A VARIABLE-ORDER FRACTAL DERIVATIVE MODEL FOR ANOMALOUS DIFFUSION

by

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This paper pays attention to develop a variable-order fractal derivative model for anomalous diffusion. Previous investigations have indicated that the medium structure, fractal dimension or porosity may change with time or space during solute transport processes, results in time or spatial dependent anomalous diffusion phenomena. Hereby, this study makes an attempt to introduce a variable-order fractal derivative diffusion model, in which the index of fractal derivative depends on temporal moment or spatial position, to characterize the previous mentioned anomalous diffusion (or transport) processes. Compared with other models, the main advantages in description and the physical explanation of new model are explored by numerical simulation. Further discussions on the dissimilitude such as computational efficiency, diffusion behavior, and heavy tail phenomena of the new model, and variable-order fractional derivative model are also offered.

Key words: *anomalous diffusion, variable-order fractal derivative, stretced Gaussian distribution, porosity-gradient*

Introduction

Nowadays, anomalous diffusion plays an important role in analysis of a variety of animate and inanimate systems [1, 2]. In most cases, the mean square displacement (MSD) of anomalous diffusion has been used to distinguish the diffusion characteristic [3, 4]. The MSD over time is usually expressed as $< x^2(t) > \infty\ t^p$, in which $0 < p < 1$ represents subdiffusion, $p = 1$ is Fickian diffusion, and $p > 1$ denotes superdiffusion. Subdiffusion has been observed in a variety of systems such as bromide transport process in a fractured granite aquifer [5], and contamination dispersion in groundwater or fractal systems [6, 7]. Meanwhile, superdiffusion exists in sediment transport, solute transport in fractured media and active motion in the biological cells of animals [8-11], *etc.*

In this field, lots of transport theories, such as multi-rate mass transfer model [12], continuous time random walk framework [13], fractional derivative model [14-16], and fractal derivative model [17-19] were proposed for anomalous diffusion/dispersion. Also, numerous experiment results illustrate that the solute transport in complex media may not keep at one single diffusive state [20, 21]. To accurately describe the transient diffusion processes, vari-

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able-order, and distributed-order fractional derivative diffusion models, along with tempered fractional derivative models, have been employed to capture these kinds of phenomena [15, 22-24]. However, all of previously mentioned models are computationally expensive and difficult for mathematical analysis in most cases. Moreover, the additional model parameters are usually unavailable from experiments or measurement, and cause extra burdens in physical analysis. Hereby, this paper will make an attempt to overcome these problems by introducing a simple model to describe the transient diffusion processes, based on the fractal derivative model.

The basic idea of fractal was introduced with the symbolic phrase *mountains are not cones, bark is not smooth, nor does lighting travel in a straight line* in Mandelbrot's book *The fractal geometry of nature*. Mandelbrot hypothesizes that many natural phenomena are statistical fractals. Based on fractal structure of porous media, Chen [17] proposed a fractal derivative model and suggested potential applications on a variety of stretced Gaussian scaling phenomena. Chen [18] and Sun *et al*. [25] improved the definition of fractal derivative and applied the fractal derivative model to characterize the water diffusion in unsaturated media. Previous research illustrated that the fractal derivative model was simple and easy-to-solve compared with fractional derivative model and could suitably describe the well-documented experimental data which exhibited stretced Gaussian distribution. However, the fractal structure of porous media and porosity-gradient materials, usually changes with time or space and yields the transient diffusion behavior [15, 19, 26-29]. Therefore, it is necessary to generalize the presented fractal derivative model to address the transient diffusion behavior which changes with time, space or other conditions. Here we name the new model as variable-order fractal derivative model, in which the index of fractal derivative changes with time, space or other conditions, corresponding to the influence of medium structure or heterogeneity variation. From physical viewpoint, the variable-order fractal derivative model means the time or space ruler varies with time or space during the solute diffusion or dispersion processes. Meanwhile, numerous experimental measurements illustrate that the geometrical structure of media varies significantly in different time or space scales, the variable-order index represents the time or space dependence of fractal characteristics.

Methodology

Definitions of the variable-order fractal derivative

The definition of fractal derivative can be written [30-32]:

$$\frac{\partial u}{\partial t^{\alpha}} = \lim_{t_1 \to t} \frac{u(t_1) - u(t)}{t_1^{\alpha} - t^{\alpha}}, \quad 0 < \alpha \tag{1}$$

To characterize the time and space dependent physical process or system, we defines the variable-order fractal derivative:

$$\frac{\partial u}{\partial t^{\alpha(x,t)}} = \lim_{t_1 \to t} \frac{u(t_1) - u(t)}{t_1^{\alpha(x,t)} - t^{\alpha(x,t)}}, \quad 0 < \alpha \tag{2}$$

A more generalized definition which can be used to describe concentration-dependent diffusion, can be written:

$$\frac{\partial u^{\beta(x,t)}}{\partial t^{\alpha(x,t)}} = \lim_{t_1 \to t} \frac{u^{\beta(x,t)}(t_1) - u^{\beta(x,t)}(t)}{t_1^{\alpha(x,t)} - t^{\alpha(x,t)}}, \quad 0 < \alpha, \quad 0 < \beta \tag{3}$$

Since the variable-order fractional derivative model has been successfully used to describe transient dispersion, we will make a comparison between two models in characterizing anomalous diffusion or dispersion. In this paper, we adopt the most commonly used variable-order fractional derivative of the Caputo type [33-35].

The properties of the fractal derivative

In order to investigate the properties of fractal derivative, we firstly consider the following functions:

$$\text{(a). } F_1(t) = t^2 \qquad \text{(b). } F_2(t) = \mathrm{e}^t \tag{4}$$

The fractal derivative of previous functions can be stated:

$$\text{(a). } \frac{\partial F_1(t)}{\partial t^\alpha} = \frac{\partial t^2}{\partial t^\alpha} = \frac{2t^{2-\alpha}}{\alpha}$$

$$\text{(b). } \frac{\partial F_2(t)}{\partial t^\alpha} = \frac{\partial \mathrm{e}^t}{\partial t^\alpha} = \frac{t^{1-\alpha}}{\alpha}\mathrm{e}^t$$

Laplace transform of time fractal derivative:

$$L\left[\frac{\partial u(x,t)}{\partial t^\alpha}\right] = L\left[\frac{\partial u(x,t)}{\partial t}\frac{\partial t}{\partial t^\alpha}\right] = \frac{1}{\alpha}L[u'(x,t)t^{1-\alpha}]$$

According to the property of Laplace transform:

$$L[f(t)g(t)] = F(s)*G(s) = \int_0^s F(s-\tau)G(\tau)\mathrm{d}\tau$$

then

$$L[u'(x,t)] = sU(x,s) - u(x,0)$$

$$L(t^{1-\alpha}) = \frac{\Gamma(2-\alpha)}{s^{2-\alpha}}$$

Hereby, the final Laplace transform expression of time fractal derivative is written:

$$L\left[\frac{\partial u(x,t)}{\partial t^\alpha}\right] = \frac{\Gamma(2-\alpha)}{\alpha s^{2-\alpha}}*[sU(x,s) - u(x,0)]$$

The variable-order fractal derivative advection-dispersion equation model

We consider the variable-order fractal derivative advection-dispersion equation model with the governing equation is stated:

$$\frac{\partial u(x,t)}{\partial t^{\alpha(x,t)}} = -A\frac{\partial u(x,t)}{\partial x} + \frac{\partial}{\partial x^{\beta(x,t)}}\left[D\frac{\partial u(x,t)}{\partial x^{\beta(x,t)}}\right] + f(x,t) \tag{5}$$

where $\alpha(x, t)\in(0,2)$, $\beta(x, t)\in(0,1]$, and $x\in\Omega$, $t > 0$, with boundary condition:

$$\frac{\partial u(x,t)}{\partial x^{\beta(x,t)}} = g(x,t) \text{ or } u(x,t) = h(x,t), \quad x \in \partial\Omega, \quad t > 0$$

and initial condition:

$$u(x,0) = w(x,t), \quad t = 0$$

Here, $u(x, t)$ means the solute concentration, $f(x, t)$ – the source or absorption term, A and D – the flow velocity and the diffusion coefficient, respectively, Ω – the spatial domain, and $\partial\Omega$ is along the boundary. Moreover, $\alpha(x, t)$ and $\beta(x, t)$ denote orders of the time and space fractal derivatives which relate to time and space, respectively.

The variable-order fractional derivative anomalous diffusion model is given by [15]:

$$\frac{\partial^{\alpha(x,t)}u(x,t)}{\partial t^{\alpha(x,t)}} = -A\frac{\partial}{\partial x}u(x,t) + \frac{\partial^{\beta(x,t)}}{\partial x^{\beta(x,t)}}\left[D\frac{\partial^{\beta(x,t)}u(x,t)}{\partial x^{\beta(x,t)}}\right] + f(x,t) \tag{6}$$

where $\alpha(x, t)\in(0,2)$, $\beta(x, t)\in(0,1]$, and $x\in\Omega$, $t > 0$, with boundary condition:

$$\frac{\partial u(x,t)}{\partial x} = g(x,t) \quad \text{or} \quad u(x,t) = h(x,t), \quad x \in \partial\Omega, \quad t > 0$$

and initial condition:

$$u(x,0) = w(x,t), \quad t = 0$$

in which $\alpha(x, t)$ and $\beta(x, t)$ denote fractional derivative orders of time and space, respectively. The other symbols and parameters are with same physical interpretations in eq. (5). Here we should notice that the eqs. (5), and (6) reduce to the classical advection-dispersion equation model when $\alpha(x, t) = \beta(x, t)=1$:

$$\frac{\partial u(x,t)}{\partial t} = -A\frac{\partial u(x,t)}{\partial x} + \frac{\partial}{\partial x}\left[D\frac{\partial u(x,t)}{\partial x}\right] + f(x,t) \tag{7}$$

The reason why we compare the fractal derivative model eq. (5) and fractional derivative model eq. (6) is that $\alpha(x, t) < 1$ and $\beta(x, t) = 1$ represents a subdiffusion while $\alpha(x, t) = 1$ and $\beta(x, t) < 1$ describes superdiffusion in both of models. However, the differences between two models are also obvious; fractal derivative is a local operator while fractional derivative is a global operator. Fractal derivative term represents the influence of geometrical structure on diffusion behavior by using the time or space rule, and fractional derivative term characterizes the history dependency and non-locality of particle random movement in heterogeneous media by employing convolution operator.

To illustrate main features of variable-order fractal derivative model, we first investigate a time fractal derivative model with the governing equation expressed:

$$\begin{cases} \dfrac{\partial u(x,t)}{\partial t^{\alpha(x,t)}} = -A\dfrac{\partial u(x,t)}{\partial x} + D\dfrac{\partial^2 u(x,t)}{\partial x^2}, \quad x \in [0,10], \quad t > 0, \quad 0 < \alpha \le 2 \\ \dfrac{\partial u(0,t)}{\partial x} = \dfrac{\partial u(10,t)}{\partial x} = 0 \\ u(x,0) = \begin{cases} 2 & (x-5)^2 \le 0.1 \\ 0 & \text{else} \end{cases} \end{cases} \tag{8}$$

Figure 1 shows the break through curves with fractal derivative $\alpha(x, t)$.

Clearly it can be seen transient of dispersion behavior from superdispersion (α = 1.4) to normal dispersion (α = 1.0) then subdispersion (α = 0.6) in the time interval $t\in(0,10]$. Here we should emphasize that time fractional derivative model describes subdispersion in most cases, while the time fractal derivative model could describe both super and subdispersion with $\alpha(x, t)\in(0, 2)$. The theory and application aspects on fractal derivative model in describing anomalous diffusion have been investigated in references [17, 18, 25].

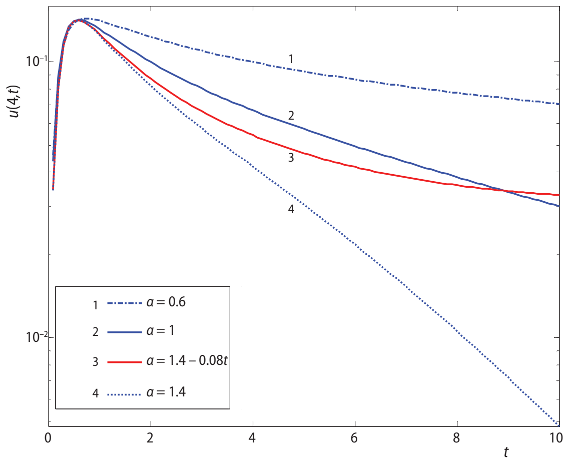

Figure 1. The dimensionless breakthrough curves of fractal derivative model at spatial location x = 4: (1) breakthrough curve with α = 0.6, (2) α = 1, (3) α = 1.4 – 0.8t, and (4) α = 1.4

Numerical results

In this section, we focus on the time variable-order fractal derivative and the time variable-order fractional derivative diffusion equation models which describe anomalous diffusion. For simplicity, we pay our attention to a 1-D diffusion problem. The time variable-order fractal derivative model is given by:

$$\begin{cases} \dfrac{\partial u(x,t)}{\partial t^{\alpha(x,t)}} = A\dfrac{\partial u(x,t)}{\partial x} + D\dfrac{\partial^2 u(x,t)}{\partial x^2}, \quad x\in[0,10], \quad t>0, \quad 0<\alpha\le 1 \\ \dfrac{\partial u(0,t)}{\partial x} = \dfrac{\partial u(10,t)}{\partial x} = 0 \\ u(x,0) = \begin{cases} 2 & (x-5)^2 \le 0.1 \\ 0 & \text{else} \end{cases} \end{cases} \tag{9}$$

The time variable-order fractional derivative equation is stated:

$$\begin{cases} \dfrac{\partial^{\alpha(x,t)} u(x,t)}{\partial t^{\alpha(x,t)}} = A\dfrac{\partial u(x,t)}{\partial x} + D\dfrac{\partial^2 u(x,t)}{\partial x^2}, \quad x\in[0,10], \quad t>0, \quad 0<\alpha\le 1 \\ \dfrac{\partial u(0,t)}{\partial x} = \dfrac{\partial u(10,t)}{\partial x} = 0 \\ u(x,0) = \begin{cases} 2 & (x-5)^2 \le 0.1 \\ 0 & \text{else} \end{cases} \end{cases} \tag{10}$$

in the eq. (10), $[\partial^{\alpha(x,t)}u(x,t)]/\partial t^{\alpha(x,t)}$ represents the variable-order fractional derivative of the Caputo type.

Since the analytical solutions of eqs. (9) and (10) can not be obtained, here employs an implicit finite difference scheme to numerically solve the previous equations. It can be proved that this numerical scheme is convergent, stable without preconditions for the variable-order fractal derivative and fractional derivative equations [36, 37].

For easy-to-implement and simplicity purpose, this study only investigates variable-orders with linear function of space or time. Solute concentration evolution curves obtained by variable-order fractal derivative model with space dependent index $\alpha(x) = 0.6 + 0.08x$ are presented in figs. 2(a) and 2(b). The space dependent index means that the geometrical structure or physical property of considered area is space dependent, which yields different diffusion behavior. The observation confirms that larger value of fractal derivative index produces faster decay of solute concentration. For example, generally speaking, solute concentration in left spatial domain, $x\in[0, 5)$, diffuse slowly than that in right spatial domain $x\in(5, 10]$. In addition, it is clear that the solute diffusion curve at spatial point ($x = 7.5$) exhibits superdiffusion feature, while the diffusion curve at ($x = 2.5$) is more like the subdiffusion phenomenon, from the observation of fig. 2(b). However, here we should point out that the solute diffusion curve obtained by using variable-order fractal derivative model is different with that of constant-order model, even though the fractal index is same at certain spatial points. The main reason is that the different fractal derivative indexes nearby influence the diffusion behavior of solute transport at present position.

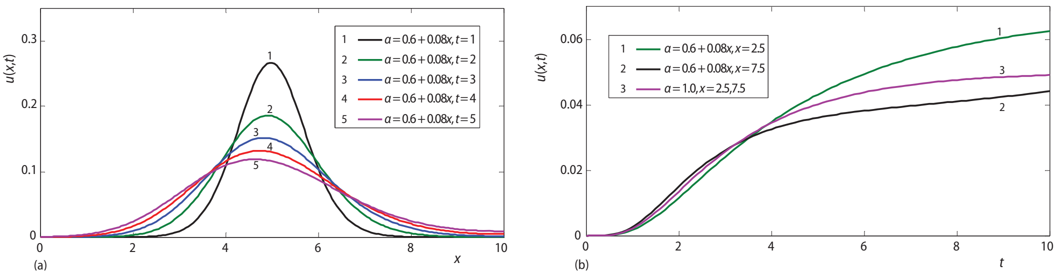

Figure 2. Solute diffusion curves obtained by using variable-order fractal derivative diffusion equation model (9) with diffusion coefficient *D* = 1.0

To explore the main property of variable-order fractal derivative model with time-dependent index, we make a comparison with variable-order fractional derivative model. There are many time-dependent factors such as medium structure or saturation, influence the diffusion behavior in solute transport. Hereby, time-dependent fractal derivative model has great application potentials in solving the real-world engineering problem. The solute diffusion curves obtained by using time-dependent fractal derivative and fractional derivative model with decreasing and increasing index functions are drawn in figs. 3(a) and 3(b). Generally speaking, the solute concentration evolution curves of variable-order fractal derivative model with $\alpha(t) \leq 1$, show a clear subdiffusion feature which can be easily observed in comparison with the classical model with $\alpha(t) = 1$. Meanwhile, fractal derivative model predicts a faster decay trend of solute concentration at the tail part, compared with fractional derivative model, fig. 3(a). Those, figs. 3(b) and 3(c) also show that the differences of numerical results of variable-order fractal derivative and fractional derivative models are not significant, which means both models can commendably describe the experimental data in many cases.

To test the computational efficiency of fractal derivative and fractional derivative models in numerical simulation, we make a comparison of computation cost with different time steps. Obviously, the computation cost of fractal derivative model is much lower than that of fractional derivative model, from the observation in tab. 1, with the computer Intel(R) Core (TM) i5-5490 CPU@3.30GHz. In addition, tab. 1 also tells us that the computation cost of fractal derivative model linearly increases with the number of nodes, but that of fractional derivative model in-

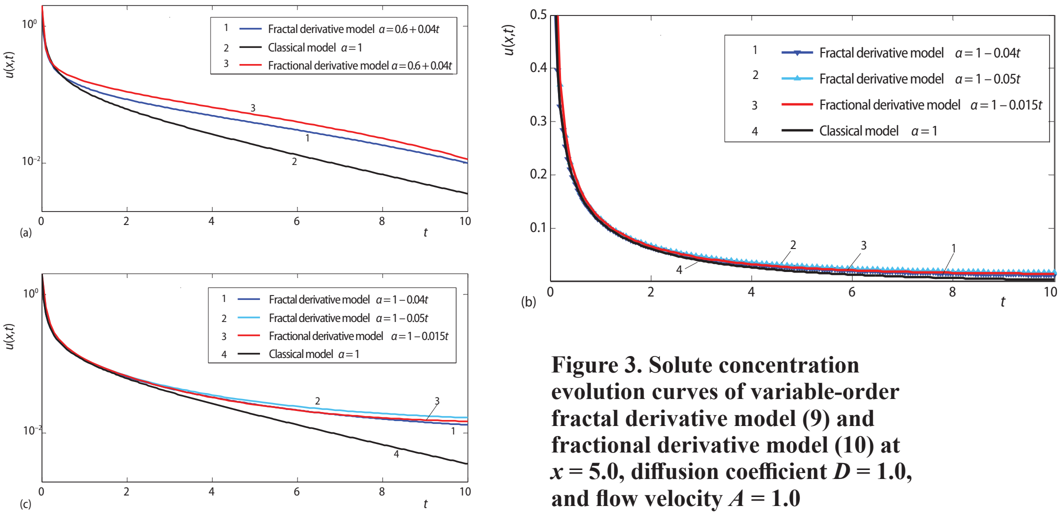

Figure 3. Solute concentration evolution curves of variable-order fractal derivative model (9) and fractional derivative model (10) at $x = 5.0$, diffusion coefficient $D = 1.0$, and flow velocity $A = 1.0$

creases dramatically with node number. The main reason lies that the fractal derivative is a local operator, while the fractional derivative is a global operator from mathematical viewpoint.

Table. 1. Comparison results of the computation cost of fractional and fractal derivative models with flow velocity $A = 1.0$ and dispersion coefficient $D = 1.0$; fractal and fractional derivative orders are $\alpha = 0.65$.

Nodes	10	100	500	1000
Fractional model [s]	0.177984	1.647346	20.922217	74.523884
Fractal model [s]	0.070087	0.507919	2.598602	10.295587

Conclusion

This paper introduces the main concept of variable-order fractal derivative and its application in anomalous diffusion modeling. From a statistical physics viewpoint, fractal derivative diffusion model is a local model, underlies the stretced Gaussian process, while the fractional derivative model corresponds to the Levy stable process. According to the comparison results, both of the variable-order fractal derivative and fractional derivative models can capture transient dispersion in heterogeneous media. But the variable-order fractal derivative model is simple to analyze and computational efficient for numerically calculation. The application potentials of variable-index fractal derivative model include a great variety of mass diffusion or transport, also heat conduction process in porosity-gradient structure, spatial or time dependent heterogeneous media.

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