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Time fractional derivative model with Mittag-Leffler function kernel for describing anomalous diffusion: Analytical solution in bounded-domain and model comparison

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ABSTRACT

Non-Fickian or anomalous diffusion had been well documented in material transport through heterogeneous systems at all scales, whose dynamics can be quantified by the time fractional derivative equations (fDEs). While analytical or numerical solutions have been developed for the standard time fDE in bounded domains, the standard time fDE suffers from the singularity issue due to its power-law function kernel. This study aimed at deriving the analytical solutions for the time fDE models with a modified kernel in bounded domains. The Mittag-Leffler function was selected as the alternate kernel to improve the standard power-law function in defining the time fractional derivative, which was known to be able to overcome the singularity issue of the standard fractional derivative. Results showed that the method of variable separation can be applied to derive the analytical solution for various time fDEs with absorbing and/or reflecting boundary conditions. Finally, numerical examples with detailed comparison for fDEs with different kernels showed that the models and solutions obtained by this study can capture anomalous diffusion in bounded domains.

1. Introduction

Fractional calculus, which is a linear integral differential operator developed by Riemann, Liouville, Caputo, Riesz, and others [1,2], generalizes the integer-order derivative to an arbitrary order [3]. Fractional diffusion equations (fDEs) or fractional advection–diffusion equations (fADEs) built upon fractional calculus can characterize anomalous or non-Fickian transport, and various methods have been developed to solve the fractional-derivative equations analytically or numerically. For example, Wyss [4] solved the fDEs in the closed form of Fox functions. Metzler and Klafter [5] considered the fDE with absorbing and reflecting boundaries using the method of variable separation. Agrawal [6] obtained a general solution for a fractional diffusion-wave equation defined in a bounded domain in space using the finite sine transform technique. Mainardi et al. [7] interpreted the related Green function as the fundamental solution for the fDEs, and then revisited the Cauchy problem for the time-fractional diffusion equation [8]. The fundamental solutions were solved using the Fourier–Laplace transform, which was the function of the Wright-type. Huang and Liu [9] derived the solution of the fADE in a half-space. Povstenko [10,11] obtained the fundamental solution to the nonhomogeneous space–time-fractional telegraph equation and the generalized Cattaneo-type telegraph equations with Caputo time fractional derivatives, respectively. Povstenko [12] presented the solutions to the time fractional diffusion-wave equations in bounded domains. Various numerical solutions have also been developed for the fDE and fADE with the absorbing or reflecting boundary [13–17]. Most of the solutions mentioned above have been successfully applied to a variety of real-world problems [18–23].

From the point of view of mathematics, the reason that the fDE or fADE can characterize anomalous transport is related to the power-law function used as the kernel of the fractional operator. This definition, however, leads to the well-known singularity problem of the fractional-derivative models, challenging their numerical solution and real-world applications. New definition of the kernel was therefore developed recently. For example, Caputo and Fabrizio [24] applied a non-singular exponential function kernel to replace the singular power-law function kernel. Further studies of this relatively new derivative were reviewed in literature [25–27], and the numerical solution was given in [28]. Sun et al.

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[29] developed a stretched exponential kernel, and then presented the numerical solution for the corresponding relaxation models. Atangana and Baleanu [30] proposed another non-singular kernel function of fractional calculus, using the Mittag-Leffler (M-L) function as the kernel. Atangana and Koca [31] and Baleanu and Fernandez [32] revisited the definition and investigated properties of the resultant fractional derivative, including the analytical solution for the related ordinary partial-differential equation. Tateishi et al. [33] solved the Cauchy problem in an infinite domain, and compared the solution for the fDEs with the power-law, exponential, and M-L function kernels. Yang et al. [37] proposed a new fractional diffusion equation with the extended Mittag-Leffler function kernel. These studies motivated us to select the promising M-L function as the kernel for the fDE and fADE models, and then derive the analytical solutions which are not available yet.

This work first revisits the M-L function kernel derivatives and reviews their properties in Section 2. In Section 3, the analytical solutions are derived for the fDEs and fADEs defined in a bounded domain (i.e., with the absorbing and/or reflecting boundary conditions). In Section 4, examples are used to explore characteristics of the density profiles with different fractional orders in the fractional-derivative model. We also compare the solution, especially the mean square displacement, of the improved fractional-derivative model with the standard model with a power-law function kernel. Analytical solutions for the fractional-derivative models with different kernels are then distinguished in Section 5. Conclusions are finally drawn in Section 6.

2. Mittag-Leffler (M-L) function

The one- and two-parameter Mittag-Leffler functions can be written as

$$\begin{cases} E_\alpha(-t^\alpha) = \sum_{k=0}^{\infty} \frac{(-t)^{\alpha k}}{\Gamma(\alpha k+1)}, \\ E_{\alpha,\beta}(-t^\alpha) = \sum_{k=0}^{\infty} \frac{(-t)^{\alpha k}}{\Gamma(\alpha k+\beta)}, \end{cases} \tag{1}$$

respectively. Some important properties of (1) which are needed in deriving the analytical solution of the time fDE in the following, including the M-L function of $x, \lambda t^\alpha$, and the Laplace transform of $t^{\beta-1}E_{\alpha,\beta}(-\lambda t^\alpha)$, are shown below (for detailed derivations, see [34]):

$$\begin{cases} E_1(x) = e^x, \\ {}_0^C D_t^\alpha E_\alpha(\lambda t^\alpha) = \lambda E_\alpha(\lambda t^\alpha), \\ L\left[t^{\beta-1}E_{\alpha,\beta}(-\lambda t^\alpha)\right] = \frac{s^{\alpha-\beta}}{s^\alpha+\lambda}, \mathrm{Re}(s) > |\lambda|^{\frac{1}{\alpha}}. \end{cases} \tag{2}$$

The fractional derivative with the M-L function kernel is defined as:

$$\begin{cases} {}_a^{ABC}D_t^\alpha f(t) = \frac{B(\alpha)}{1-\alpha}\int_a^t \frac{df(\tau)}{d\tau} E_\alpha\left[-\alpha\frac{(t-\tau)^\alpha}{1-\alpha}\right]d\tau, \\ {}_a^{ABR}D_t^\alpha f(t) = \frac{B(\alpha)}{1-\alpha}\frac{d}{dt}\int_a^t f(\tau)E_\alpha\left[-\alpha\frac{(t-\tau)^\alpha}{1-\alpha}\right]d\tau, \end{cases} \tag{3}$$

where the superscript "ABC" denotes the Atangana and Baleanu definition of the Caputo fractional derivative, "ABR" denotes the Atangana and Baleanu definition of the Riemann-Liouville fractional derivative [32], the index α denotes the order of the time fractional derivative, $B(\alpha)$ is a function used for normalization, and $E_\alpha(\cdot)$ denotes the single-parameter M-L function. Here the Caputo representation makes a huge advantage since it allows the traditional initial condition to be remained in the governing equation [2]. For example, applying the Laplace transform on both sides of Eq. (3), we obtain

$$L\left[{}_a^{ABC}D_t^\alpha f(t)\right] = \frac{B(\alpha)s^{\alpha-1}\left[s\tilde{f}(s) - f(0)\right]}{(1-\alpha)s^\alpha+\alpha}, \tag{4}$$

where s is the Laplace transform parameter, $\tilde{f}(s)$ is the Laplace transform of $f(t)$, and $f(0)$ defines the initial distribution of $f(t)$. Therefore, we may solve anomalous transport described for example by anomalous diffusion equations or telegraph equations in a finite space domain.

We consider the following time-fractional advection-diffusion equation in a finite domain:

$$\begin{cases} {}_0^{ABC}D_t^\alpha u(x,t) = k\frac{\partial^2 u(x,t)}{\partial x^2}, & 0 \le x \le L, t>0, 0<\alpha\le 1, \\ {}_0^{ABC}D_t^\alpha u(x,t) = -\nu\frac{\partial u(x,t)}{\partial x} + k\frac{\partial^2 u(x,t)}{\partial x^2}, & 0 \le x \le L, t>0, 0<\alpha\le 1, \end{cases} \tag{5}$$

where the density $u(x, t)$ can represent the (normalized) concentration of pollutants in surface water or groundwater; the symbol ${}_0^{ABC}D_t^\alpha$ denotes the fractional operator with the M-L function kernel respecting to t; and ν and k denote the constant drift velocity and the diffusion coefficient, respectively. Eq. (5) reduces to the classical diffusion equation when $\alpha = 1$, as expected.

3. Solutions to the fractional derivative models

In this section, we solve the time fDE and the time fADE in finite domains. Notably, the analytical solution of the fractional-derivative model may change with the boundary condition. The absorbing boundary and reflecting boundary [5,15,35] have been widely used for real-world processes. Therefore, we investigate the analytical solution for the fractional-derivative models with these two boundary conditions and their combination.

3.1. The fDE with two reflecting boundaries

The model with the initial and boundary conditions can be written as:

$$\begin{cases} {}_0^{ABC}D_t^\alpha u(x,t) = k\frac{\partial^2 u(x,t)}{\partial x^2}, & 0 \le x \le L, t>0, 0<\alpha\le 1, \\ u(x,0) = \phi(x), & 0 \le x \le L, \\ u_x(0,t) = u_x(L,t) = 0, & t>0, \end{cases} \tag{6}$$

whose analytical solution can be derived using the method of variable separation. Assuming $u(x,t) = X(x)T(t)$, the resulting equation

$$\frac{{}_0^{ABC}D_t^\alpha T(t)}{kT(t)} = \frac{X''(x)}{X(x)} = -\lambda \tag{7}$$

can be separated into several eigenequations

$$\begin{aligned} &{}_0^{ABC}D_t^\alpha T(t) + \lambda k T(t) = 0, \\ &X''(x) + \lambda X(x) = 0, \quad X'(0) = X'(L) = 0. \end{aligned} \tag{8}$$

Given the zero-value Neumann boundary condition defined in (6), the Sturm-Liouville problem has eigenvalues

$$\lambda_n = \left(\frac{n\pi}{L}\right)^2, \quad n = 0, 1, \ldots \tag{9}$$

and the following eigenfunctions

$$X_n(x) = C_n\cos\frac{n\pi x}{L}, \quad n = 0, 1, \ldots \tag{10}$$

where C_n denotes an arbitrary constant. Given the eigenvalue λ_n, the corresponding temporal eigenfunctions $T(t)$ can be derived using the Laplace transform

$$\hat{T}_n(s) = T_n(0)\frac{\frac{B(\alpha)}{B(\alpha)-A_n+A_n\alpha}s^{\alpha-1}}{s^\alpha - \frac{A_n\alpha}{B(\alpha)-A_n+A_n\alpha}}, \quad n = 1, 2, \ldots, \tag{11}$$