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Variable-order fractional differential operators in anomalous diffusion modeling

HongGuang Sun [a,b,*], Wen Chen [a], YangQuan Chen [b]

[a] Institute of Soft Matter Mechanics, Department of Engineering Mechanics, Hohai University, No.1 XiKang Road, Nanjing, Jiangsu 210098, China

[b] Center for Self-Organizing and Intelligent Systems (CSOIS), Department of Electrical and Computer Engineering, Utah State University, 4160 Old Main Hill, Logan, UT 84322-4160, USA

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ABSTRACT

The purpose of this paper is to offer a unified discussion of variable-order differential operators in anomalous diffusion modeling. The characteristics of the new models, in contrast to constant-order fractional diffusion models, change with time, space, concentration or other independent quantities. We introduced a classification of variable-order fractional diffusion models based on the possible physical origins which prompt the variable-order. Some potential applications of the variable-order fractional diffusion models are also discussed.

1. Introduction

Anomalous diffusion phenomena are observed in various physical, chemical and biological situations, which have motivated the development of new mathematical and physical models [1]. It has been widely studied both by statistical methods and differential equation models [2,3]. Fractional diffusion equations account for typical "anomalous" features which are observed in many systems, e.g. in the cases of dispersive transports in amorphous semiconductors, porous medium, colloid, proteins, biosystems or even in ecosystems [4,5]. In this study, we focus on the differential equation models of anomalous diffusion which govern many physical phenomena such as heat, mass or electron transfer; pollutants or liquid transport through porous media.

Up until now, the constant-order (CO) fractional kinetic equations have been considered in most cases and received tremendous success in anomalous diffusion modeling and other fields [1,6–8]. However, it has become clear that further theoretical and numerical investigations are required in order to incorporate adequate tools for the description of more complicated (or more realistic) stochastic diffusion processes [9]. There are a large class of physical, biological and physiological diffusion phenomena that the CO fractional diffusion equation with constant coefficients is not equipped to characterize. The typical features of these phenomena are that they are complex to analysis and the diffusion behaviors

* Corresponding author at: Institute of Soft Matter Mechanics, Department of Engineering Mechanics, Hohai University, No.1 XiKang Road, Nanjing, Jiangsu 210098, China. Tel.: +86 13621586259.
E-mail address: sunhongguang08@gmail.com (H. Sun).

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depend on the time evolution, space variation or even system parameters [10]. In recent years, some authors employed the distributed-order (DO) fractional operator to depict the decelerating/accelerating diffusion processes and obtained some valuable results [11,12]. One of the time DO fractional diffusion equations can be stated as follows [12]

$$\int_0^1 p(\beta)[D_t^{\beta} c(x,t)]\mathrm{d}\beta = \frac{\partial^2 c(x,t)}{\partial x^2}, \quad \int_0^1 p(\beta)\mathrm{d}\beta = 1. \tag{1}$$

The DO fractional differential operator was first mentioned by Caputo [13,14] in 1967, and further studied by Bagley [15], Lorenzo [16], Chechkin [17], Diethelm [18], etc. It can precisely depict the long time behavior of the diffusion process. But this kind of models still belong to the CO fractional differential equation models. In addition, we will explain that the DO model is not the ideal tool to depict the decelerating/accelerating diffusion processes.

The fractional calculus has allowed the operations of integration and differentiation to any complex orders. This fact enables us to consider the order of the fractional derivatives to be a function of time, space or some other variables, rather than a constant of arbitrary order [16,19]. Compared with CO fractional systems, the investigation of variable-order (VO) systems has not received much attention. Samko et al. first proposed the concept of VO operator and investigated the mathematical properties of VO integration and differentiation operators of Riemann–Liouville type [20–22]. Lorenzo and Hartley generalized different types of VO fractional operator definitions and made some theoretical studies via the iterative Laplace transform [16]. Coimbra et al. investigated the dynamics and control of nonlinear viscoelasticity oscillator via VO operator [23,24]. Ingman et al. employed the time dependent VO operator to model the viscoelastic deformation process [25,26]. Pedro et al. studied the motion of particles suspended in a viscous fluid with drag force is determined using the VO calculus [27]. Kobelev et al. investigated the statistical and dynamical systems with fixed and variable memories, the fractal dimension of considered system is variable with time and coordinate [28]. However, to the best of the authors' knowledge, the comprehensive investigation of the VO operators in the anomalous diffusion modeling is still not reported in the literature. The only related work is implemented by Chechkin et al. who introduced the space dependent VO derivative into the differential equation of diffusion process in inhomogeneous media with the assumption that the waiting-time probability density function (PDF) is space dependent in the continuous time random walk (CTRW) scheme [9]. Therefore, in this study, we will make an investigation of VO operator in complex anomalous diffusion modeling.

Variable-order differential operator (VODO) model can be employed as a powerful tool in complex anomalous diffusion modeling. For example, VODO is eligible to depict the time dependent diffusion process, the tracer transfer in inhomogeneous medium and the anomalous diffusion in intermediate turbulence. If we consider the anomalous diffusion processes in oscillating external field, the VODO will also be a promising approach [29]. Moreover, we believe that the VODO is the more suitable model to simulate the generalized decelerating/accelerating diffusion processes.

The main structure of the paper is organized as follows: In Section 2, four different types of VODO models in anomalous diffusion modeling are presented, and the numerical simulation is taken to demonstrate diffusion properties of such systems. We further state and discuss our findings in Section 3. Finally, we end up this paper by some remarks in Section 4.

2. Variable-order time-fractional diffusion models

The simple constant fractional differential order anomalous diffusion equation in one dimension can be written as follow

$$\frac{\partial^{\alpha} c(x,t)}{\partial t^{\alpha}} = K\frac{\partial^{\beta} c(x,t)}{\partial^{\beta} x}, \quad 0 < \alpha \le 1, 1 < \beta \le 2, \tag{2}$$

where K is the diffusion coefficient, $c(x, t)$ represents the concentration or probability density function of particle [30].

However, this simple model is inapplicable when encountering the more complex diffusion process, hence we prefer the novel approach of VODO model instead. Considering different situations of diffusion process, we classify the VODO models into four different types: time dependent, space dependent, concentration dependent and system parameter dependent models. For simplicity, in this study we focus on the time-fractional diffusion equation.

2.1. Time dependent variable-order model

In many diffusion phenomena, the diffusion behavior changes with the time evolution. Particularly, it becomes more Fickian with the time in some diffusion processes (from anomalous diffusion to normal diffusion) [31,32]. This kind of phenomena extensively exist in experimental measurements of various fields, such as biophysics, plasma physics, and econophysics [33]. In addition, still in some diffusion processes the diffusion rate decreases with the time climbing (from normal diffusion to sub-diffusion). From the traditional viewpoints, most scholars are apt to integer order derivative equations associated with time dependent diffusion coefficient to simulate the time dependent diffusion process [34,35]. However, we believe this approach does not capture the origin of the problems. Though in some special experimental cases, this method can provide a good data fitting, it cannot be extended to the general formulation for time dependent diffusion processes. As an alternative approach, the time dependent VO model is the right choice to depict this type of diffusion phenomena.

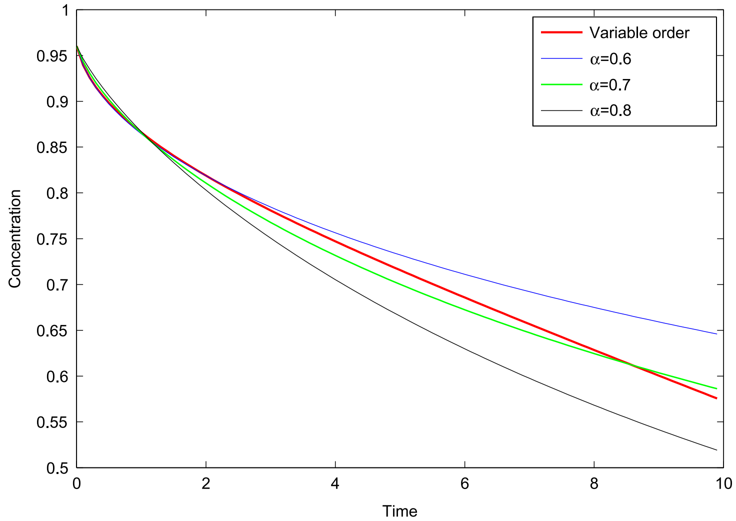

Fig. 1. The diffusion behaviors of time dependent VODO model and constant-order model at $x = 0.6$. The dotted line (blue line in the web version), the dot-dashed line (green line in the web version) and the dashed line (black line in the web version) represent the concentration curve with $\alpha = 0.6$, $\alpha = 0.7$ and $\alpha = 0.8$. The solid line (red line in the web version) represents the concentration evolution curve with VO function in (7).

There are several definitions of the VODO [36]. Here we adopt the definition of the VODO suggested by Coimbra [23],

$$D_t^{\alpha(t)} f(t) = \frac{1}{\Gamma(1-\alpha(t))} \int_{0+}^{t} \frac{f'(\tau)\mathrm{d}\tau}{(t-\tau)^{\alpha(t)}} + \frac{(f(0+)-f(0-))t^{-\alpha(t)}}{\Gamma(1-\alpha(t))}, \quad 0 < \alpha(t) < 1. \tag{3}$$

Different from other definitions in mathematics, this definition only needs the initial condition with integer derivative orders which can be easily used in physical field. Moreover, if $\alpha(t)$ is a constant, it can be reduced to the constant-order Caputo definition [23]. This definition means that the memory rate of system changes with time and is determined by the current time instant. It looks as if we have different memory abilities in the different time periods. The time-fractional diffusion equation which employs this definition can be stated as

$$D_t^{\alpha(t)} c(x,t) = K \frac{\partial^2 c(x,t)}{\partial x^2}, \quad 0 < \alpha(t) < 1. \tag{4}$$

Furthermore, we can consider the derivative order having the memory of its history, then the order of $\alpha(t)$ should be changed into $\alpha(t, \tau)$. The definition which accounts for this property can be stated as follows [26]

$$_{*}D_t^{\alpha(t)} f(t) = \frac{d}{dt} \int_0^t \frac{(t-\tau)^{\alpha(t-\tau)}}{\Gamma[1-\alpha(t-\tau)]} f(t-\tau)\mathrm{d}\tau, \quad 0 < \alpha(t) < 1. \tag{5}$$

One of the important characteristics of this operator is the behavior in which the operator accounts for the order memory. Two types of memories are attributed to the operator, the first is the fading memory of the whole operator, and the second is the memory involving the derivative order history [16]. The main difference between (3) and (5) is that the VO has no memory of past orders in the first definition, but the second one has the memory of its order history.

For simplicity, we will concentrate our attention on the first definition (3). To further illustrate the behavior of this model, we consider the following diffusion equation

$$\begin{cases} D_t^{\alpha(t)} c(x,t) = K \dfrac{\partial^2 c(x,t)}{\partial x^2}, & 0 < x < L, \\ c(x,0) = \sin\left(\dfrac{x\pi}{L}\right), & 0 \le x \le L, \\ c(0,t) = c(L,t) = 0, & t > 0. \end{cases} \tag{6}$$

In the above, $0 < \alpha(t) < 1$ is the VO defined by (3). Assuming $L = 10$, $K = 1.0$, and $\alpha(t)$ has the following expression

$$\alpha(t) = \alpha_0 + p \frac{t}{T_{\max}}, \tag{7}$$

where p is the proportional parameter, $T_{\max}$ is the measured time length and $\alpha_0 = 0.6$. Employing the Crank–Nicholson scheme [37], we can get the diffusion curve of the VODO model with $p = 0.2$ shown in the Fig. 1. The stability and accuracy of this scheme can be verified by the techniques in the [38–40].

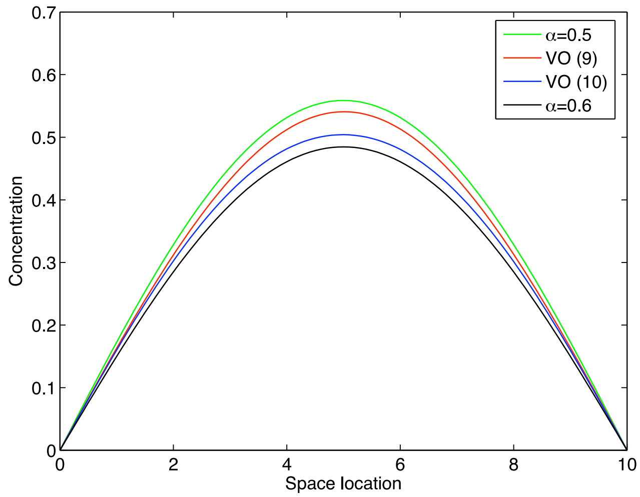

Fig. 2. The comparison of two types of space dependent VO models and CO model at $t = 10$. The dotted line (green line in the web version) and the dashed line (black line in the web version) represent the concentration curves with $\alpha = 0.5$ and $\alpha = 0.6$; the solid line (red line in the web version) and the dot-dashed line (blue line in the web version) represent the concentration curve with VO functions in (9) and (10).

From the Fig. 1, we can observe that the diffusion behavior of VODO model shifts from $\alpha = 0.6$ to $\alpha = 0.8$. It means that this model can depict the diffusion process which exhibits accelerating sub-diffusion. With other forms of the VO function $\alpha(t)$, one can also depict the decelerating sub-diffusion, decelerating/accelerating super-diffusion or other anomalous diffusion processes.

2.2. Space dependent variable-order model

Anomalous diffusion in complex medium is a rapidly growing issue of scientific research which is very important in various fields of science and engineering applications including geophysics, environmental science, hydrology, biological systems and protein dynamics [41]. Some typical examples include heat conduction and fluid flow in porous media, propagation of seismic waves. Therefore, the investigations of diffusion behavior in porous media especially in the inhomogeneous or anisotropic medium are of fundamental significance. This type of diffusion is currently modeled by nonlinearity to statistical mechanics and memory formalisms [42].

In the homogeneous medium, the CO diffusion model is efficient. But in the complex medium, the heterogeneities of the medium cause variations of permeability in different spatial positions. In this situation, the space dependent VO model is the eligible approach which can correctly describe location dependent diffusion processes. The space dependent time derivative term represents the memory rate depending on the space location in the considered diffusion system. The similar cases are corresponding to the space dependent waiting time PDF in the CTRW model. The definition of the space dependent VO derivative can be derived by replacing $\alpha(t)$ with $\alpha(x)$ in (3), consequently, one can obtain the following diffusion equation

$$D_t^{\alpha(x)} c(x,t) = K \frac{\partial^2 c(x,t)}{\partial x^2}, \quad 0 < \alpha(x) < 1. \tag{8}$$

In order to further interpret the space dependent VODO model and show the difference between the VO model and CO model, we adopt two types of order functions

$$\alpha_1(x) = \alpha_0 + \left| \beta \left(\frac{x}{L} - 0.5 \right) \right|, \tag{9}$$

$$\alpha_2(x) = \begin{cases} \alpha_0 + \beta \dfrac{x}{L}, & 0 < x < L/2, \\ \alpha_0 + \beta \left(1 - \dfrac{x}{L} \right), & L/2 \le x < L. \end{cases} \tag{10}$$

Assuming the same initial and boundary conditions, parameter value with the Eq. (6) and $\beta = 0.2$, $\alpha_0 = 0.5$, we can obtain the concentration curve in Fig. 2.

From Fig. 2, we observe that if the derivative order is bigger in the spatial location where exactly is the high concentration domain, the diffusion behavior is more notable.

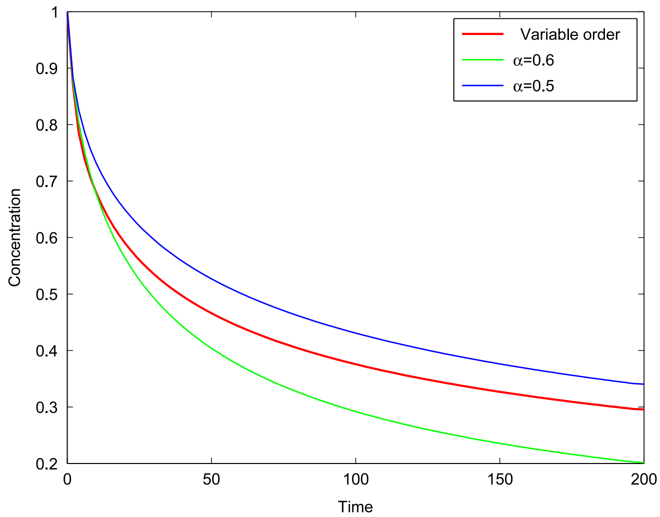

Fig. 3. The diffusion behaviors of concentration dependent VODO model and CO model at $x = 0.5$. The dashed line (blue line in the web version) and the dotted line (green line in the web version) represent the concentration curve with $\alpha = 0.5$ and $\alpha = 0.6$; the solid line (red line in the web version) represents the concentration evolution curve with VO function in (12).

2.3. Concentration dependent variable-order model

In some physical, chemical and biological diffusion processes, the concentration plays a dominating role in deciding the diffusion pattern [43]. For instance, the diffusion and transport of macromolecules (such as protein, medicine) in biological tissues; the diffusion process related to the chemical reaction, the concentration of the reactant will shape the main characteristics of the chemical diffusion process. Therefore, the study of the concentration dependent diffusion process is of great significance in anomalous diffusion modeling.

Concentration dependent diffusion processes have attracted much attention in statistical physics and chemical field. In traditional approaches, the researchers usually adopt the nonlinear or variable coefficient partial differential equations. Blackband and Mansfield explored an expression of the concentration dependent diffusion coefficient via nuclear magnetic resonance (NMR) imaging method [44]. De Azevedo et al. investigated the time-fractional diffusion equation with concentration dependent diffusion coefficient [45]. However, this type of model is hard for analysis, and even harder for numerical simulation of real engineering applications. Because the diffusion coefficient function usually contains several free parameters which cannot be obtained from physical analysis or experimental measurement [46]. As an alternative approach, the concentration dependent diffusion process can be considered as the diffusion system in which the memory rate changes with the concentration. A concentration dependent time derivative α can capture the complexity that would otherwise be coded by a complex concentration dependent K. It enable us to employ the concentration dependent VO equation model to handle this special type of diffusion processes

$$D_t^{\alpha[c(x,t)]} c(x,t) = K \frac{\partial^2 c(x,t)}{\partial x^2}, \quad 0 < \alpha[c(x,t)] < 1. \tag{11}$$

In the above equation, the definition of the concentration dependent VO derivative can be derived by replacing $\alpha(t)$ with $\alpha[c(x,t)]$ in (3). To investigate the behavior of the new model, one adopts the VO function as follows

$$\alpha[c(x,t)] = \alpha_0 + p \frac{c(x,t)}{C_{\max}}. \tag{12}$$

Assuming the same initial and boundary conditions, parameter values with the Eq. (6) and $p = 0.1$, $\alpha_0 = 0.5$, we can obtain the concentration curve in Fig. 3 which accounts for the decelerating sub-diffusion process. It means that the diffusion behavior, which is close to some real-world diffusion processes, will become more and more slow with concentration descending.

2.4. System parameter dependent variable-order model

In many real-world diffusion processes, the system parameter may change with time and space. For example, when we consider the anomalous diffusion in the turbulence, because it is a dissipative system, the Reynolds number *Re* determines the diffusion pattern especially in the laminar–turbulent transition. The similar situation happens in the transport of passive tracers carried by fluid flow in porous medium or in the transmission medium with fractal structure. The fractal dimension *D* or the Hurst number *H* changes with time or space in its transport process. Still in the heat conduction, electron transfer or pollutant transplant, the changes of the temperature, external force field or other system parameters will remodel the system behavior [47]. Finally, the behavior of these diffusion or transport processes in response to system parameter changes can be better described using VO elements rather than time or space varying coefficients. Some applications of fractional operator also imply that the derivative order perhaps is not a constant, but a function of system parameters [27].

We can simply employ the following equation to depict this type of diffusion behavior

$$D_t^{\alpha[f(x,t)]}c(x,t) = K\frac{\partial^2 c(x,t)}{\partial x^2}, \quad 0 < \alpha[f(x,t)] < 1. \tag{13}$$

In the above, the function $f(x,t)$ could be $Re(x,t)$, $H(x,t)$, $D(x,t)$ or other independent functions.

If the considered diffusion or transport system is interfered by some noises (e.g. oscillating external field or unstable system parameters), these noises inevitably cause the fluctuation of the whole system. The behaviors of system will show deviations from the CO fractional differential model pattern. In these cases, the random-order (e.g. $\alpha(x,t) = \alpha_0 + \epsilon_{x,t}$, $\epsilon_{x,t}$ is small random variable) time differential operator model may be the more physically appropriate approach [48].

3. Discussions

Different forms of the VO fractional equations can be used to properly characterize different real-world diffusion processes. For example, the diffusion models with the time dependent VO derivative can better describe the diffusion processes whenever they get more anomalous or more Fickian in the course of time. Similarly the diffusion models involving the space dependent VO derivative can properly describe the situations in which the diffusion rate is variable with the space location. In addition, the concentration and system parameter dependent VO models can properly depict some special diffusion processes which may exhibit significantly diverse anomalous behaviors.

The VODO model can serve as an effective mathematical framework for the description of various real-world anomalous diffusion processes in transitional regimes or other particular situations. It can exhibit certain special features of some physical processes which remain unnoticed in other models. However, the mathematical foundations of VO operator are still immature; the theoretical analysis and numerical schemes for VO operator are still incipient [49]. On the other hand, though the applications of VODO model have been reported in several fields, it is clear that there are still considerable potential physical applications that motivate further development and implementation of VO operators.

The classification of VODO model is not unique and we only considered the VO model involving time derivative. The VO may be attributed to the variation in the space differential terms which is left as our further research effort.

4. Conclusion

The main message of this paper is that various complex anomalous diffusion processes can be depicted by the VODO model. In addition, the VODO model is classified into four types: time dependent, space dependent, concentration dependent and system parameter dependent models.

Our further investigations include the statistical mechanism corresponding to the appearance of VO fractional derivative in the fractional diffusion models. Specifically, we will look into the continuous time random walk (CTRW) frameworks with the time dependent waiting-time probability density functions (PDF) or time (or space) dependent jump length PDFs.

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