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Research paper

Solutions for a mass transfer process governed by fractional diffusion equations with reaction terms

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We investigate the behavior of a mass transfer process governed by a set of fractional diffusion equations coupled by appropriate reaction terms. The presence of memory effects in the diffusive term is also considered. For this set of equations, we obtain solutions and analyze the influence of the reaction terms on the spreading of these solutions. Particularly, we observe that for reversible reaction processes the reaction terms play an important role for intermediate times and for long times the processes are essentially governed by the bulk equations. These results show a rich class of behaviors which can be connected to sub- or superdiffusive regime.

1. Introduction

Many situations of interest existing in physics [1–3], chemistry [4], and biology [5–7] have shown that the anomalous diffusion phenomenon [1] plays an important role with direct consequences on the dynamic behavior of these systems. One of the most important characteristics of the anomalous diffusion, when the central limit theorem is satisfied, remains on the nonlinear dependence on the mean square displacement, e.g., $\langle (x-\langle x\rangle)\rangle^2 \sim t^\alpha$ with $\alpha \neq 1$, which is usually related to the non-Markovian features manifested by these systems. On the other hand, there are situations characterized by the Lévy distributions, asymptotically characterized by power-laws, which do not satisfy the central limit theorem and consequently have a divergent behavior of the mean square displacement. In order to describe these systems, several approaches have been previously reported in the literature, such as the generalized Langevin equations [8,9], nonlinear diffusion equations [10–13], master equations, and the fractional diffusion equations [14–22]. In this context, reaction diffusion problems have also been investigated [23–29], due to the importance of chemical reactions in scientific and industrial applications. Toward this, we devote this manuscript to analyze the behavior of a mass transfer process [30] governed of a set of fractional diffusion equations coupled by appropriate reaction terms. More precisely, we investigate the following set of diffusion equations, which has been used to describe a subdiffusion limited reaction system:

$$\frac{\partial^\gamma}{\partial t^\gamma}\rho_1(x,t) = \frac{\partial^2}{\partial x^2}\int_{-\infty}^{\infty} dx'\mathcal{D}_1(x-x')\rho_1(x',t) - r_1\rho_1(x,t) + r_2\rho_2(x,t)\ , \tag{1}$$

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$$\frac{\partial^\gamma}{\partial t^\gamma}\rho_2(x,t) = \frac{\partial^2}{\partial x^2}\int_{-\infty}^{\infty} dx'\mathcal{D}_2(x-x')\rho_2(x',t) + r_1\rho_1(x,t) - r_2\rho_2(x,t) \;, \tag{2}$$

where $0 < \gamma < 1$. In these equations, $\rho_1(x, t)$ and $\rho_2(x, t)$ represent two different diffusing systems (e.g., substances, particles or species), $\mathcal{D}_1(x)$ and $\mathcal{D}_2(x)$ are the diffusion coefficients for each species and the reaction rates, and r_1 and r_2, are connected with the reaction process, which in this case can be represented by the reversible reaction $1 \rightleftharpoons 2$ or an irreversible process, e.g., $1 \to 2$. The fractional time operator considered is the Caputo's one [31]. These equations may be obtained from a random walk by considering the following coupled balance equations

$$\begin{aligned}\rho_1(x,t) = {} & \Phi(t)\rho_1(x,0) + \int_{-\infty}^{\infty} dx'\int_0^t dt'\Psi(x-x',t-t')\rho(x',t') \\ & - \int_0^t dt'\Phi_{r_1}(t-t')\rho_1(x,t') + \int_0^t dt'\Phi_{r_2}(t-t')\rho(x,t'),\end{aligned} \tag{3}$$

$$\begin{aligned}\rho_2(x,t) = {} & \Phi(t)\rho_2(x,0) + \int_{-\infty}^{\infty} dx'\int_0^t dt'\Psi(x-x',t-t')\rho_2(x',t') \\ & - \int_0^t dt'\Phi_{r_1}(t-t')\rho_1(x,t') - \int_0^t dt'\Phi_{r_2}(t-t')\rho_2(x,t'),\end{aligned} \tag{4}$$

where $\Phi(t) = 1 - \int_0^t \int_{-\infty}^{\infty} \Psi(x,t')dt'dx$, $\Phi_{r_1}(t) = r_1\Phi(t)$, and $\Phi_{r_2}(t) = r_2\Phi(t)$. In Eqs. (3) and (4), $\Psi(x, t')$ represents a probability density function from which the waiting time distribution and jumping probability can be obtained, i.e., $\omega(t) = \int_{-\infty}^{\infty} \Psi(x,t)dx$ and $\lambda(x) = \int_0^{\infty} \Psi(x,t)dt$. It is worth mentioning that both, the fractional time derivative and the memory effect present in the diffusive term, change the properties of the waiting time and the jumping probability distributions. For Eqs. (1) and (2), we analyze the mean square displacement for the case $\mathcal{D}_1(x) \neq 0$ with $\mathcal{D}_2(x) = 0$, when the limit central theorem is verified. We also analyze the spreading of the system and obtain exact solutions for the cases $\mathcal{D}_1(x) \propto 1/|x|^{\mu_1 - 1}$ with $\mathcal{D}_2(x) = 0$ and $\mathcal{D}_1(x) \propto 1/|x|^{\mu_1 - 1}$ and $\mathcal{D}_2(x) \propto 1/|x|^{\mu_2 - 1}$ $(1 < \mu_1, \mu_2 \leq 2)$. Note that these choices for the kernels present in the diffusive term lead to situations characterized by distributions asymptotically governed by power – laws such as the Lévy distributions, which may be connected to a random walk with long tailed jump probability density. In addition, for $\mu_1 \neq 2$ and $\mu_2 \neq 2$ we have an interplay among different regimes during the time evolution of the solutions obtained for these species. These developments are performed in Sections 2 and in 3, we present our conclusions.

2. Diffusion equation and reaction terms

Let us analyze the behavior of the previous set of fractional diffusion equations with linear reaction terms by firstly considering the case characterized by $\mathcal{D}_1(x) \neq 0$ with $\mathcal{D}_2(x) = 0$ and afterwards, the case where $\mathcal{D}_1(x) \neq 0$ with $\mathcal{D}_2(x) \neq 0$. In the first case, one can assume that one of the species remains somehow immobile in the bulk, while in the second case both species can diffuse in the bulk. For this case, the Eqs. (1) and (2) can be rewritten as

$$\frac{\partial^\gamma}{\partial t^\gamma}\rho_1(x,t) = \frac{\partial^2}{\partial x^2}\int_{-\infty}^{\infty} dx'\mathcal{D}_1(x-x')\rho_1(x',t) - r_1\rho_1(x,t) + r_2\rho_2(x,t) \;, \tag{5}$$

$$\frac{\partial^\gamma}{\partial t^\gamma}\rho_2(x,t) = r_1\rho_1(x,t) - r_2\rho_2(x,t) \;, \tag{6}$$

with $r_1 \neq 0$ and $r_2 \neq 0$ characterizing a reversible first order reaction process present in the bulk. This set of equations can be related to an intermittent motion where the reaction terms can be related to the rate of switching the particles from the diffusive mode to the resting mode r_1 or switching them from the resting to the movement r_2. It can also be regarded as a problem in diffusion in which some of the diffusing substances become immobilized as the diffusion proceeds, or a problem in chemical kinetics in which the rate of reaction depends on the rate of supply of one of the reactants by diffusion.

Before obtaining the solutions for $\rho_1(x, t)$ and $\rho_2(x, t)$ from the previous set of diffusion equations, we analyze the behavior of the second moment and, consequently, the time dependence exhibited by the mean square displacement. In order to perform this analysis, we consider that the distributions obtained from these equations satisfy the central limit theorem. For Eqs. (5) and (6), typical situations which may verify this theorem are usually characterized by $\int_{-\infty}^{\infty} dx\mathcal{D}_{1(2)}(x) = const$. By taking into account this requirement and the boundary conditions $\rho_1(\pm\infty, t) = 0$ and $\rho_2(\pm\infty, t) = 0$, it is possible to show that the dynamic of the second moment for both species is governed by the following equations:

$$\frac{\partial^\gamma}{\partial t^\gamma}\langle x^2\rangle_1 = 2\mathcal{I}_{\mathcal{D}_1}\mathcal{S}_1(t) - r_1\langle x^2\rangle_1 + r_2\langle x^2\rangle_2 \;, \tag{7}$$

$$\frac{\partial^\gamma}{\partial t^\gamma}\langle x^2\rangle_2 = r_1\langle x^2\rangle_1 - r_2\langle x^2\rangle_2 \;, \tag{8}$$