Physica A 447 (2016) 467–481

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Modeling diffusive transport with a fractional derivative without singular kernel

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HIGHLIGHTS

- Fractional calculus is applied to the diffusion and the diffusion–advection equation.
- The Caputo–Fabrizio fractional derivative is applied.
- The generalization of the equations in space–time exhibits anomalous behavior.
- To keep the dimensionality an auxiliary parameter σ is introduced.
- The numerical solutions are obtained using the numerical Laplace transform algorithm.

ARTICLE INFO

Article history:
Received 28 July 2015
Received in revised form 6 November 2015
Available online 29 December 2015

Keywords:
Fractional calculus
Non-local transport processes
Non-Fickian diffusion
Caputo–Fabrizio fractional derivative
Dissipative dynamics
Anomalous diffusion

ABSTRACT

In this paper we present an alternative representation of the diffusion equation and the diffusion–advection equation using the fractional calculus approach, the spatial-time derivatives are approximated using the fractional definition recently introduced by Caputo and Fabrizio in the range $\beta, \gamma \in (0; 2]$ for the space and time domain respectively. In this representation two auxiliary parameters σ_x and σ_t are introduced, these parameters related to equation results in a fractal space–time geometry provide an entire new family of solutions for the diffusion processes. The numerical results showed different behaviors when compared with classical model solutions. In the range $\beta, \gamma \in (0; 1)$, the concentration exhibits the non-Markovian Lévy flights and the subdiffusion phenomena; when $\beta = \gamma = 1$ the classical case is recovered; when $\beta, \gamma \in (1; 2]$ the concentration exhibits the Markovian Lévy flights and the superdiffusion phenomena; finally when $\beta = \gamma = 2$ the concentration is anomalous dispersive and we found ballistic diffusion.

1. Introduction

Fractional Calculus (FC) generalizes the concept of a derivative operator of integer order to a derivative operator of arbitrary order (real or complex), this mathematical formulation was developed by Fourier, Liouville, Abel, Riemann, Lacroix, Grünwald, Riesz, among many others [1–3]. The dynamical systems of fractional order are non-conservative and involve

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http://dx.doi.org/10.1016/j.physa.2015.12.066
0378-4371/

non-local operators which yield new information about their behavior, many problems in physical science, electromagnetism, electrochemistry, diffusion and general transport theory can be solved by the fractional calculus approach [4–17]. It has been demonstrated that the fractional order modeling is particularly useful to represent systems where the memory plays a significant role, this quality is the most significant advantage [18–20]. Diffusive transport can be seen as the average of the random motions of a huge number of individual molecules in a system. Diffusive transport has a number of important implications in the nature. If we consider the case of one-dimensional diffusion, a concentration gradient produces a net transport in one direction, and the rate of transport is directly proportional to the magnitude of this gradient, the Diffusion Equation (DE) is the governing equation of this process [20]. The advection is a transport mechanism of a substance due to the fluid's bulk motion. The Diffusion–Advection Equation (DAE) describes the tendency of the particles to be moved along by the fluid (the convective terms arise when changing from Lagrangian to Eulerian frames) and the diffusion refers to the dissipation/loss of a particle's property (such as momentum) due to internal frictional forces characterized, in this equation by the concentration-dependent diffusion coefficient [21]. In this context the DE, DAE and Fokker–Planck equation in space–time were suggested based on local FC theory [22–31]. These representations arise in continuous-time random walks. A random walk is a mathematical formalization of a path that consists of a succession of random steps. Random walks are related to the diffusion models and within the fractional approach it is possible to include external fields and transport in the phase space within the same approach [22]. A Lévy flight, also referred as Lévy motion, is a random walk in which the step-lengths have a heavy-tailed probability distribution. In a dimension greater than one, the steps are defined in terms of a probability distribution [23]. Mainardi in Ref. [24] presented the interpretation of the corresponding Green function as a probability density for the particular cases of space-fractional, time-fractional and neutral-fractional diffusion, the fundamental equation was obtained from the conventional diffusion equation by replacing the second-order space derivative with a Riesz–Feller derivative and the first-order time derivative with a Caputo derivative. Gorenflo reported in Ref. [25] the time fractional diffusion equation obtained from a fractional Fick law, the fundamental solution was interpreted as a probability density of a non-Markovian stochastic process and was related to a phenomenon of slow anomalous diffusion. In recent papers of Luchko [26–28], the generalized time-fractional diffusion equation with variable coefficients was considered. The author showed the existence and uniqueness of the solution for the initial boundary value problem of the generalized time-fractional diffusion equation; the Fourier method was used to construct a formal solution. Liu [30] used the Riemann–Liouville and Grünwald–Letnikov definitions of fractional derivatives to analyze the Fokker–Planck equation, the equation was transformed into a system of ordinary differential equations that presented numerical results of the space Fokker–Planck equation; in the work [31] the authors proposed an alternative construction for the space–time fractional DAE considered derivatives of Caputo type of order $\beta, \gamma \in (0, 1]$, the results revealed Lévy flights (non-Markovian version) and the phenomena of subdiffusion. Other applications of FC for modeling diffusive transport are given in Refs. [32–41].

The Riemann–Liouville definition entails physically unacceptable initial conditions (fractional order initial conditions) [42]; conversely for the Caputo representation, the initial conditions are expressed in terms of integer-order derivatives having direct physical significance [43], these definitions have the disadvantage that their kernel had singularity, this kernel includes memory effects and therefore both definitions cannot accurately describe the full effect of the memory. Due to this inconvenience, Michele Caputo and Mauro Fabrizio in Ref. [44] present a new definition of fractional derivative without singular kernel, the Caputo–Fabrizio (CF) fractional derivative, this derivative possesses very interesting properties, for instance, the possibility to describe fluctuations and structures with different scales. Furthermore, this definition allows for the description of mechanical properties related with damage, fatigue, material heterogeneities and structures at different scales. Properties and applications of this new fractional derivative are reviewed in detail in the papers [45–48].

The aim of this work is developed a new representation of the fractional DE and DAE applying the CF fractional derivative, the order of the derivative being considered is $\beta, \gamma \in (0; 2]$ for space–time domain respectively, we employ the idea suggested in Refs. [4,5] to construct dimensional correct fractional differential equations, this alternative representation preserves the physical dimensionality of the equation for any value taken by the exponent of the fractional derivative.

The paper is organized as follows. In the next section, we recall the CF fractional derivative. In Section 3, the alternative representation of the fractional DAE and DE is performed. Finally, some concluding remarks are drawn in Section 5.

2. Basic tools

The CF definition of fractional derivative is based on the convolution of a first order derivative and the exponential function, the CF fractional derivative of order $\gamma \in [0; 1]$ is defined as follows [44,45]

$$ {}^{CF}_{0}\mathcal{D}^{\gamma}_{t} f(t) = \frac{M(\gamma)}{1-\gamma} \int_0^t \dot{f}(\alpha) \exp\Big[-\frac{\gamma(t-\alpha)}{1-\gamma}\Big] \mathrm{d}\alpha, \tag{1} $$

where $\frac{\mathrm{d}^{\gamma}}{\mathrm{d}t^{\gamma}} = {}^{CF}_{0}\mathcal{D}^{\gamma}_{t}$ is a CF derivative with respect to t, $M(\gamma)$ is a normalization function such that $M(0) = M(1) = 1$, in this fractional derivative the exponential function helps to reduce the risk of singularity, furthermore, the derivative of a constant is equal to zero and the kernel does not have singularity for $t = \alpha$.

If $n \geq 1$ and $\gamma \in [0, 1]$, the CF fractional derivative, ${}^{CF}_{0}\mathcal{D}^{(\gamma+n)}_{t} f(t)$ of order $(n + \gamma)$ is defined by

$$ {}^{CF}_{0}\mathcal{D}^{(\gamma+n)}_{t} f(t) = {}^{CF}_{0}\mathcal{D}^{(\gamma)}_{t} ({}^{CF}_{0}\mathcal{D}^{(n)}_{t} f(t)). \tag{2} $$