_i, t_{n+1}) - c(x_i, 0) = \frac{1}{\Gamma (\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \tau)^{\alpha-1} F(x_i, \tau, c(x_i, \tau)) d\tau
\]
\[
= \frac{1}{\Gamma (\alpha)} \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} F(x_i, \tau, c(x_i, \tau)) d\tau
\]
(23)
A Lagrange polynomial \( (P_j (t)) \) is then considered for polynomial interpolation,
\[
P_j (t) = \frac{t - t_j}{t_j - t_{j-1}} f(x_i, t_j, c(x_i, t_j)) - \frac{t - t_j}{t_j - t_{j-1}} F(x_i, t_{j-1}, c(x_i, t_{j-1}))
\]
(24)
Applying the Lagrange polynomial \( (P_j (t)) \) to Eq. (23),
\[
c(x_i, t_{n+1}) - c(x_i, 0)
\]
\[
= \frac{1}{\Gamma (\alpha)} \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} \left[ \frac{t - t_j}{t_j - t_{j-1}} F(x_i, t_j, c(x_i, t_j)) - \frac{t - t_j}{t_j - t_{j-1}} F(x_i, t_{j-1}, c(x_i, t_{j-1})) \right] d\tau
\]
(25)
Simplifying notation,
\[ c_i^{n+1} - c_i^0 = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} (t_{n+1} - \tau)^{\alpha-1} \left[ \frac{t-t_{j+1}}{t_{j+1}-t_j} F \left( x_i, t_j, c_i^j \right) \right] d\tau \]  
\tag{26}

Applying the numerical approximation determined by \[50\], the following is obtained,

\[ c_i^{n+1} - c_i^0 = \frac{(\Delta t)\alpha}{\Gamma(\alpha+2)} \sum_{j=0}^{n} \left[ F(x_i, t_j, c_i^j)\{(n-j+1)^\alpha(n-j+2+\alpha) - (n-j)^\alpha(n-j+2+2\alpha)\} - F(x_i, t_{j-1}, c_i^{j-1})\{(n-j+1)^{\alpha+1} - (n-j)^{\alpha}(n-j+1+\alpha)\} \right] \]  
\tag{27}

Remembering the defined function \( F(x, t, c(x, t)) \) (Eq. 20), and applying standard finite difference approximations, namely a central difference and second-order approximation, the following is obtained

\[ F \left( x_i, t_j, c_i^j \right) = V^\beta F(x_i) \left( \frac{c_{i+1}^j - c_{i-1}^j}{2\Delta x} \right) + D^\beta_c (x_i) \left( \frac{c_{i+1}^j - 2c_i^j + c_{i-1}^j}{(\Delta x)^2} \right) \]  
\tag{28}

and,

\[ F \left( x_i, t_{j-1}, c_{i-1}^j \right) = V^\beta F(x_i) \left( \frac{c_{i+1}^{j-1} - c_{i-1}^{j-1}}{2\Delta x} \right) + D^\beta_c (x_i) \left( \frac{c_{i+1}^{j-1} - 2c_i^{j-1} + c_{i-1}^{j-1}}{(\Delta x)^2} \right) \]  
\tag{29}

Substituting back into Eq. (27),

\[ c_i^{n+1} - c_i^0 = \frac{(\Delta t)^\alpha}{\Gamma(\alpha+2)} \sum_{j=0}^{n} \left[ \left( V^\beta F(x_i) \left( \frac{c_{i+1}^j - c_{i-1}^j}{2\Delta x} \right) + D^\beta_c (x_i) \left( \frac{c_{i+1}^j - 2c_i^j + c_{i-1}^j}{(\Delta x)^2} \right) \right) \left\{ (n-j+1)^\alpha(n-j+2+\alpha) \right\} - \left( V^\beta F(x_i) \left( \frac{c_{i+1}^{j-1} - c_{i-1}^{j-1}}{2\Delta x} \right) + D^\beta_c (x_i) \left( \frac{c_{i+1}^{j-1} - 2c_i^{j-1} + c_{i-1}^{j-1}}{(\Delta x)^2} \right) \right\} \left\{ (n-j)^{\alpha+1} - (n-j)^{\alpha}(n-j+1+\alpha) \right\} \right] d\tau \]  
\tag{30}

Therefore, the alternative numerical approximation method by \[50\], considers smaller integration-based time steps \( t_j \) within each approximation time step \( t_n \). From this perspective, the method has the potential to capture a larger memory and improve accuracy.

7. Simulation. To test the applicability of the fractional order and fractal dimension, a fractional and fractal model is simulated for a simple transport problem in the software programme Maple. 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 \( C_0 \) is 10 mg/l. The initial condition and boundary conditions for the defined problem are

\[
\begin{align*}
  c(x, 0) &= C_0 \\
  c(0, t) &= C_0 \cdot \exp(\lambda t) \\
  c(L, t) &= 0
\end{align*}
\]  
\[
\begin{cases}
  x \geq 0 \\
  t \geq 0
\end{cases}
\]
The presence of two non-local parameters, namely the fractional order ($\alpha$) and fractal dimension ($\beta$), increases the number of parameter combinations in the simulation, compared to the sole consideration of either a fractional or fractal derivative. The velocity and dispersivity are highly sensitive to these parameters and a simulation of the potential combinations is performed to explore the relationship. The fractional and 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 3 to Figure 7, and the suitable $\alpha, \beta$ combinations tabulated in Table 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 3). When the fractional order is at $\alpha = 1$, and the derivative in time becomes an integer-order, the fractal dimension is applicable 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 4, 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 the additional influence of a fractional order in time is a control on the breakthrough curve peak, while the fractal dimension controls the degree of tailing in 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 5 for fractional order $\alpha = 0.8$, and in Figure 8 for fractional order $\alpha = 0.7$. However, the range of appropriate fractal dimensions decreases systematically (Table 1).

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 and 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 simulated time. This eventually causes instabilities as this rapid movement along the line becomes unrealistic. The result of this rapid transport can be 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 simulation time (Figure 7).

The simulated fractional and fractal advection-dispersion model highlights the importance of selecting appropriate combinations of fractional order and fractal dimension. Considering the suggestion of using fractal dimensions greater than 0.5, the range of appropriate fractional order and fractal dimension for the combined fractional and fractal model should be stricter due to the cumulative increase in velocity/dispersion. A final recommendation is refined based on the simulations to an optimal fractional order and fractal dimension of $0.7 \leq \alpha, \beta \leq 1$.

8. Conclusions. A fractional and fractal advection-dispersion model is established from the individual fractional, and fractal advection-dispersion equations previously developed, producing an efficient tool to model anomalous diffusion with the same non-local advantages. However, the fractional and fractal model has two parameters to consider, the fractional order ($\alpha$) and the fractal dimension ($\beta$), and this increases
the number of parameter combinations available for simulation. An investigation

Figure 3. 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 4. Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order $\alpha = 0.9$ (simplifies to a local order), and varying fractal dimensions ($0.5 \leq \beta \leq 1$).

on the influence of the fractal dimension on the velocity/dispersivity found the
velocity/dispersivity increases exponentially with a decrease in the fractal order. A recommendation to use a fractal dimension above 0.5 was made based on the
Fig. 6. Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order \( \alpha = 0.7 \) (simplifies to a local order), and varying fractal dimensions \((0.7 \leq \beta \leq 1)\)

| Fractional order | Fractal dimension |
|------------------|-------------------|
|                  | \( \beta = 1 \) | \( \beta = 0.9 \) | \( \beta = 0.8 \) | \( \beta = 0.7 \) | \( \beta = 0.6 \) | \( \beta = 0.5 \) | \( \beta = 0.4 \) |
| \( \alpha = 1 \) | x                 | x                 | x                 | x                 | x                 | x                 | x                 |
| \( \alpha = 0.9 \) | x                 | x                 | x                 | x                 | x                 | x                 | x                 |
| \( \alpha = 0.8 \) | x                 | x                 | x                 | x                 | x                 | x                 | x                 |
| \( \alpha = 0.7 \) | x                 | x                 | x                 | x                 | x                 | x                 | x                 |
| \( \alpha = 0.6 \) | x                 | x                 | x                 | x                 | x                 | x                 | x                 |
| \( \alpha = 0.5 \) | x                 | x                 | x                 | x                 | x                 | x                 | x                 |
| \( \alpha = 0.4 \) | x                 | x                 | x                 | x                 | x                 | x                 | x                 |

Table 1. Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order \( \alpha = 0.7 \) (simplifies to a local order), and varying fractal dimensions \((0.7 \leq \beta \leq 1)\).

evaluation. The established relationship highlighted the importance of selecting appropriate parameter combinations. From the simulations, it is found that the
Figure 7. Simulation results illustrated for distance (m) in the x-direction along a line over time (d) for the fractional order \( \alpha = 0.6, 0.5 \) (simplifies to a local order), and varying fractal dimensions \((0.8 \leq \beta \leq 1)\)

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 \( 0.7 \leq \alpha, \beta \leq 1 \).

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Received April 2019; revised October 2020.

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