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Solutions for a sorption process governed by a fractional diffusion equation

E.K. Lenzi [a,b,*], M.A.F. dos Santos [a], D.S. Vieira [c], R.S. Zola [c,d], H.V. Ribeiro [c,d]

[a] Departamento de Física, Universidade Estadual de Ponta Grossa - Ponta Grossa, PR 87030-900, Brazil
[b] National Institute of Science and Technology for Complex Systems - Rio de Janeiro, RJ 22290-180, Brazil
[c] Departamento de Física, Universidade Estadual de Maringá - Maringá, PR 87020-900, Brazil
[d] Departamento de Física, Universidade Tecnológica Federal do Paraná - Apucarana, PR 86812-460, Brazil

HIGHLIGHTS

- Solutions for a fractional diffusion equation and anomalous diffusion.
- Sorption process governed by a generalized kinetic equation.
- Exact solutions for a fractional diffusion equation with the Green function approach.
- Analytical solutions for the mean square displacement and survival probability.

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ABSTRACT

We investigate a sorption process where one substance spreads out through another having possibility of chemical reaction between them. So as to describe this process, we have considered the bulk dynamics governed by a fractional diffusion equation, where the reaction term may describe an irreversible or a reversible process. This reaction term represents a generalization of the first order kinetic equation taking memory effects into account. The analytical solutions for the mean square displacement, survival probability and probability density of the particles we have obtained show a rich class of behaviors connected to anomalous diffusion.

1. Introduction

Nowadays, anomalous diffusion plays an important role in several fields of science, ranging from physics to biology. For instance, protein motion in living cells [1], passive movements of biomolecules or vesicles in cells, diffusion of water and other substances in muscles [2], cardiac electrical propagation [3], electrical response [4,5], and transport properties of particles on complex structures [6]. One of the main characteristics present in this phenomenon is the non-linear time dependence exhibited by the mean square displacement. This behavior is often modeled as a power-law dependence [7,8]. In this context, continuous time random walk [9], generalized Langevin equations and fractional diffusion equations (see Refs. [10–18]) have been analyzed and applied in several situations, such as molecular diffusion *in vivo* [10,19], in membrane cells [20,21], subdiffusion in thin membranes [22] and chemotaxis diffusion [23]. For these situations, the mean-square displacement, in general, is characterized by $\sigma_x^2(t) \sim t^\alpha$, being the superdiffusion ($\alpha > 1$) commonly related, for example,

* Corresponding author at: Departamento de Física, Universidade Estadual de Ponta Grossa - Ponta Grossa, PR 87030-900, Brazil.
E-mail address: ervinkaminskilenzi@gmail.com (E.K. Lenzi).

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to active transport [24–27], while the subdiffusive behavior ($\alpha < 1$) may be related to the molecular crowding [28] and fractal structure [29]. Thus, the comprehension of the formal aspects present in these formalisms is a relevant point to establish connections between models and experimental results.

Here, we investigate a sorption process where one substance spreads out through another having also the possibility of chemically reacting by considering a general situation which can be related to a random walk with a long tailed distributions, i.e., the waiting time and the jumping probability distributions are asymptotically characterized by a power-law behavior. A random walk with this characteristic leads, as reported in Refs. [11,12], to fractional diffusion equations usually applied in anomalous diffusion. Thus, this analysis enables one to investigate, by incorporating this behavior, processes connected to anomalous diffusion which are not suitable described in term of the usual approach. In particular, it has been used to investigate diffusion, adsorption kinetics, and the effect on the molecular rearrangement of the anisotropic molecules on the surface [30]. It can also be applied to biological systems [31] such as for living cells, where chemical reactions and diffusion take place in crowded environment [32], thus, justifying the anomalous behavior [33] embedded in our system. For this, we consider that the density of particles is governed by the following fractional diffusion equation,

$$\frac{\partial}{\partial t}\rho(x,t) = \mathcal{K}_{\gamma\,0}\mathcal{D}_t^{1-\gamma}\left(\frac{\partial^\mu}{\partial|x|^\mu}\rho(x,t)\right) - \frac{\partial}{\partial t}\Gamma(x,t) \tag{1}$$

where $\mathcal{K}_\gamma$ is the diffusion coefficient, $0 < \gamma \le 1$ (for $\gamma = 1$ usual diffusion, $0 < \gamma < 1$ subdiffusion), and the fractional time derivative is the Riemann–Liouville [34]. The spatial fractional derivative is considered in the Riesz–Weyl representation [34] with $1 < \mu \le 2$. In Eq. (1), $\rho(x,t)$ represents the density of diffusing particles whereas $\Gamma(x,t)$ is connected to the density of absorbed particles. The last term may represent the process of a substance being absorbed by another as well as the possibility of these substances reacting chemically. This process can thus be understood either as diffusion in which part of the substance becomes immobilized or as a chemical kinetics problem in which the rate of reaction depends on the supply rate of one of the reactants by diffusion. Examples involving diffusion into living cells and microorganisms can be found in biology and biochemistry [35]. In order to accomplish these contexts, we consider, for $\Gamma(x,t)$, the following general kinetic equation:

$$\frac{\partial}{\partial t}\Gamma(x,t) = \int_0^t k_f(t-t')\rho(x,t')\mathrm{d}t' - \int_0^t k_b(t-t')\Gamma(x,t')\mathrm{d}t', \tag{2}$$

where $k_f(t)$ and $k_b(t)$, respectively, are the rate of the forward and backward reactions. Thus, the immobilized solute is formed at a rate proportional to the concentration of solute free to diffuse, and disappears at a rate proportional to its own concentration. This feature lead us to an alternance between periods of diffusive transport and resting times which are governed by $k_f(t)$ and $k_b(t)$. Eq. (2) has as particular case several situations worked out in Refs. [36,37] and, from a phenomenological point of view, the choice of kernel in Eq. (2) could be related, for example, to surface irregularities [38], which is an important factor in adsorption–desorption, diffusion, and catalysis processes. In addition, Eqs. (1) and (2) generalize the ones used in the fluorescence recovery after photobleaching (FRAP), a widely used experimental method to explore binding interactions in cells both in vitro and in vivo [39].

2. Fractional diffusion equation and solutions

We start discussing the time dependent solutions of Eq. (1) subjected to the previous boundary conditions. In order to solve this problem, we use the Laplace ($\mathcal{L}\{\rho(x,t)\} = \overline{\rho}(x,s)$ and $\mathcal{L}^{-1}\{\overline{\rho}(x,s)\} = \rho(x,t)$) and Fourier ($\mathcal{F}\{\rho(x,t)\} = \tilde{\rho}(k,t)$ and the $\mathcal{F}^{-1}\{\tilde{\rho}(k,t)\} = \rho(x,t)$) transforms. Applying the Fourier transform, Eqs. (1) and (2) can be written as

$$-\mathcal{K}_\gamma|k|^\mu{}_0\mathcal{D}_t^{1-\gamma}\left(\tilde{\rho}(k,t)\right) - \frac{\partial}{\partial t}\tilde{\Gamma}(k,t) = \frac{\partial}{\partial t}\tilde{\rho}(k,t) \tag{3}$$

and

$$\frac{\partial}{\partial t}\tilde{\Gamma}(k,t) = \int_0^t k_f(t-t')\tilde{\rho}(k,t')\mathrm{d}t' - \int_0^t k_b(t-t')\tilde{\Gamma}(k,t')\mathrm{d}t'. \tag{4}$$

Now by using the Laplace transform

$$\overline{\tilde{\rho}}(k,s) = \left(\tilde{\rho}(k) + \frac{k_b(s)}{s+k_b(s)}\tilde{\Gamma}(k,0)\right)\overline{\tilde{\mathcal{G}}}(k,s), \tag{5}$$

$$\overline{\tilde{\mathcal{G}}}(k,s) = \frac{1}{s+\mathcal{K}_\gamma s^{1-\gamma}|k|^\mu + \overline{\Upsilon}(s)}, \tag{6}$$

where $\overline{\tilde{\mathcal{G}}}(k,s)$ represents the Green function in the Fourier–Laplace space of Eq. (1) and

$$\overline{\tilde{\Gamma}}(k,s) = \frac{1}{s+\overline{k}_b(s)}\left(\overline{k}_f(s)\overline{\tilde{\rho}}(k,s) + \tilde{\Gamma}(k,0)\right), \tag{7}$$

with $\overline{\Upsilon}(s) = s\bar{k}_f(s)/(s + \bar{k}_b(s))$, and the initial condition of the system depends on $\tilde{\rho}(k)$ and $\tilde{\Gamma}(k, 0)$ which, for simplicity, are given by $\tilde{\rho}(k) = \rho_i$ and $\tilde{\Gamma}(k, 0) = \Gamma_i$ (where $\rho_i + \Gamma_i = 1$).

Note that the processes described by Eq. (1) with the Green function given by Eq. (6) may also be related to a random walk [11,9,17,18], as we have previously mentioned in the introduction. For instance, in the absence of the reaction term ($k_b(t) = k_f(t) = 0$), by performing a direct comparison between the Green function, Eq. (6), and the continuous time random walk approach presented in Ref. [17] (or Ref. [18]), we obtain $\overline{\psi}(s) = 1/(1 + \tau^{\gamma} s^{\gamma})$ (τ is characteristic time scale) and $\tilde{\lambda}(k) = 1 - \mathcal{K}_{\gamma}\tau^{\gamma}|k|^{\mu}$. These results show that the fractional derivatives have a direct influence on the waiting time and the jumping probability distribution. The presence of the reaction term ($k_b(t) \neq 0$ and $k_f(t) \neq 0$) implies in a creation and annihilation processes where there is addition or removal of the walkers at the start of the waiting time between steps. In this sense, for the initial conditions $\rho(x, 0) = \delta(x)$ and $\Gamma(x, 0) = 0$, by using the random walk approach presented in Ref. [18] (see also Ref. [40]) is possible to connect Eqs. (1) and (2) with the processes described by the balance equations

$$\rho(x,t) = \Phi(t)\delta(x) + \int_{-\infty}^{\infty} dx' \int_0^t dt' \psi(t-t')\lambda(x-x')\rho(x',t') + \int_0^t dt' \Phi_b(t-t')\Gamma(x,t') - \int_0^t dt' \Phi_f(t-t')\rho(x,t') \tag{8}$$

$$\Gamma(x,t) = \int_0^t dt' \int_0^{t'} d\tilde{t} k_f(t'-\tilde{t})\rho(x,\tilde{t}) - \int_0^t dt' \int_0^{t'} d\tilde{t} k_b(t'-\tilde{t})\Gamma(x,\tilde{t}) \tag{9}$$

where $\Phi(t) = 1 - \int_0^t \psi(t)dt$, $\Phi_b(t) = \int_0^t dt' \Phi(t-t')k_b(t')$, and $\Phi_f(t) = \int_0^t dt' \Phi(t-t')k_f(t')$. After some calculations, these equations can be simplified to

$$\rho(x,t) = \Phi(t)\delta(x) + \int_{-\infty}^{\infty} dx' \int_0^t dt' \psi(t-t')\lambda(x-x')\rho(x',t') + \int_0^t dt' \Phi(t-t')\mathcal{R}(x,t') \tag{10}$$

with

$$\mathcal{R}(x,t) = -\frac{\partial}{\partial t}\int_0^t dt' \mathcal{M}(t-t')\rho(x,t'), \tag{11}$$

where the memory function $\mathcal{M}(t)$ is given by $\mathcal{M}(t) = \mathcal{L}^{-1}\{k_b(s)/(s + k_f(s))\}$. In particular, by considering the asymptotic limit of $t \to \infty$ ($s \to 0$), for $k_b(s)/(s + k_f(s)) \sim \kappa =$ const, Eq. (10) can be simplified to a fractional diffusion equation and, for $k_b(s)/(s + k_f(s)) \sim 1/s^{\gamma}$, it can be reduced to Eq. (43) of Ref. [18] where a nonnegative behavior for $\rho(x, t)$ is exhibited.

From the previous results it is possible to obtain, in the Laplace space, some quantities of interest such as the mean square displacement, i.e., $\Delta_x^2(t) = \langle (x - \langle x \rangle)^2 \rangle$, for $\mu = 2$ and the survival probability $\mathcal{S}(t)$, which is connected to the mobile particle present in the bulk. For the mean square displacement, it is possible to show that

$$\overline{\Delta}_x^2(s) = \frac{2\mathcal{K}_{\gamma}}{s^{1+\gamma}}\left(\rho_i + \frac{k_b(s)}{s + k_b(s)}\Gamma_i\right)\left(\frac{s + k_b(s)}{s + k_b(s) + k_f(s)}\right)^2. \tag{12}$$

Eq. (12) indicates that the distribution of particles spreads out depending on the parameters $k_b(s)$ and $k_f(s)$, thus, different behaviors are found depending on the choice of the parameters. This feature can be verified, for example, for the cases characterized asymptotically ($s \to 0$ or $t \to \infty$) by power-laws which imply in $\bar{k}_b(s) \sim k_b s^{\eta_b}$ and $\bar{k}_f(s) \sim k_f s^{\eta_f}$ with $0 < \eta_f < \eta_b < 1$ leading to

$$\Delta_x^2(t) \sim \begin{cases} \dfrac{2\mathcal{K}_{\gamma}}{\Gamma(1+\gamma)} t^{\gamma}, & t \ll t_c \\ \dfrac{2\mathcal{K}_{\gamma}}{\Gamma(1+\xi)}\left(\dfrac{k_b}{k_f}\right)^2 t^{\xi}, & t \gg t_c \end{cases} \tag{13}$$

calculated for the initial condition $\rho_i = 1$ and $\Gamma_i = 0$ with $\xi = \gamma - 2(\eta_b - \eta_f)$. Here, $t_c = \left(\frac{\Gamma(1+\gamma)}{\Gamma(1+\xi)}\left(\frac{k_b}{k_f}\right)^2\right)^{\frac{1}{2(\eta_b-\eta_f)}}$ is the crossover time between the two regimes manifested when these rates are considered. Note that the behavior for $t \gg t_c$ can be subdiffusive ($0 < \gamma - 2(\eta_b - \eta_f) < 1$), superdiffusive ($1 < \gamma - 2(\eta_b - \eta_f)$) or stationary ($\gamma = 2(\eta_b - \eta_f)$). The last condition for ξ implies that the particles present in the bulk and the kinetic process given by Eq. (2) reach an equilibrium situation. For the cases characterized by constant rates, we have the asymptotic limit governed by the diffusive term which depends on γ, as illustrated in Fig. 1. The initial condition of the system may also lead to an anomalous behavior for short times, as shown in Fig. 1(b). This point is also illustrated in Fig. 1 by considering that the system is initially immobilized, i.e., $\Gamma_i = 1$ and $\rho_i = 0$, producing an anomalous spreading of the particles for short times ($t \ll (1+\gamma)k_f/(k_f + k_b)^2$) as the particles are released by a physical or chemical process. In particular, in this limit, the spreading of the system is governed by $\Delta_x(t) \sim 2k_f\mathcal{K}_{\gamma}t^{1+\gamma}/\Gamma(1+\gamma)$. It is also interesting to mention that the behavior manifested, for example, by the black solid

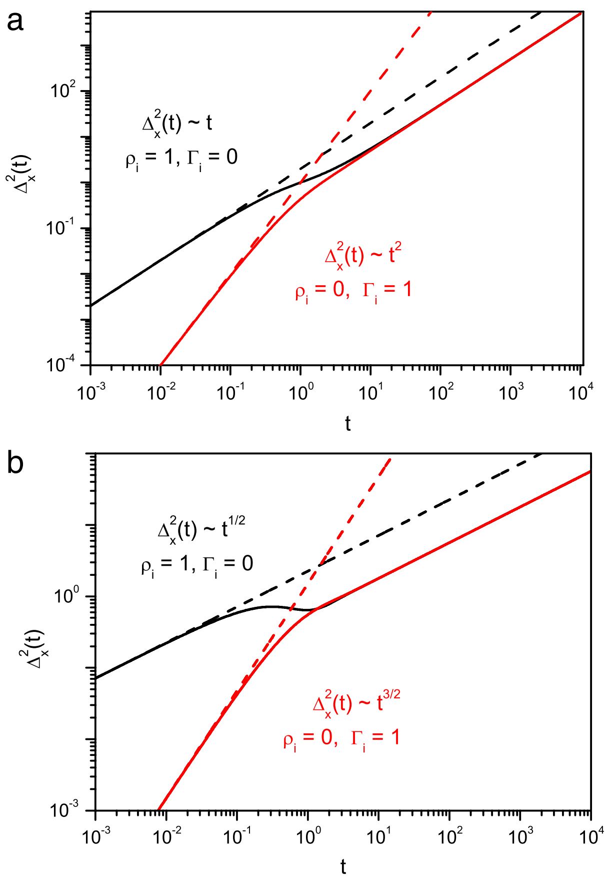

Fig. 1. Behavior of the mean square displacement versus t by considering two different initial conditions and constant rates. We consider $\gamma = 1$ in (a) and $\gamma = 1/2$ in (b). For simplicity, it is assumed that $k_f = 1$, $k_b = 1$, and $\mathcal{K}_\gamma = 1$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

line in Fig. 1(a) may represent the effect of molecular crowding on diffusion in the cytoplasm [41], where for small times a usual diffusion is manifested and is followed by an anomalous and a usual diffusion with an effective diffusion coefficient. The other line (red) in Fig. 1(a) represents the expected behavior when the substance in initially binding. For the case $\mu \neq 2$, we illustrate the behavior of $1/\rho^2(x,t)$ as a measure of the spreading of the system (see, Fig. 2). We observe that, for the initial condition $\rho_i = 1$ with $\Gamma_i = 0$, the behavior for short and long times is governed by $1/\rho^2(x,t) \sim t^{2/\mu}$. For the case $\rho_i = 0$ with $\Gamma_i = 1$, only the asymptotic behavior is governed by $1/\rho^2(x,t) \sim t^{2/\mu}$.

The survival probability, defined as $\mathcal{S}(t) = \int_{-\infty}^{\infty} \rho(x,t)dx = \tilde{\rho}(0,t)$, which in the above context reflects the quantity of particles mobile present in the bulk, is given by

$$\overline{\mathcal{S}}(s) = \left(\rho_i + \frac{k_b(s)}{s + k_b(s)}\Gamma_i\right) \frac{s + k_b(s)}{s(s + k_b(s) + k_f(s))}. \tag{14}$$

Eq. (14) depends on the reaction processes in the bulk and does not show dependence on the diffusive term since the system is not limited (or confined). Fig. 3 illustrates the behavior of Eq. (14) for different $k_b(t)$ and $k_f(t)$. For the previous case, asymptotically characterized by $k_b(s) \sim k_b s^{\eta_b}$ and $k_f(s) \sim k_f s^{\eta_f}$, however with $0 < \eta_b < \eta_f < 1$,

$$\mathcal{S}(t) \sim \frac{k_b}{k_f} t^{\alpha} E_{\alpha,1+\alpha}\left(-\frac{k_b}{k_f} t^{\alpha}\right), \tag{15}$$

calculated for $\rho_i = 1$ and $\Gamma_i = 0$, $\alpha = \eta_f - \eta_b$, where $E_{\alpha,\beta}(x)$ is the generalized Mittag-Leffler function [34] (for details, see Appendix). The case $k_b(s) \sim k_b/s^{\eta_b}$ with $k_f(s) \sim k_f/s^{\eta_f}$, for the same initial condition, leads us to

$$\mathcal{S}(t) \sim E_{\alpha}\left(-\frac{k_f}{k_b} t^{\alpha}\right). \tag{16}$$

From the asymptotic behavior shown by Eqs. (15) and (16), it is possible to observe two situations: the particles are sorbed and after desorbed (Eq. (15) with $\mathcal{S}(t) \rightarrow$ const for $t \rightarrow \infty$) or the particles are absorbed and, consequently, immobilized (Eq. (16), with $\mathcal{S}(t) \rightarrow 0$ for $t \rightarrow \infty$).

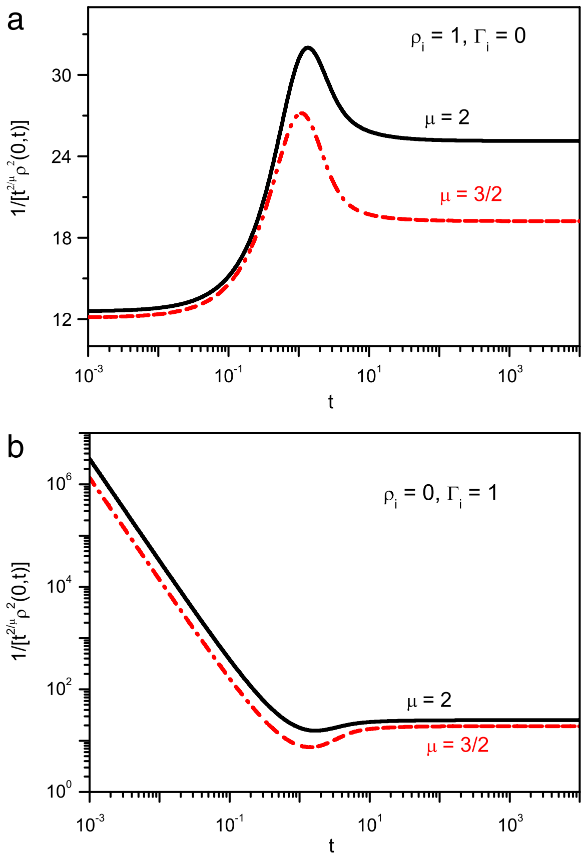

Fig. 2. Behavior of $1/\left[t^{2/\mu}\rho^2(0,t)\right]$ versus t by considering two different initial conditions and constant rates. We consider, for simplicity, $\gamma = 1$, $k_f = 1$, $k_b = 1$, and $\mathcal{K}_\gamma = 1$.

Now, let us perform in Eq. (6) the inverse of the Fourier and the Laplace transforms. First, we focus on the Green function that can be written as follows:

$$\bar{\tilde{\mathcal{G}}}(k,s) = \frac{1}{s+\mathcal{K}_\gamma s^{1-\gamma}|k|^\mu} + \sum_{n=1}^{\infty}\frac{(-\overline{\Upsilon}(s))^n}{\left(s+\mathcal{K}_\gamma s^{1-\gamma}|k|^\mu\right)^{n+1}}. \tag{17}$$

The first term of Eq. (17) corresponds to the Green function of the fractional diffusion equation in the absence of the reaction term. The second term is the contribution of the reaction term or the spreading of the system. By applying the inverse Laplace transform, we obtain

$$\tilde{\mathcal{G}}(k,t) = E_\gamma\left(-\mathcal{K}_\gamma t^\gamma|k|^\mu\right) + \sum_{n=1}^{\infty}\frac{(-1)^n}{\Gamma(1+n)}\int_0^t dt'\Lambda_n(t-t')t'^n H_{1,1}^{1,2}\left[\mathcal{K}_\gamma t'^\gamma|k|^\mu \middle|_{(0,\ 1)\ (-n,\gamma)}^{(-n,1)}\right], \tag{18}$$

where $H_{p,q}^{m,n}\left[x\middle|_{(b,\ B)}^{(a,A)}\right]$ is the Fox H function [42] (for details, see Appendix), $\Lambda_n(t) = \Upsilon(t)$ for $n = 1$ and

$$\Lambda_n(t) = \int_0^t dt_{n-1}\Upsilon(t-t_{n-1})\int_0^{t_{n-1}} dt_{n-2}\Upsilon(t_{n-2}-t_{n-3})\cdots\int_0^{t_2} dt_1\Upsilon(t_2-t_1)\Upsilon(t_1) \tag{19}$$

for $n > 1$, and

$$\Upsilon(t) = k_f(t) - \int_0^t dt' k_f(t-t')\int_0^{t'} d\bar{t}k_b(\bar{t}) + \int_0^t dt' k_f(t-t')\sum_{n=2}^{\infty}(-1)^n\int_0^{t'} dt_{n-1}I_{k_b}(t'-t_{n-1})$$
$$\times\int_0^{t_{n-1}} dt_{n-2}I_{k_b}(t_{n-2}-t_{n-1})\cdots\int_0^{t_2} dt_1 I_{k_b}(t_2-t_1)I_{k_b}(t_1), \tag{20}$$

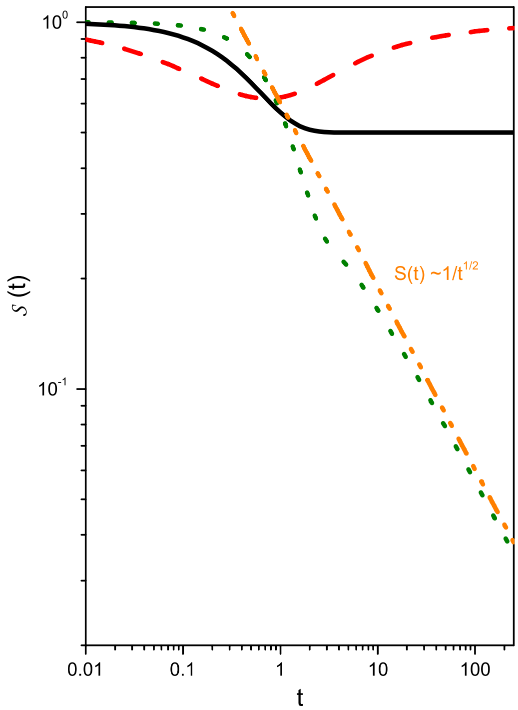

Fig. 3. Behavior of $\mathcal{S}(t)$ by considering different $k_f(t)$ and $k_b(t)$. The red (dashed), black (solid), and green (dotted) lines corresponds to the cases $k_f(s) \sim \bar{k}_f s^{\eta_f}$, $k_b(s) = \bar{k}_b$, $k_f(s) = \bar{k}_f$, $k_b(s) = \bar{k}_b$, and $k_f(s) = \bar{k}_f/s^{\eta_f}$, $k_b(s) = \bar{k}_b$. Note that, depending on the choice of rates, the survival probability may exhibit different asymptotic behaviors, i.e., we may have $\mathcal{S}(t) \to$ const or $\mathcal{S}(t) \to 1/t^{\delta}$ $(0 < \delta < 1)$ for $t \to \infty$. For simplicity, we consider $\bar{k}_f = 1$, $\eta_f = 1/2$, $\rho_i = 1$, $\Gamma_i = 0$, and $\bar{k}_b = 1$ in arbitrary unities.

where $I_{k_b}(t) = \int_0^t dt' k_b(t')$. The inverse Fourier transform of Eq. (18) yields

$$\mathcal{G}(x,t) = \frac{1}{\mu|x|} H^{2,1}_{3,3}\left[\frac{|x|}{(\mathcal{K}_\gamma t^\gamma)^{\frac{1}{\mu}}}\left|\begin{matrix}\left(1,\frac{1}{\mu}\right),\left(1,\frac{\gamma}{\mu}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1,\frac{1}{\mu}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right] + \sum_{n=1}^{\infty}\frac{(-1)^n}{\mu|x|\Gamma(1+n)}\int_0^t dt' \Lambda(t-t')t'^n H^{2,1}_{3,3}\left[\frac{|x|}{(\mathcal{K}_\gamma t^\gamma)^{\frac{1}{\mu}}}\left|\begin{matrix}\left(1,\frac{1}{\mu}\right),\left(1+n,\frac{\gamma}{\mu}\right),\left(1,\frac{1}{2}\right)\\(1,1),\left(1+n,\frac{1}{\mu}\right),\left(1,\frac{1}{2}\right)\end{matrix}\right.\right] \quad (21)$$

(see Fig. 4) and, consequently, the distribution for an arbitrary initial condition is given by

$$\rho(x,t) = \int_{-\infty}^{\infty} dx' \rho(x',0)\mathcal{G}(x-x',t) + \int_0^t dt' \int_{-\infty}^{\infty} dx' \Gamma(x',0)\Pi(t')\mathcal{G}(x-x',t-t') \quad (22)$$

with

$$\Pi(t) = I_{k_b}(t) + \sum_{n=1}^{\infty}(-1)^n \int_0^t dt_{n-1} I_{k_b}(t-t_{n-1}) \int_0^{t_{n-1}} dt_{n-2} I_{k_b}(t_{n-1}-t_{n-2}) \cdots \int_0^{t_2} dt_1 I_{k_b}(t_2-t_1) I_{k_b}(t_1). \quad (23)$$

Fig. 5 shows the behavior of the distribution when the reaction term is considered. Note that the distribution presents an anomalous spreading more evidenced when the initial condition of the system is characterized by $\rho_i = 0$ and $\Gamma_i = 1$. Fig. 6 shows the behavior of $\rho(x,t)$ for different functions $k_f(t)$ and $k_b(t)$.

3. Conclusions

We have investigated a fractional diffusion equation in the presence of a reaction term. The reaction term is given by a kinetic equation where $k_f(t)$ and $k_b(t)$ may represent the rates connected to adsorption, desorption and absorption processes. We obtained the solution for $k_f(t)$ and $k_b(t)$ arbitraries and investigated how these quantities can influence the diffusion of the system as illustrated in Figs. 1 and 5 for the mean square displacement and the distribution. In particular, Fig. 1 shows that, depending on the initial condition, the system for short times can exhibit an anomalous diffusion even for

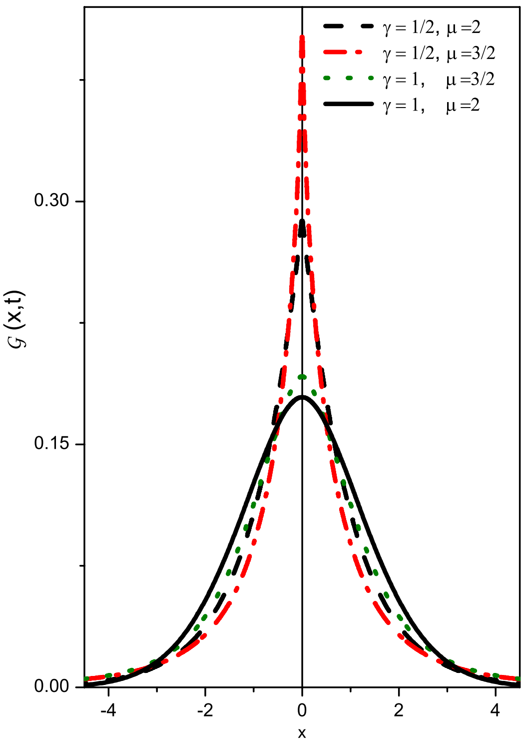

Fig. 4. Behavior of $\mathcal{G}(x,t)$ versus x by considering different values of μ and γ. For simplicity, we consider $k_f(t)=k_f'=1,\ k_b(t)=k_b'=1,\ \mathcal{K}_\gamma=1$, and $t=1$ in arbitrary unities. We can observe that a direct influence of γ and μ on the shape of the Green function.

$\Gamma(x,t)$ governed by an usual kinetic equation, i.e., $k_f(t)\propto\delta(t)$ and $k_b(t)\propto\delta(t)$, and, for long times, be dominated by the regime imposed by the diffusive term. A stationary state can also be manifested depending on the choice of $k_f(t)$ and $k_b(t)$ as shown by Eq. (13). These points have a direct consequence on the survival probability reflecting the quantity of mobile particles present in the bulk.

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Appendix

The Fox H function (or H-function) may be defined in terms of the Mellin–Branes type integral [11,42]

$$H^{m,n}_{p,q}\left[x\left|^{(a_p,A_p)}_{(b_q,B_q)}\right.\right]=H^{m,n}_{p,q}\left[x\left|^{(a_1,A_1),\ldots,(a_p,A_p)}_{(b_1,B_1),\ldots,(b_q,B_q)}\right.\right]=\frac{1}{2\pi\mathrm{i}}\int_L\chi(\xi)x^{-\xi}\mathrm{d}\xi$$

$$\chi(\xi)=\frac{\Pi^m_{j=1}\Gamma\left(b_j-B_j\xi\right)\Pi^n_{j=1}\Gamma\left(1-a_j+A_j\xi\right)}{\Pi^q_{j=m+1}\Gamma\left(1-b_j+B_j\xi\right)\Pi^p_{j=n+1}\Gamma\left(a_j-A_j\xi\right)}\tag{24}$$

where m, n, p and q are integers satisfying $0\le n\le p$ and $1\le m\le q$. It may also be defined by its Mellin transform

$$\int_0^\infty H^{m,n}_{p,q}\left[ax\left|^{(a_p,A_p)}_{(b_q,B_q)}\right.\right]x^{\xi-1}\mathrm{d}x=a^{-\xi}\chi(\xi).\tag{25}$$

Here, the parameters have to be defined such that $A_j>0$ and $B_j>0$ and $a_j(b_h+\nu)\neq B_h(a_j-\lambda-1)$ where $\nu,\lambda=0,1,2,\ldots,\ h=1,2,\ldots,m$ and $j=1,2,\ldots,m$. The contour L separates the poles of $\Gamma\left(b_j-B_j\xi\right)$ for $j=1,2,\ldots,m$ from those of $\Gamma\left(1-a_j+A_j\xi\right)$ for $j=1,2,\ldots,n$ [42]. The H-function is analytic in x if either (i) $x\neq 0$ and $M>0$ or (ii) $0<|x|<1/B$ and $M=0$, where $M=\sum_{j=1}^q B_j-\sum_{j=1}^p A_j$ and $B=\prod_{j=1}^p A_j^{A_j}\prod_{j=1}^q B_j^{-B_j}$.

Some useful properties of the Fox H function found in Refs. [11,42] are listed below.

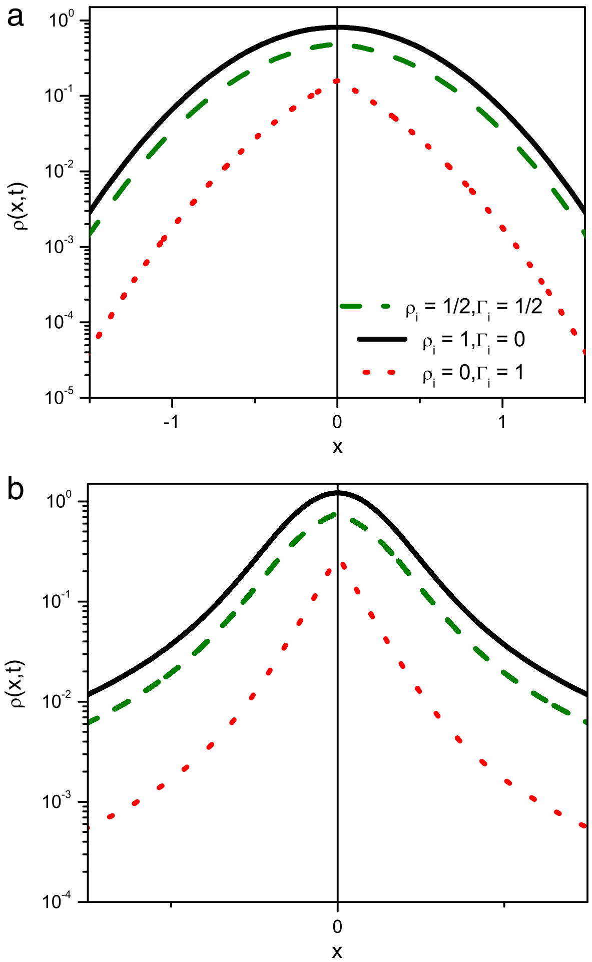

Fig. 5. Behavior of $\rho(x,t)$ by considering different initial conditions. (a) illustrates the case $\mu = 2$ and (b) the case $\mu = 3/2$. For simplicity, we consider $k_f = 1$, $k_b = 1$, $\gamma = 1$, $t = 0.1$, and $\mathcal{K}_\gamma = 1$ in arbitrary unities.

(i) The H-function is symmetric in the pairs $(a_1, A_1), \ldots, (a_p, A_p)$, likewise $(a_{n+1}, A_{n+1}), \ldots, (a_p, A_p)$; in $(b_1, B_1), \ldots, (b_q, B_q)$ and in $(b_{n+1}, B_{n+1}), \ldots, (b_q, B_q)$.

(ii) For $k > 0$

$$H^{m,n}_{p,q}\left[x\left|^{(a_p,A_p)}_{(b_q,B_q)}\right.\right] = kH^{m,n}_{p,q}\left[x^k\left|^{(a_p,kA_p)}_{(b_q,kB_q)}\right.\right] . \quad (26)$$

(iii) The multiplication rule is

$$x^k H^{m,n}_{p,q}\left[x\left|^{(a_p,A_p)}_{(b_q,B_q)}\right.\right] = H^{m,n}_{p,q}\left[x\left|^{(a_p+kA_p,A_p)}_{(b_q+kB_q,B_q)}\right.\right] . \quad (27)$$

(iv) For $n \geq 1$ and $q > m$,

$$H^{m,n}_{p,q}\left[x\left|^{(a_1,A_1)(a_2,A_2)\cdots(a_p,A_p)}_{(b_1,B_1)\cdots(b_{q-1},B_{q-1})(a_1,A_1)}\right.\right] = H^{m,n-1}_{p-1,q-1}\left[x\left|^{(a_2,A_2)\cdots(a_p,A_p)}_{(b_1,B_1)\cdots(b_{q-1},B_{q-1})}\right.\right] . \quad (28)$$

(v) The relation between the generalized Mittag-Leffler function and the Fox H function is given by

$$E_{\alpha,\beta}(x) = \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(\beta+\alpha n)} = H^{1,1}_{1,2}\left[-x\left|^{(0,1)}_{(0,1)(1-\beta,\alpha)}\right.\right] . \quad (29)$$

It is also interesting to note that $E_{\alpha,1}(x) = E_\alpha(x)$.

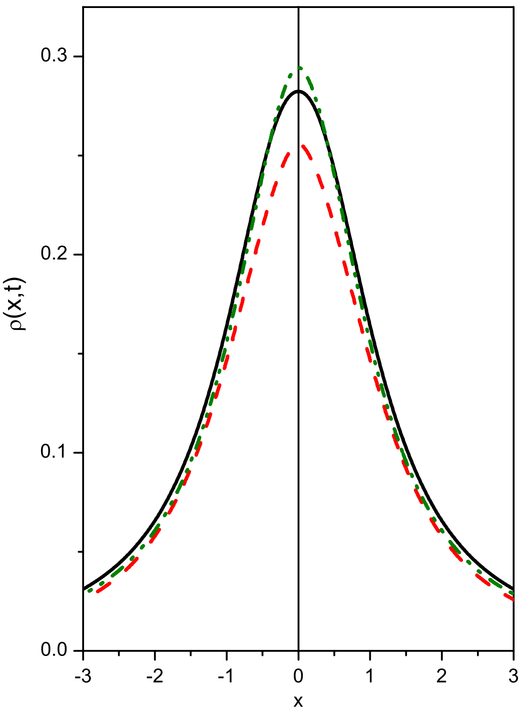

Fig. 6. Behavior of $\rho(x,t)$ versus x by considering different $k_f(t)$ and $k_b(t)$. The black, red, and green line correspond to $k_f(t) = k'_f e^{-t}$ with $k_b(t) = k'_b e^{-t}$, $k_f(t) = k'_f$ with $k_b(t) = k'_b e^{-t}$, and $k_f(t) = k'_f$ with $k_b(t) = k'_b$, respectively. For simplicity, we consider $k'_f = 5$, $k'_b = 1/2$, $\gamma = 1$, $\mu = 1.1$, $t = 1/2$, and $\mathcal{K}_\gamma = 2$ in arbitrary unities. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

(vi) If the poles of $\prod_{j=1}^{m} \Gamma\left(b_j - B_j\xi\right)$ are simple, the following series expansion is valid:

$$H_{p,q}^{m,n}\left[x\left|\begin{matrix}(a_p,A_p)\\(b_q,B_q)\end{matrix}\right.\right] = \sum_{h=1}^{m}\sum_{\nu=0}^{\infty}\frac{(-1)^\nu x^{(b_h+\nu)/B_h}}{\nu! B_h}\frac{\Pi_{j=1,j\neq h}^{m}\Gamma\left(b_j-\frac{B_j}{B_h}(b_h+\nu)\right)}{\Pi_{j=m+1}^{q}\Gamma\left(1-b_j+\frac{B_j}{B_h}(b_h+\nu)\right)} \times \frac{\Pi_{j=1}^{n}\Gamma\left(1-a_j+\frac{A_j}{B_h}(b_h+\nu)\right)}{\Pi_{j=n+1}^{p}\Gamma\left(a_j-\frac{A_j}{B_h}(b_h+\nu)\right)}. \tag{30}$$

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