Solutions for a non-Markovian diffusion equation

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ABSTRACT

Solutions for a non-Markovian diffusion equation are investigated. For this equation, we consider a spatial and time dependent diffusion coefficient and the presence of an absorbent term. The solutions exhibit an anomalous behavior which may be related to the solutions of fractional diffusion equations and anomalous diffusion.

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1. Introduction

One of the most important phenomena present in the nature is the diffusion which is a stochastic process. Depending on the conditions or the characteristics of the system it may be Markovian or non-Markovian. A typical diffusive process which may be related to a Markovian process is the one with mean square displacement proportional to the time, i.e., $\langle (x - \langle x \rangle)^2 \rangle \sim t$. On the other hand, systems with anomalous diffusion have an unusual spreading and, consequently, the mean square displacement is not proportional to the time and in some cases is not finite. This manner, the stochastic processes which govern these system with anomalous diffusion has non-Markovian characteristics. Physical situations connected to anomalous diffusion may be found in porous substrate [1], diffusion of high molecular weight polyisopropylacrylamide in nanopores [2], highly confined hard disk fluid mixture [3], fluctuating particle fluxes [4], diffusion on fractals [5], ferrofluid [6], nanoporous material [7], and colloids [8].

Several approaches have been used for investigating these phenomena with usual or anomalous diffusion. They are essentially the Langevin equations [9], master equations [10], random walks [11], Fokker–Planck equations with spatial and time dependent coefficients, and its extensions by considering nonlinear terms [12] or fractional derivatives [13,14]. The study of these formalism has also been performed by considering several situations such as the presence of external forces [15,16], reaction terms [17–19], linear response [20], and surface effects [21,22] to comprehend the formalism and the potential applications to physical systems. In this direction, we devote this work to investigate the solutions for the non-Markovian diffusion equation:

$$\frac{\partial}{\partial t}\rho(x,t) = \int_0^t dt' \frac{\partial}{\partial x}\left(\mathcal{D}(x, t-t')\frac{\partial}{\partial x}\rho(x,t')\right) - \int_0^t dt'\alpha(t-t')\rho(x,t'), \tag{1}$$

where the (dimensionless) diffusion coefficient is given by $\mathcal{D}(x,t) = \bar{\mathcal{D}}(t)|x|^{-\eta}$ and $\alpha(t)$ is an (dimensionless) absorbent term which may be, for example, related to a reaction process. The solutions for Eq. (1) are investigated by considering the boundary condition $\rho(\pm\infty, t) = 0$ and the initial condition $\rho(x,0) = \bar{\rho}(x)$, which is normalized, i.e., $\int_{-\infty}^{\infty} dx\, \rho(x,0) = \int_{-\infty}^{\infty} dx\, \bar{\rho}(x) = 1$. Note that this equation has the diffusive term different from the one worked out in [23] which considers the presence of spatial fractional derivatives and, consequently, is not able to describe situations with a nonconstant diffusion coefficient, i.e., inhomogeneous situations. In addition, it may be obtained from the Comb-Model by employing the procedure presented in [24,25] with suitable changes. Eq. (1) is also related to several

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contexts, in particular, the fractional diffusion equations [13,14], fractional diffusion equations of distributed order [26,27], and Cattaneo equation [28,29] by a convenient choice of the time dependence present in the diffusion. For this equation, we obtain solutions by using the Green function approach and by choosing appropriate time dependent forms of the diffusion coefficient and the absorbent term. In particular, our analysis extends the results found in [30–33]. These developments are done in Section 2 and in Section 3 we present our conclusions.

2. Non-Markovian diffusion equation

Let us start our analysis about the solutions and the survival probability by substituting in Eq. (1) the diffusion coefficient $\mathcal{D}(x,t) = \bar{\mathcal{D}}(t)|x|^{-\eta}$ and considering the absence of the absorbent term. For this case, Eq. (1) may be written as

$$\frac{\partial}{\partial t}\rho(x,t) = \int\limits_0^t dt'\,\bar{\mathcal{D}}(t-t')\frac{\partial}{\partial x}\left(|x|^{-\eta}\frac{\partial}{\partial x}\rho(x,t')\right). \tag{2}$$

Note that we are considering an arbitrary time dependence to the diffusion coefficient and later on we discuss possible choices of the diffusion coefficient. In order to find the solution for this equation subjected to these conditions, we may use the Laplace transform and, after, the Green function approach. By applying the Laplace transform, it is possible to reduce the integro-differential Eq. (2) to an inhomogeneous ordinary differential equation which can be solved with the Green function approach. Applying the Laplace transform, we obtain

$$\bar{\mathcal{D}}(s)\frac{d}{dx}\left(|x|^{-\eta}\frac{d}{dx}\rho(x,s)\right) = s\rho(x,s) - \rho(x,0). \tag{3}$$

The solution to Eq. (3) can be written as

$$\rho(x,s) = \int\limits_{-\infty}^{\infty} dx'\,\mathcal{G}(x,x',s)\bar{\rho}(x'), \tag{4}$$

with the Green function determined by the following equation

$$\bar{\mathcal{D}}(s)\frac{d}{dx}\left(|x|^{-\eta}\frac{d}{dx}\mathcal{G}(x,s)\right) - s\mathcal{G}(x,s) = \delta(x-x'), \tag{5}$$

and subjected to the condition $\mathcal{G}(\pm\infty, x', s) = 0$. In order to solve Eq. (5), we may use the eigenfunctions which are obtained from the Sturm–Liouville problem [34] related to the spatial operator of this equation, i.e.,

$$\frac{d}{dx}\left(|x|^{-\eta}\frac{d}{dx}\Psi(k,x)\right) = -k^2\Psi(k,x), \tag{6}$$

subjected to the required boundary conditions. Performing some calculations by using well-established formulas [35], and taking the boundary condition $\Psi(\pm\infty, t) = 0$ into account, it is possible to show that this equation has as solution the functions

$$\Psi_+(k,x) = |x|^{\frac{1}{2}(1+\eta)}J_{-\nu}\left(\frac{2|k|}{2+\eta}|x|^{\frac{1}{2}(2+\eta)}\right) \tag{7}$$

and

$$\Psi_-(k,x) = x|x|^{\frac{1}{2}(\eta-1)}J_\nu\left(\frac{2|k|}{2+\eta}|x|^{\frac{1}{2}(2+\eta)}\right). \tag{8}$$

In Eqs. (7) and (8), the signs $+$ and $-$ refer, respectively, to the even and odd functions, $J_\nu(x)$ is the Bessel function, $\nu = (1+\eta)/(2+\eta)$, and k is a constant (eigenvalue) which is related to the Sturm–Liouville problem of the spatial operator. In this manner, after some calculations by using the orthogonality condition of these eigenfunctions, it is possible to show that the solution to Eq. (5) is given by

$$\mathcal{G}(x,x',s) = \frac{1}{2(2+\eta)}\sum_{i=-,+}\int\limits_{-\infty}^{\infty} dk\,|k|\Psi_i(k,x')\Psi_i(k,x)\Phi(k,s) \tag{9}$$

with $\Phi(k,s) = 1/(s + \bar{\mathcal{D}}(s)k^2)$.

Notice that to perform the inverse Laplace transform for an arbitrary dependence on $\mathcal{D}(s)$ leads us to cumbersome calculations. To circumvent this difficulty, we have to make a choice of the diffusion coefficient which can be motivated by the physical situation under investigation. Typical dependencies for the diffusion coefficient are $\bar{\mathcal{D}}(t) = \tilde{\mathcal{D}}t^{\gamma-2}/\Gamma(\gamma-1)$ ($\bar{\mathcal{D}}(s) = \tilde{\mathcal{D}}s^{1-\gamma}$), $\bar{\mathcal{D}}(t) = \tilde{\mathcal{D}}e^{-t/\tau}/\tau$ ($\bar{\mathcal{D}}(s) = \tilde{\mathcal{D}}/(1+s\tau)$) and $\bar{\mathcal{D}}(t) = \tilde{\mathcal{D}}\delta(t)$ ($\bar{\mathcal{D}}(s) = \tilde{\mathcal{D}}$) which correspond, respectively, to the fractional diffusion [13], Cattaneo equation [28, 29], and the usual diffusion equation [36], as discussed before. It is also possible to consider other time dependencies for the diffusion coefficient such as the ones related to the fractional diffusion equations of distributed order [26,27]. In this context, we expect that Eq. (2) exhibits different diffusive regimes depending on the time dependence considered. This feature can be verified, for example, by evaluating the variance, i.e., $\sigma^2 = \langle(x - \langle x\rangle)^2\rangle$, for the simplified situation characterized by the initial condition $\rho(x,0) = \delta(x)$ with $\eta = 0$ without loss of generality. In particular, for this case, $\sigma^2 = 2\int_0^t dt'(t-t')\bar{\mathcal{D}}(t')$ which, for $\bar{\mathcal{D}}(t) = \tilde{\mathcal{D}}\delta(t)$, recovers the usual spreading,
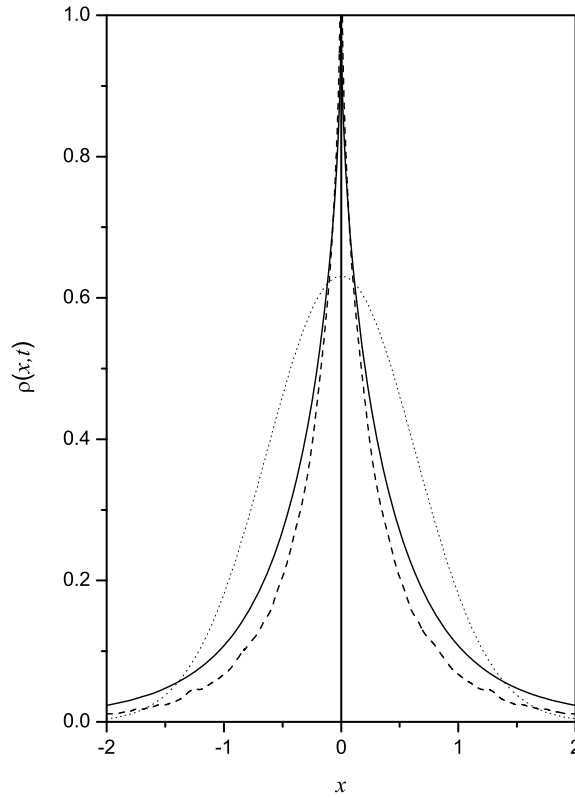
Fig. 1. Behavior of $\rho(x,t)$ versus x is illustrated. The solid line corresponds the case $\tilde{\mathcal{D}} = 1$ and $\mathcal{D}_\gamma = 1$, with $\eta = -1/2$ and $\gamma = 2/3$, and the dashed line is the case $\tilde{\mathcal{D}} = 0$ and $\mathcal{D}_\gamma = 2$, with $\eta = -1/2$ and $\gamma = 2/3$. The dotted line is the usual case, i.e., $\tilde{\mathcal{D}} = 1$ and $\mathcal{D}_\gamma = 1$, with $\eta = 0$ and $\gamma = 1$. We also consider, for simplicity, the initial condition $\rho(x,0) = \delta(x)$.

and for other choice lead us to an anomalous diffusion. In what follows, we consider the diffusion coefficient $\bar{\mathcal{D}}(s) = \mathcal{D}_\gamma s^{1-\gamma} + \tilde{\mathcal{D}}(s)$ ($\bar{\mathcal{D}}(t) = \mathcal{D}_\gamma t^{\gamma-2}/\Gamma(\gamma - 1) + \tilde{\mathcal{D}}(t)$), with $\tilde{\mathcal{D}}(s)$ arbitrary, enabling us to cover several situations. For this case, we obtain

$$\Phi(k,t) = E_\gamma\left(-\mathcal{D}_\gamma k^2 t^\gamma\right) + \sum_{n=1}^{\infty} \frac{(-1)^n}{\Gamma(1+n)\mathcal{D}_\gamma^n} \int_0^t dt' \, \Upsilon_n(t-t') H_{1,2}^{1,1}\left[\mathcal{D}_\gamma k^2 t^\gamma \Big|_{(n,1)\,(0,\gamma)}^{(n,1)}\right], \tag{10}$$

with

$$\Upsilon_n(t) = \int_0^t dt_n \, \Lambda(t-t_n) \int_0^{t_n} dt_{n-1} \, \Lambda(t_n - t_{n-1}) \cdots \int_0^{t_2} dt_1 \, \Lambda(t_2 - t_1)\Lambda(t_1), \tag{11}$$

and $\Lambda(t) = (1/\Gamma(1-\gamma)) \int_0^t dt' \, \tilde{\mathcal{D}}(t')/(t-t')^\gamma$, where $H_{p,q}^{m,n}[x|_{(b_1,B_1),\ldots,(b_q,B_q)}^{(a_1,A_1),\ldots,(a_p,A_p)}]$ is the Fox H function [37]. For the particular case $\bar{\mathcal{D}}(s) = \tilde{\mathcal{D}} + \mathcal{D}_\gamma s^{1-\gamma}$ ($\bar{\mathcal{D}}(t) = \tilde{\mathcal{D}}\delta(t) + \mathcal{D}_\gamma t^{\gamma-2}/\Gamma(\gamma-1)$), which corresponds to a mixing between the usual and the fractional relaxation, the above equation may be simplified to

$$\Phi(k,t) = \sum_{n=0}^{\infty} \frac{(-\mathcal{D}k^2 t)^n}{\Gamma(1+n)} H_{1,2}^{1,1}\left[\mathcal{D}_\gamma k^2 t^\gamma \Big|_{(-n,1)\,(-n,\gamma)}^{(0,1)}\right] \tag{12}$$

(see Fig. 1). To investigate the influence of the effects introduced by the spatial and time dependencies present in the diffusion coefficient we may analyze the asymptotic behavior of the variance for short and long times. It is possible to show that $\sigma^2 \propto t^{2\gamma/(2+\eta)}$ for short times and $\sigma^2 \propto t^{2/(2+\eta)}$ for long times. These approximated results show that the spreading of the distribution for long times is essentially governed by the spatial dependence present in the diffusion coefficient and may be subdiffusive or superdiffusive depending on η. The behavior for short times manifests the effect of the time dependence present in the diffusion coefficient, i.e., the dominant term exhibits a dependence on γ. In particular, for this case of short times, the behavior of the diffusive process may be subdiffusive or superdiffusive depending on the value of $2\gamma/(2+\theta)$. From Eq. (12) the exponential relaxation is recovered for $\mathcal{D}_\gamma = 0$, i.e., $\Phi(k,t) = e^{-\mathcal{D}k^2 t}$, and for $\tilde{\mathcal{D}} = 0$ the relaxation is governed by the Mittag-Leffler function, i.e., $\Phi(k,t) = E_\gamma(-\mathcal{D}_\gamma k^2 t^\gamma)$, as expected. For these two cases the Green function may be written as follows:

$$\mathcal{G}(x,x',t) = \frac{|xx'|^{\frac{1}{2}(1+\eta)}}{2(2+\eta)\mathcal{D}t} e^{-\frac{1}{(2+\eta)^2\mathcal{D}t}(|x|^{2+\eta}+|x'|^{2+\eta})}\left(I_{-\nu}\left(\frac{2|xx'|^{\frac{1}{2}(2+\eta)}}{(2+\eta)^2\mathcal{D}t}\right) + \frac{xx'}{|xx'|}I_\nu\left(\frac{2|xx'|^{\frac{1}{2}(2+\eta)}}{(2+\eta)^2\mathcal{D}t}\right)\right), \tag{13}$$

for the case $\mathcal{D}_\gamma = 0$, where $I_\nu(x)$ is the Bessel function of modified argument. For the case $\tilde{\mathcal{D}} = 0$, we obtain

$$\mathcal{G}(x, x', s) = \frac{1}{2(2+\eta)} \sum_{i=-,+} \int_{-\infty}^{\infty} dk \, |k| \Psi_i(k, x') \Psi_i(k, x) E_\gamma(-\mathcal{D}_\gamma k^2 t^\gamma). \tag{14}$$

Equation (14), after applying the identities presented in [38], may also be written as

$$\mathcal{G}(x, x', s) = \frac{2+\eta}{2|x|^{2+\eta}} |xx'|^{\frac{1}{2}(1+\eta)} \left\{ H_{2,[0:1],0,[0:2]}^{1,0,1,1,1} \left[\begin{array}{c|c} |\frac{x'}{x}|^{2+\eta} & \frac{(2-\nu}{2}, 1); (\frac{2+\nu}{2}, 1) \\ \frac{(2+\eta)^2 \mathcal{D}_\gamma t^\gamma}{|x|^{2+\eta}} & --; (0,1) \\ & (-\frac{\nu}{2}, 1); (\frac{\nu}{2}, 1); (0,1), (0,\gamma) \end{array} \right] \right.$$

$$\left. + \frac{xx'}{|xx'|} H_{2,[0:1],0,[0:2]}^{1,0,1,1,1} \left[\begin{array}{c|c} |\frac{x'}{x}|^{2+\eta} & (\frac{2+\nu}{2}, 1); (\frac{2-\nu}{2}, 1) \\ \frac{(2+\eta)^2 \mathcal{D}_\gamma t^\gamma}{|x|^{2+\eta}} & --; (0,1) \\ & (\frac{\nu}{2}, 1); (-\frac{\nu}{2}, 1); (0,1), (0,\gamma) \end{array} \right] \right\}, \tag{15}$$

where

$$H_{E,[A:C],F,[B,D]}^{L,M,M_1,N,N_1} \left[\begin{array}{c|c} x & (\varepsilon_1, \omega_1), \ldots, (\varepsilon_E, \omega_E) \\ & (a_1, \alpha_1), \ldots, (a_A, \alpha_A); (c_1, \gamma_1), \ldots, (c_C, \gamma_C) \\ y & (\xi_1, \varpi_1), \ldots, (\xi_F, \varpi_F) \\ & (b_1, \beta_1), \ldots, (b_B, \beta_B); (d_1, \delta_1), \ldots, (d_C, \delta_D) \end{array} \right], \tag{16}$$

is the generalized Fox H function [38].

Let us now incorporate the presence of an absorbent term to the previous analysis. In order to obtain the solution for this case, we also employ the above procedure based on the Laplace transform to simplify the integro-differential equation and the Green function approach. In this case, the solution is formally given by Eq. (4) with the Green function governed by equation

$$\bar{\mathcal{D}}(s) \frac{d}{dx} \left(|x|^{-\eta} \frac{d}{dx} \mathcal{G}(x, s) \right) - (s + \alpha(s)) \mathcal{G}(x, s) = \delta(x - x'), \tag{17}$$

and subjected to the condition $\mathcal{G}(\pm\infty, x', s) = 0$. The solution to Eq. (17) is given by

$$\mathcal{G}(x, x', s) = \frac{1}{2(2+\eta)} \sum_{i=-,+} \int_{-\infty}^{\infty} dk \, |k| \Psi_i(k, x') \Psi_i(k, x) \tilde{\Phi}(k, s) \tag{18}$$

with

$$\tilde{\Phi}(k, s) = \frac{1}{s + \bar{\mathcal{D}}(s) k^2 + \alpha(s)}. \tag{19}$$

Similarly to the situations analyzed for Eq. (2), we have to perform a choice of the diffusion coefficient and the absorbent term to avoid cumbersome calculations. For simplicity, we consider $\bar{\mathcal{D}}(s) = \tilde{\mathcal{D}} s^{1-\gamma}$ ($\bar{\mathcal{D}}(t) = \tilde{\mathcal{D}} t^{\gamma-2}/\Gamma(1-\gamma)$), with $\alpha(s)$ arbitrary, to perform the inverse Laplace transform. Note that the choice performed to the diffusion coefficient is connected to the fractional diffusion equations. After some calculations, for this case, it is possible to show that

$$\Phi(k, t) = E_\gamma(-\mathcal{D}_\gamma k^2 t^\gamma) + \sum_{n=1}^{\infty} \frac{(-1)^n}{\Gamma(1+n)} \int_0^t dt' \, \Omega_n(t - t') t'^{n\gamma} H_{1,2}^{1,1} \left[\mathcal{D}_\gamma k^2 t'^\gamma \Big|_{(0,1)\ (-n\gamma,\gamma)}^{(0,1)} \right], \tag{20}$$

with

$$\Omega_n(t) = \int_0^t dt_n \, \Theta(t - t_n) \int_0^{t_n} dt_{n-1} \, \Theta(t_n - t_{n-1}) \cdots \int_0^{t_2} dt_1 \, \Theta(t_2 - t_1) \Theta(t_1), \tag{21}$$

and $\Theta(t) = (1/\Gamma(1-\gamma)) \int_0^t dt' \, \alpha(t')/(t - t')^\gamma$. In Eq. (20), the first term is the Mittag–Leffler function, typical function which characterizes the time relaxation of the fractional diffusion equation, and the second term is due to the absorbent term which modifies the spreading of the system. In addition, depending on the choice of $\alpha(t)$ we may relate the solution with other contexts such as the solutions of the fractional diffusion equation of distributed order. In particular, for the case $\alpha(t) = \bar{\alpha} t^{\omega-1}/\Gamma(\omega)$ ($\bar{\alpha}$ is a nonnegative constant), Eq. (20) may be simplified to

$$\Phi(k, t) = E_\gamma(-\mathcal{D}_\gamma k^2 t^\gamma) + \sum_{n=1}^{\infty} \frac{(-\alpha)^n}{\Gamma(1+n)} H_{1,2}^{1,1} \left[\mathcal{D}_\gamma k^2 t^\gamma \Big|_{(0,1)\ (-(1-\omega)n,\gamma)}^{(0,1)} \right]. \tag{22}$$

Figure 2 shows the behavior of the solution by accomplishing Eq. (22) for typical values of γ, η, and ω, by considering, for simplicity, the initial condition $\rho(x, 0) = \delta(x)$. It is worth mentioning that the nonlocal form of the absorption term considered here produces an anomalous spreading of the solution which can be verified by the shape of the distributions in Fig. 2. In fact, it illustrates the effects on
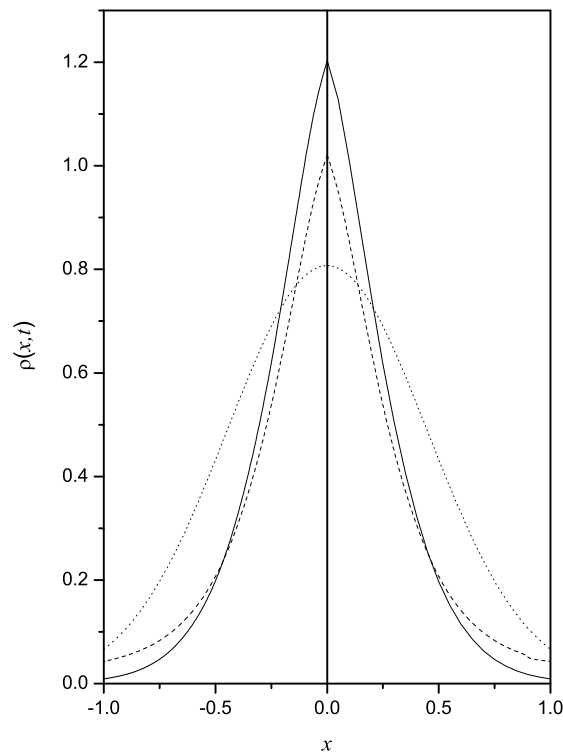
Fig. 2. This figure illustrates $\rho(x,t)$ versus x by considering the presence of an absorbent term, i.e., the time dependent function given by Eq. (22) and two typical values of ω, with $\gamma = 1$. The dashed line corresponds the case $\omega = 1/3$, with $\eta = -1/2$, whereas the solid line is the case $\omega = 1/2$, with $\eta = -1/2$. The dotted line is the usual case, i.e., $\omega = 1$ and $\eta = 0$. We also consider, for simplicity, $\mathcal{D}_\gamma = 1$ and $\bar{\alpha} = 1$.

the spreading of the system due to the spatial and time dependencies presented by the diffusion coefficient and the effects introduced by the absorbent term which is nonlocal. In particular, in the absence of the absorbent term the variance of the system is governed by the equation $\sigma^2 \propto t^{2\gamma/(2+\eta)}$. By incorporating the previous absorbent term, the asymptotic behavior of the variance is $\sigma^2 \propto t^{2\gamma/(2+\eta)}$, for short times, and, for long times, it is given by $\sigma^2 \propto t^{\bar{\omega}+\varepsilon} E_{\bar{\omega},1+\varepsilon}^{(1)}(-\bar{\alpha}t^{\bar{\omega}})$, with $\bar{\omega} = 1 + \omega$, $\varepsilon = 2(\gamma - 1 - \omega)/(2+\eta)$ and $E_{\alpha,\beta}^{(n)}(x) = d^n E_{\alpha,\beta}(x)/dx^n$ where $E_{\alpha,\beta}(x)$ is the Mittag-Leffler function [39].

3. Discussions and conclusions

We have investigated the solutions for a non-Markovian diffusion equation with a spatial and time dependent diffusion coefficient in presence of an absorbent term. We first worked out the situations without absorbent term by performing the following choice $\bar{\mathcal{D}}(t) = \mathcal{D}_\gamma t^{\gamma-2}/\Gamma(\gamma-1) + \tilde{\mathcal{D}}(t)$ for the time dependence of the diffusion coefficient. The solution for this case was formally obtained and some particular situations showing an anomalous spreading due to the presence of the time or the spatial dependencies present in the diffusion coefficient were analyzed. In addition, we remark that the results found in this context extend results found in [30–33] by incorporating fractional derivatives or spatial dependence on the diffusion coefficient. After that, we have incorporated an absorbent term in the diffusion equation and discussed that this additional term may be related to several physical situations and, in particular, to the fractional derivative of distributed order. For this case, we have also obtained an exact solution. We hope that the results found here may be useful to investigate situations where the anomalous diffusion is present.

Acknowledgements

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