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Fractional diffusion equations coupled by reaction terms

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HIGHLIGHTS

- Solutions for a set of fractional diffusion equations with reaction terms.
- Interplay between different diffusive regimes and anomalous diffusion.
- Asymptotic behavior governed by long tailed distributions.

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ABSTRACT

We investigate the behavior for a set of fractional reaction–diffusion equations that extend the usual ones by the presence of spatial fractional derivatives of distributed order in the diffusive term. These equations are coupled via the reaction terms which may represent reversible or irreversible processes. For these equations, we find exact solutions and show that the spreading of the distributions is asymptotically governed by the same the long-tailed distribution. Furthermore, we observe that the coupling introduced by reaction terms creates an interplay between different diffusive regimes leading us to a rich class of behaviors related to anomalous diffusion.

1. Introduction

Anomalous diffusion has been reported in several contexts such as fractal globules [1], molecular crowding [2], particles transported by parallel flows [3], brain metabolites [4], and particle tracking [5]. One of the main characteristics of this phenomenon is the unusual time dependence of the mean square displacement that can be, *e.g.*, nonlinear $\langle (x-\langle x\rangle)^2\rangle \sim t^{\alpha}$, with $\alpha < 1$ and $\alpha > 1$ corresponding to sub- and superdiffusion, or not well defined as occurs with Lévy distributions, which are characterized by a long-tailed distributions. In this context, the fractional calculus has proved to be a powerful tool in scenarios such as tumor growth [6], electrical response [7], solute transport [8], living cells [9], anomalous transport in biological cells [10], solar cosmic-ray transport [11], and diffusion-controlled surfactant adsorption [12] by extending the usual approaches to noninteger differential operators. Typical examples are the fractional diffusion equations [13], which display a wide variety of behaviors that can be connected to anomalous diffusion. The fractional equations are also related to random walks, where the fractional operators appear as a consequence of the behavior exhibited by the waiting time and/or the jumping probabilities distributions, generally characterized by long-tailed distributions. These distributions cause the

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divergence of low-order moments, and consequently the hypotheses underlying the central limit theorem are not valid. In particular, fractional order in the spatial derivative (Laplacian) of a diffusion equation can be connected to Lévy distributions in the jumping probabilities, leading to a divergent behavior in the variance. Another interesting point is the behavior obtained from these equations when reaction terms are considered [14–23]. Reaction terms have been used to investigate several situations related to pattern formation [24,25], fluorescence recovery after photobleaching [26], non-Fickian phenomena related to astronomical phenomena [27], solute transport subject to bimolecular reactions [28], and ecology [29]. Thus, the analysis of fractional diffusion equations, especially those with reaction terms, is of the great interest from the analytical and numerical point of view due to the large number of scenarios which can be connected.

Here, we investigate a two component system governed by fractional diffusion equations with reaction terms, which may represent a reversible or irreversible process depending on the choice of the rates. In particular, we consider the following equations

$$\frac{\partial}{\partial t}\rho_1(x,t)=\int_1^{\mu_1}d\overline{\mu}_1\mathcal{D}_1(\overline{\mu}_1)\frac{\partial^{\overline{\mu}_1}}{\partial|x|^{\overline{\mu}_1}}\rho_1(x,t)-k_1\rho_1(x,t)+k_2\rho_2(x,t), \tag{1}$$

$$\frac{\partial}{\partial t}\rho_2(x,t)=\int_1^{\mu_2}d\overline{\mu}_2\mathcal{D}_2(\overline{\mu}_2)\frac{\partial^{\overline{\mu}_2}}{\partial|x|^{\overline{\mu}_2}}\rho_2(x,t)+k_1\rho_1(x,t)-k_2\rho_2(x,t), \tag{2}$$

where $1 < \mu_1 \leq 2$ and $1 < \mu_2 \leq 2$. The constants k_1 and k_2 may be related to reversible (forward and backward) reactions, *i.e.*, $1 \rightleftharpoons 2$, or irreversible reactions, *i.e.*, $1 \to 2$. The fractional operator is the Riesz–Weyl [30] one, which encompasses situations characterized by long-tailed distributions in connection to the Lévy distributions. The functions $\mathcal{D}_1(\overline{\mu}_1)$ and $\mathcal{D}_2(\overline{\mu}_2)$ are the distributions related to the index $\overline{\mu}_1$ and $\overline{\mu}_2$. In particular, we shall consider that $\mathcal{D}_1(\overline{\mu}_1)=\mathcal{D}_{\mu_1'}\delta(\overline{\mu}_1-\mu_1')+\mathcal{D}_{\mu_1}\delta(\overline{\mu}_1-\mu_1)$ and $\mathcal{D}_2(\overline{\mu}_2)=\mathcal{D}_{\mu_2'}\delta(\overline{\mu}_2-\mu_2')+\mathcal{D}_{\mu_2}\delta(\overline{\mu}_2-\mu_2)$. This choice leads us to an interplay between the regimes characterized by the different index, $\mu_{1(2)}$ and $\mu'_{1(2)}$. In this scenario, a reaction process occurs, and consequently the regime manifested by one processes influences the other due to the coupling produced by the reaction terms. In Section 2, we find exact solutions for this set of equations and discuss the spreading of the distributions in different scenarios. The discussions and conclusions are presented in Section 3.

2. Diffusion and reaction

We investigate the behavior of Eqs. (1) and (2) by considering different scenarios. We first consider the case $\mathcal{D}_1(\overline{\mu}_1)\neq 0$ and $\mathcal{D}_2(\overline{\mu}_2)=0$, followed by the case in which $\mathcal{D}_1(\overline{\mu}_1)\neq 0$ and $\mathcal{D}_2(\overline{\mu}_2)\neq 0$. In both cases, we obtain exact solutions in terms of the Fox H-functions [30] and analyze the spreading of the solutions.

2.1. The case $\mathcal{D}_1(\overline{\mu}_1)\neq 0$ and $\mathcal{D}_2(\overline{\mu}_2)=0$

We start the case $\mathcal{D}_1(\overline{\mu}_1)\neq 0$ and $\mathcal{D}_2(\overline{\mu}_2)=0$ by assuming an infinite medium where all relevant quantities are diffusing in one dimension, *i.e.*, the x direction with $-\infty < x < \infty$. Eqs. (1) and (2) for this case can be written as

$$\frac{\partial}{\partial t}\rho_1(x,t)=\int_1^{\mu_1}d\overline{\mu}_1\mathcal{D}_1(\overline{\mu}_1)\frac{\partial^{\overline{\mu}_1}}{\partial|x|^{\overline{\mu}_1}}\rho_1(x,t)-k_1\rho_1(x,t)+k_2\rho_2(x,t), \tag{3}$$

$$\frac{\partial}{\partial t}\rho_2(x,t)=k_1\rho_1(x,t)-k_2\rho_2(x,t). \tag{4}$$

These equations represent a process where one substance may be sorbed or chemically react with another kind of substance that is diffusing. Thus, this case corresponds to a diffusion problem in which some of the diffusing substance is immobilized as the diffusion proceeds, or as a problem in chemical kinetic in which the rate of the reaction depends on the supply rate of one of the reactants by diffusion. In both situations, the quantities k_1 and k_2 are relevant to define the rate related to these processes. For these equations, it is possible to show that

$$\int_{-\infty}^{\infty}dx\rho_1(x,t)+\int_{-\infty}^{\infty}dx\rho_2(x,t)=\text{const.}, \tag{5}$$

implying that the number of particles is conserved in this system. In order to find the solution for this set of equations, from the formal point of view, we may use the Fourier and Laplace transform yielding

$$\rho_1(k,s)=\frac{(s+k_2)\,\rho_1(k,0)}{s(s+k_1+k_2)+(s+k_2)\mathcal{I}_1(k;\mu_1,\mu_1')}, \tag{6}$$

$$\rho_2(k,s)=\frac{k_1}{s+k_2}\rho_1(k,s) \tag{7}$$