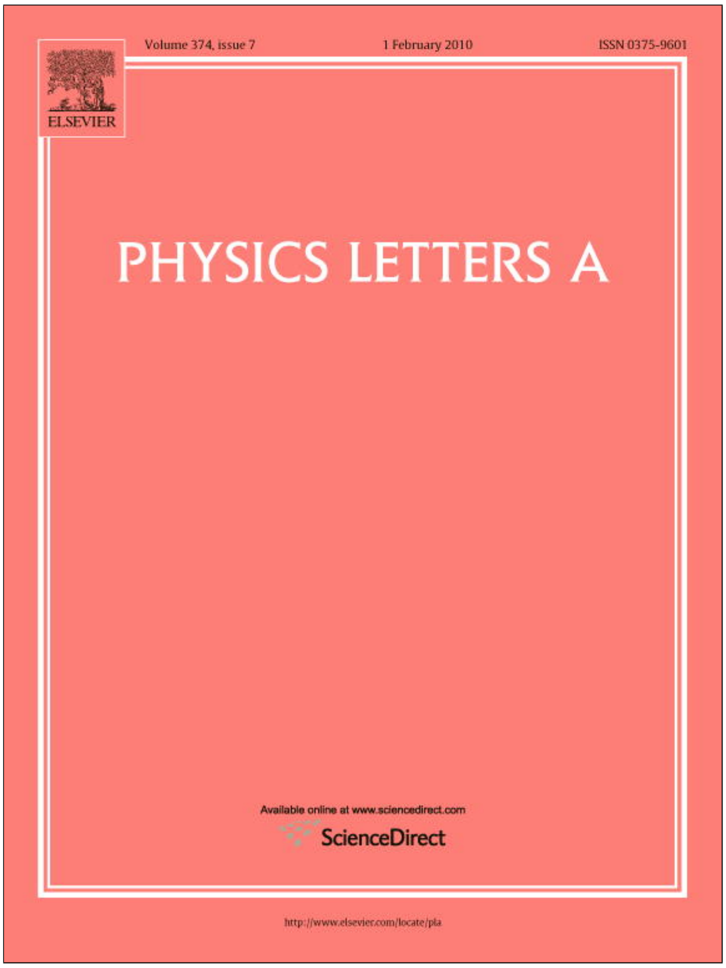
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On mean square displacement behaviors of anomalous diffusions with variable and random orders

HongGuang Sun [a,c,*], Wen Chen [a], Hu Sheng [b,c], YangQuan Chen [c]

[a] Institute of Soft Matter Mechanics, Department of Engineering Mechanics, Hohai University, No. 1 XiKang Road, Nanjing, Jiangsu 210098, China
[b] Department of Electronic Engineering, Dalian University of Technology, Dalian 116024, China
[c] 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

Mean square displacement (MSD) is used to characterize anomalous diffusion. Recently, models of anomalous diffusion with variable-order and random-order were proposed, but no MSD analysis has been given so far. The purpose of this Letter is to offer a concise derivation of MSD functions for the variable-order model and the random-order model. Numerical results are presented to illustrate the analytical results. In addition, we show how to establish a variable-random-order model for a given MSD function which has clear application potentials.

1. Introduction

Anomalous diffusion and its related phenomena have been observed in various physical fields, such as tracer transfer in underground water, dispersive transports in amorphous semiconductors, seepage in soil or rocks, turbulence, etc. [1–4]. The features of anomalous diffusion include history dependence, long-range correlation and heavy tail characteristics [5,6]. These features can be accommodated well by using fractional calculus as shown, e.g. in [6,7], where the fractional calculus is used to characterize the phenomena having the properties of long memory and spatial nonlocality. It is not surprising that fractional diffusion equations have been widely used to depict and simulate anomalous diffusion processes [7–9].

In order to deal with the diffusion processes in which the diffusion behaviors depend on time evolution, space variation or system parameters, the variable-order diffusion models were proposed [10–13]. The concept of variable-order operator was first introduced by Samko in 1993 [14] and has received much attention in the fields of viscoelasticity [15], viscoelastic deformation [16], viscous fluid [17], etc. Nowadays, it has been employed as a powerful tool in complex anomalous diffusion modeling. In addition, to depict the diffusion processes under oscillating external field, we contributed a random-order diffusion model [18]. However, the distinguishing advantages and features of two models, i.e., the variable-order model and the random-order model in anomalous diffusion modeling are still unclear and require further research investigation.

Mean square displacement (MSD) is well known as an important tool to characterize anomalous diffusion processes [19–21]. Many properties of anomalous diffusion can be explored by the analysis of MSD. The constant-order fractional diffusion equations are widely used to describe anomalous diffusion processes where the characteristic displacement scales as a constant power of time $\langle x^2(t)\rangle \propto t^{\alpha}$, where α is a constant. In this study, we investigate the MSD behaviors for variable-order and random-order diffusion models. Moreover, we propose a new time fractional diffusion model with clear application potentials. The new model integrates the advantages of variable-order and random-order diffusion models.

The main structure of the Letter is as follows: In Section 2, definitions and properties of variable-order and random-order operators are presented. The derivations and further discussions about the MSDs of variable-order and random-order time fractional diffu-

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

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sion models are given in Section 3. This Letter ends up with some remarks in the last section.

2. Definitions and properties of variable-order and random-order operators

Here we just recall the most typical definitions which are easy-to-use in physics. The Caputo-type variable-order derivative definition suggested by Coimbra is stated as follows [15],

$$ {}^C D_0^{\alpha(t)} f(t) = \frac{1}{\Gamma(1-\alpha(t))} \int_{0_+}^{t} \frac{f'(\tau)\,d\tau}{(t-\tau)^{\alpha(t)}} + \frac{(f(0_+) - f(0_-))t^{-\alpha(t)}}{\Gamma(1-\alpha(t))}, \quad 0 < \alpha(t) < 1. \tag{1} $$

For the sake of simplicity, assuming the property of function $f(t)$ at $t = 0$ is good enough, then we can state the following Caputo-type definition

$$ {}^C D_{0+}^{\alpha(t)} f(t) = \frac{1}{\Gamma(1-\alpha(t))} \int_{0}^{t} \frac{f'(\tau)\,d\tau}{(t-\tau)^{\alpha(t)}}, \quad 0 < \alpha(t) < 1. \tag{2} $$

The Riemann–Liouville-type variable-order definition in which the differential order has memory of itself [16,22], is seldomly used, so it is not discussed here.

The definition of variable-order integration proposed by Samko is presented as below [14,23]

$$ I_{0+}^{\alpha(t)} f(t) = \frac{1}{\Gamma(\alpha(t))} \int_{0}^{t} (t-\tau)^{\alpha(t)-1} f(\tau)\,d\tau, $$
$$ \mathrm{Re}\big(\alpha(t)\big) > 0. \tag{3} $$

The definition of the Caputo-type random-order derivative is stated as follows

$$ D_{0+}^{\alpha_0+\epsilon_t} f(t) = \frac{1}{\Gamma(1-\alpha_0-\epsilon_t)} \int_{0}^{t} \frac{f'(\tau)\,d\tau}{(t-\tau)^{\alpha_0+\epsilon_t}}, $$
$$ p(\epsilon_t \mid 0 < \alpha_0 + \epsilon_t \leqslant 1) = 1, \tag{4} $$

where $p(.)$ denotes probability density function. In this definition, we should emphasize that the noise term can be represented in two different types: the first is independent with time, that is, the noise term has no relation with time evolution; the second is dependent with time, which means different time instants correspond to different types of noises. The definition of random-order integration can be obtained via replacing $\alpha(t)$ by $\alpha_0 + \epsilon_t$ in (3).

Then, we present following properties for the above definitions which will be used in the next section.

Properties.

(1) $ {}^C D_{0_+}^{\alpha(t)} t^\beta = \dfrac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha(t)+1)} t^{\beta-\alpha(t)}, \quad 0 < \alpha(t) < 1.$

(2) $ I_{0_+}^{\alpha(t)}\big({}^C D_{0_+}^{\alpha(t)} f(t)\big) = f(t) - f(0), \quad 0 < \alpha(t) < 1.$

Proof. (1) By using the definition of Caputo-type fractional derivative (2), one can get

$$ {}^C D_{0_+}^{\alpha(t)} t^\beta = \frac{1}{\Gamma(1-\alpha(t))} \int_0^t (t-\tau)^{-\alpha(t)} \big(\tau^\beta\big)'\,d\tau $$
$$ = \frac{\beta}{\Gamma(1-\alpha(t))} \int_0^t (t-\tau)^{-\alpha(t)} \tau^{\beta-1}\,d\tau $$

Let $\tau = \varepsilon t$, according to the definition of beta function [24], we can get

$$ {}^C D_{0_+}^{\alpha(t)} t^\beta = \frac{\beta t^{\beta-\alpha(t)}}{\Gamma(1-\alpha(t))} \int_0^1 (1-\varepsilon)^{-\alpha(t)} \varepsilon^{\beta-1}\,d\varepsilon $$
$$ = \frac{B(1-\alpha(t),\beta)}{\Gamma(1-\alpha(t))} t^{\beta-\alpha(t)} $$
$$ = \frac{\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha(t))} t^{\beta-\alpha(t)}, \tag{5} $$

where B is the beta function which is defined as follows

$$ B(z,\nu) = \int_0^1 \tau^{z-1}(1-\tau)^{\nu-1}\,d\tau \quad \big(\mathrm{Re}(z) > 0, \mathrm{Re}(\nu) > 0\big). \tag{6} $$

(2) By using the property of Caputo-type definition, we can get

$$ I_{0_+}^{\alpha(t)}\big({}^C D_{0_+}^{\alpha(t)} f(t)\big) = I_{0_+}^{\alpha(t)}\big(I_{0_+}^{1-\alpha(t)} f'(t)\big) $$
$$ = \int_0^t f'(\tau)\,d\tau = f(t) - f(0). $$

With the similar method, we can prove that the random-order definitions also have the above properties. □

3. Mean square displacement behaviors of time fractional diffusion models

First, we consider the variable-order time fractional diffusion equation

$$ \begin{cases} D_{0_+}^{\alpha(t)} c(x,t) = K \dfrac{\partial^2 c(x,t)}{\partial x^2}, & -\infty < x < +\infty,\ t > 0, \\ c(x,0) = \delta(x), \quad c(\pm\infty,t) = 0, & \dfrac{\partial c(\pm\infty,t)}{\partial x} = 0, \end{cases} \tag{7} $$

where $\delta(x)$ is the Dirac delta function, $0 < \alpha(t) \leqslant 1$ denotes variable-order time fractional derivative, K is a generalized diffusion coefficient, $c(x,t)$ represents concentration of interest.

The primary difficulty to obtain the MSD of the variable-order diffusion process lies in the fact that the Fourier and Laplace transforms of variable-order equation are hard, if not impossible, to perform. Therefore, in this study, we devise the following method to obtain the MSD. First, as in [24,25], we perform integration of Eq. (7) with $\int_{-\infty}^{\infty} x^2\,dx$, which leads to

$$ \int_{-\infty}^{\infty} x^2\, {}^C D_{0_+}^{\alpha(t)} c(x,t)\,dx = \int_{-\infty}^{\infty} x^2 K \frac{\partial^2 c(x,t)}{\partial x^2}\,dx. \tag{8} $$

That is

$$ {}^C D_{0_+}^{\alpha(t)} \langle x^2(t) \rangle = \int_{-\infty}^{\infty} x^2 K \frac{\partial^2 c(x,t)}{\partial x^2}\,dx. \tag{9} $$

Clearly, (9) can be simplified into the following form

$$ {}^C D_{0_+}^{\alpha(t)} \langle x^2(t) \rangle = 2K. \tag{10} $$

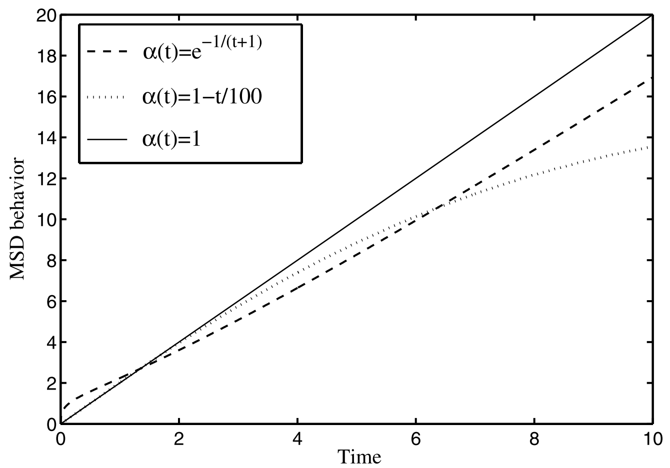

Fig. 1. The MSD behaviors of variable-order time fractional diffusion equation with different variable-order functions, $K = 1$. The solid line represents the MSD behavior with time derivative order $\alpha = 1$. The dashed line denotes MSD behavior with the variable-order function $\alpha(t) = e^{-1/(t+1)}$, it represents the diffusion process shifts from subdiffusion to normal diffusion. The dotted line denotes MSD behavior with the variable-order function $\alpha(t) = 1 - t/100$, it represents the diffusion process shifts from normal diffusion to subdiffusion.

By applying the integration of order $\alpha(t)$ to the both sides of (10), we can get

$$\langle x^2(t)\rangle = \langle x^2(0)\rangle + \frac{1}{\Gamma(\alpha(t))}\int_0^t (t-\tau)^{\alpha(t)-1} K\,d\tau. \tag{11}$$

Since $c(x,0) = \delta(x)$, one can get $\langle x^2(0)\rangle = 0$. Finally, we obtain

$$\langle x^2(t)\rangle = \frac{2Kt^{\alpha(t)}}{\Gamma(\alpha(t)+1)}. \tag{12}$$

From the above expression, we can know that, different with the MSD function of constant-order fractional diffusion model, the exponential term in the right-hand side of (12) is a function of time rather than a constant. In addition, for illustration, we can show different types of MSD behaviors (Fig. 1) for different variable-order functions. The feature shown in Fig. 1 demonstrates that many real-world diffusion or diffusion related processes which exhibit accelerating or decelerating diffusion behaviors can be better depicted by the variable-order fractional diffusion models or advection–diffusion models.

We know that many diffusion processes are usually characterized by the Hurst exponent. The corresponding MSD is usually expressed as $\langle x^2(t)\rangle \propto t^{2H}$, $H \in (0,1)$, when $H = 0.5$ it becomes the MSD represents normal diffusion process. But, in some cases, it cannot be well characterized by a single constant Hurst exponent [25]. From (12), we can observe that it is more reasonable to investigate the diffusion process via a time-dependent Hurst exponent $H(t)$. Thereby, it becomes clear that why we should investigate the fractional Brownian motion with time-dependent Hurst exponent [26,27]. In general, when we investigate the fractional Brownian motion, the Hurst exponent is considered as a constant which satisfies $H \in (0,1)$ and $H \neq 0.5$. However, in some real-world situations, the Hurst exponent usually changes with time, then it is more reasonable to consider the multi-fractional Brownian motion with a function $H(\cdot)$ depending on the time variable t: $X(t) = B(t, H(t))$ [28]. In addition, to deal with the diffusion or diffusion related processes in the disordered medium which have fractal structures, we usually construct the MSD by a function of fractal dimension. But it is difficult to model the diffusion process in which the fractal dimension changes with time [29,30]. In this situation, the variable-order fractional equation model may be a better choice [31].

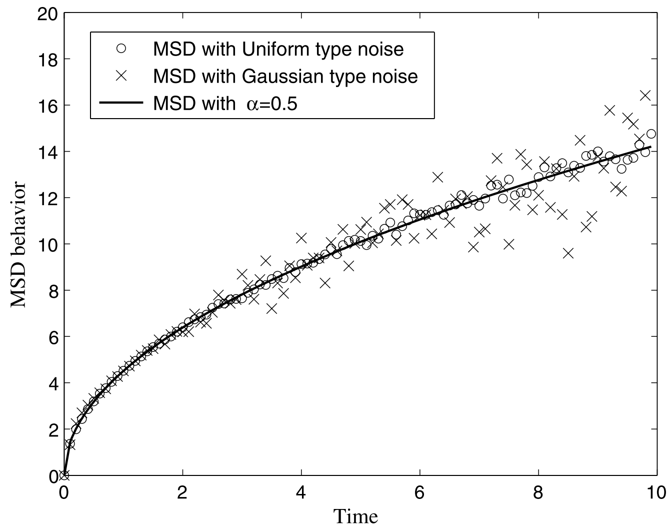

Fig. 2. The MSD of the time fractional diffusion equation with derivative order includes Uniform or Gaussian-type noises. Uniform-type noise: $\xi = \gamma_1(u - 0.5)$, $\gamma_1 = 0.04$, and $u \in (0,1)$, is a uniform random number. Gaussian-type noise: $\xi = 2\gamma_2\sqrt{-\ln u_1}\sin\phi$, where $\phi = \pi(u_2 - 1/2)$, and $u_1, u_2 \in (0,1)$ are uniform random numbers, $\gamma_2 = 0.04$ is scale parameter.

Moreover, in addition to MSD, we can look into the general expression of n-order displacement of the variable-order time fractional diffusion equation model, which can be stated as

$$\langle x^{2n}(t)\rangle = (2n)!\frac{Kt^{n\alpha(t)}}{\Gamma(1+n\alpha(t))}, \quad n \in Z^+. \tag{13}$$

Next, we investigate the MSD behavior of random-order time fractional diffusion equation model. The master equation can be stated as

$$\begin{cases} \dfrac{\partial^{\alpha_0+\epsilon_t} c(x,t)}{\partial t^{\alpha_0+\epsilon_t}} = K\dfrac{\partial^2 c(x,t)}{\partial x^2}, \\ p(\epsilon_t \mid 0 < \alpha_0 + \epsilon_t < 1) = 1, \quad t > 0, \\ c(x,0) = \delta(x), \quad c(\pm\infty, t) = 0, \quad \dfrac{\partial c(\pm\infty, t)}{\partial x} = 0, \end{cases} \tag{14}$$

where $p(.)$ denotes probability density function. In the above equation, we assume that the noise is random with time evolution but independent with the time. It means that the memory rate at every time instant is independent. For example, the system memory rate in this situation jumps from $\alpha_0 + \epsilon_{t_1}$ to $\alpha_0 + \epsilon_{t_2}$ then to $\alpha_0 + \epsilon_{t_3}$, and so on.

The mean square displacement can be obtained by integration of (14) with $\int_{-\infty}^{\infty} x^2\,dx$, which leads to

$${}_C D_0^{\alpha_0+\epsilon_t}\langle x^2(t)\rangle = \int_{-\infty}^{\infty} x^2 K\frac{\partial^2 c(x,t)}{\partial x^2}\,dx. \tag{15}$$

Then, we can get

$${}_C D_0^{\alpha_0+\epsilon_t}\langle x^2(t)\rangle = 2K, \tag{16}$$

and hence,

$$\langle x^2(t)\rangle = \langle x^2(0)\rangle + \frac{1}{\Gamma(\alpha_0+\epsilon_t)}\int_0^t (t-\tau)^{\alpha_0+\epsilon_t-1} K\,d\tau. \tag{17}$$

Finally, we get

$$\langle x^2(t)\rangle = \frac{2Kt^{\alpha_0+\epsilon_t}}{\Gamma(\alpha_0+\epsilon_t+1)}. \tag{18}$$

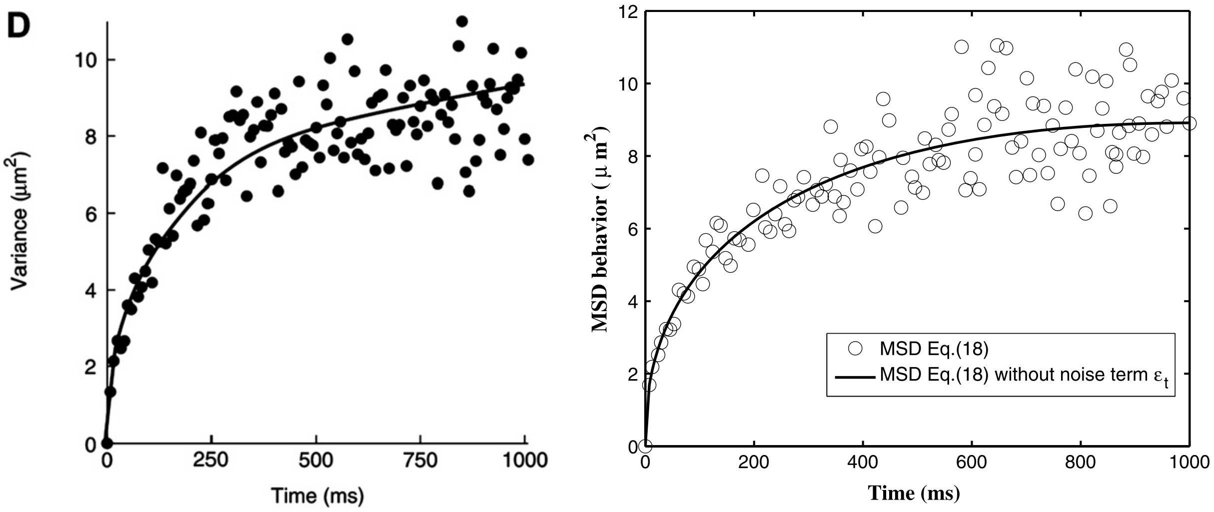

Fig. 3. Left: The MSD of calcium ions diffusion in dendrites presented in Ref. [30]. Right: The best fitting result using (19). Solid line: $\langle x^2(t)\rangle = 2 * 0.33t^{0.41-t/20000}/\Gamma(0.41 - t/20000 + 1)$. Circle: $\langle x^2(t)\rangle = 2 * 0.33t^{0.41-t/20000+\epsilon_t}/\Gamma(0.41 - t/20000 + \epsilon_t + 1)$, ϵ_t obeys Gaussian distribution with 0 mean and the variance of 0.019.

Clearly, the popular MSD behavior of constant-order fractional model is changed in random-order diffusion system. The MSD in (18) has a more complex relationship with a random exponential term. For illustration purpose, assuming $K = 1$, we study two types of noises: the first one is uniform distribution noise and the second one is the Gaussian-type noise. Then we can draw the MSD curves in Fig. 2. From Fig. 2, as expected, we find that the Gaussian-type noise causes more fluctuations than uniform type noise even with the same scale parameter. Meanwhile, system fluctuations increase with the time evolution for both types of noises.

Putting together, we can consider the MSD function in (12) or (18) having the time-dependent order $\alpha(t)$ and the noise term ϵ_t. The MSD function corresponding to this combined case has the following form

$$\langle x^2(t)\rangle = \frac{2Kt^{\alpha(t)+\epsilon_t}}{\Gamma(\alpha(t)+\epsilon_t+1)}. \tag{19}$$

The new type of MSD behavior especially exists in chemical-physics and biophysical fields [30,32]. For example, in Ref. [30], the authors investigated the diffusion behavior of calcium ions (Ca^{2+}) within dendrites. If we only consider diffusion behavior in this process, we can observe obvious fluctuation feature of the considered diffusion process from Fig. 3 (left). In addition, the authors in Ref. [30] also stated that the diffusion pattern changes with time evolution which implies that the exponential term in the right-hand side of (19) should be a function of time. So we can fit this experimental data using (19). From our data fitting, the best MSD curve is shown in Fig. 3 (right). The comparison of experimental data and fitting result prompts us that this specific diffusion process studied in Ref. [30] can be much better characterized by (19).

Now, let us turn to the discussion of the fractional order equation model corresponding to (19). Generally speaking, there are several types of fractional diffusion models and advection–diffusion models which could yield the MSD in the form of (19). Here, we just give the corresponding time fractional diffusion model. From the derivation processes of the variable-order model and the random-order model, we can obtain the following master equation corresponding to (19)

$$\begin{cases} \dfrac{\partial^{\alpha(t)+\epsilon_t}c(x,t)}{\partial t^{\alpha(t)+\epsilon_t}} = K\dfrac{\partial^2 c(x,t)}{\partial x^2}, \\ p(\epsilon_t \mid 0 < \alpha(t)+\epsilon_t < 1) = 1, \quad t > 0, \\ c(x,0) = \delta(x), \quad c(\pm\infty,t) = 0, \quad \dfrac{\partial c(\pm\infty,t)}{\partial x} = 0, \end{cases} \tag{20}$$

where again $p(.)$ denotes probability density function.

Because the time derivative order includes both the time variable term and the random noise term in this model, we name this model as variable–random-order time fractional diffusion equation model which has combined the advantages of variable-order model and random-order model. Hereby, it provides us with a new modeling approach when we deal with complex real-world diffusion processes which may change over time and may subject to fluctuating noise.

4. Conclusions

Variable-order and random-order fractional diffusion models are the improved forms of constant-order fractional diffusion models. The advantages and characteristics of these two new models have attracted much attention by researchers. Since the MSD behavior is a basic aspect to characterize anomalous diffusion, we made a brief investigation about MSD for the two new models. From the analysis and numerical simulation of MSD behaviors of these two models, we have known that the variable-order model is powerful in depicting the time-dependent anomalous diffusion, and the random-order model is able to characterize the effect of fluctuating noise in the diffusion process. Furthermore, the variable-random-order diffusion model may be more powerful in tackling the real-world diffusion process as demonstrated by restudying the diffusion MSD data in [30], which is practically interesting.

In this study, we have studied the MSD behaviors of variable-order and random-order time fractional diffusion models. The future research work will focus on the MSD behaviors of variable-order spatiotemporal fractional diffusion equation models and their practical applications.

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