SOLUTIONS FOR A FRACTIONAL DIFFUSION EQUATION WITH RADIAL SYMMETRY AND INTEGRO-DIFFERENTIAL BOUNDARY CONDITIONS

by

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The solutions for a dimensional system with radial symmetry and governed by a fractional diffusion equation have been investigated. More specifically, a spherical system was considered, being defined in the semi-infinity interval [R, ∞) and subjected to surface effects described in terms of integro-differential boundary conditions which has many practical applications. The analytical solutions were obtained by using the Green function approach, showing a broad range of different behaviors which can be related to anomalous diffusion. The analyses also considered the influence of the parameters of the analytical solution in order to describe a more realistic scenario.

Key words: *fractional derivative, diffusion equation, anomalous diffusion*

Introduction

Recently, fractional calculus [1-4] has played a significant role to investigate several scenarios in engineering [5-7], biology [8, 9], and physics [10]. In this context, the situations connected to anomalous diffusion [11] have received as much attention as the usual approach [12, 13] does not provide a suitable description of the experimental results behavior, requiring a proper and more realistic mathematical representation. In order to address this issue, by using fractional calculus, the diffusion equation (or Fokker-Planck equation) and the Langevin equation have been successfully extended and, consequently, employed to investigate several important scenarios as previously reported in [14-21]. In these studies, one of the main features is the nonlinear time dependence exhibited by the mean-square displacement which is usually characterized by $\langle (r-\langle r\rangle)^2\rangle \sim t^{\alpha}$. The superdiffusion occurs for $\alpha > 1$, being commonly related, for example, to active transport [22-25], while the subdiffusive behavior, $\alpha < 1$, may be related to the molecular crowding [26] and fractal structures [27].

This paper reports the solutions of a fractional diffusion equation by taking into account the dimensional case with spherical symmetry and subjected to an integro-differential boundary condition which can be related to surface effects such as absorption, adsorption

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and/or desorption on a surface in contact with the particles present in the bulk. It can also recover the usual Robin boundary condition and be related to a reaction process [28]. Thus, for the particles in the bulk, one can consider them to be governed by the fractional diffusion equation:

$$\frac{\partial}{\partial t}\rho(r,t) = \mathcal{K}_{\gamma 0}\mathcal{D}_t^{1-\gamma}[\nabla^2\rho(r,t)] \tag{1}$$

where K_γ is the diffusion coefficient, $0 < \gamma \leq 1$ (for $\gamma = 1$ usual diffusion, $0 < \gamma < 1$ subdiffusion), and the fractional time derivative is the Riemann-Liouville [3], defined by:

$${}_0\mathcal{D}_t^{\overline{\alpha}}[\rho(r,t)] = \frac{1}{\Gamma(n-\overline{\alpha})}\frac{\mathrm{d}^n}{\mathrm{d}t^n}\int_0^t \mathrm{d}t' \frac{\rho(r,t')}{(t-t')^{1+\overline{\alpha}-n}} \tag{2}$$

with $n-1 < \overline{\alpha} < n.$ The initial condition is given by $\rho(r,0) = \varphi(r),$ where $\varphi(r)$ is initially normalized, and the boundary conditions considered here are given by:

$$\mathcal{K}_\gamma\, {}_0\mathcal{D}_t^{1-\gamma}\left[\frac{\partial}{\partial r}\rho(r,t)\right]\bigg|_{r=\mathcal{R}} = \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \mathrm{d}t'\kappa(t-t')\rho(\mathcal{R},t') \tag{3}$$

$$\rho(r,t)\big|_{r=\infty} = \Phi(t) \tag{4}$$

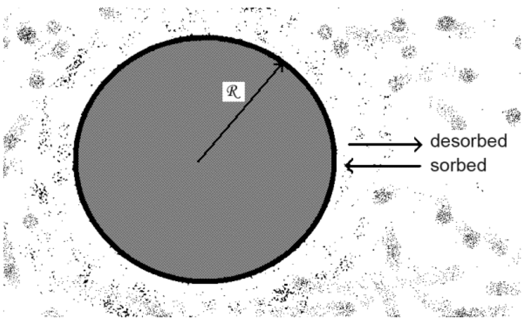

Figure 1. A possible application of the formalism where the particles are sorbed, and may be desorbed by an spherical surface

where $\Phi(t)$ is an arbitrary time dependent function. Note that the boundary condition represented by eq. (3) may be related to several situations, for example [14, 16, 17, 28], depending on the choice of parameter γ and function $\kappa(t)$. From a phenomenological point of view, the choice of the kernel function in eq. (3) can be related, for example, to the surface irregularity [29] which is an important issue in adsorption-desorption, diffusion, and catalysis [30, 31]. Figure 1 presents a representation of the adsorption-desorption phenomena considering a spherical particle.

In the paper, the section *Fractional diffusion equation and solutions* is devoted to the investigation of the solutions and the processes related to eq. (1) taking into account the boundary conditions given by eqs. (3) and (4).

Fractional diffusion equation and solutions

The first step starts with the discussion regarding the time dependent solutions of eq. (1) subjected to the previous boundary conditions. In order to face this problem, one can use the Laplace transform $\mathcal{L}\{\rho(r,t)\} = \overline{\rho}(r,s),$ and $\mathcal{L}^{-1}\{\overline{\rho}(r,s)\} = \rho(r,t),$ and the Green function approach. After applying the Laplace transform, the previous equations can be rewritten:

$$\mathcal{K}_\gamma s^{1-\gamma}\nabla^2\overline{\rho}(r,s) = s\overline{\rho}(r,s) - \rho(r,0) \tag{5}$$

and

$$\mathcal{K}_\gamma s^{1-\gamma}\frac{\partial}{\partial r}\bar{\rho}(r,s)\Big|_{r=\mathcal{R}} = s\bar{\kappa}(s)\bar{\rho}(\mathcal{R},s) \tag{6}$$

$$\bar{\rho}(r,s)\Big|_{r=\infty} = \bar{\Phi}(s) \tag{7}$$

By using Green function approach, the solution of eq. (5), subjected to the conditions given by eqs. (6) and (7), can be formally written:

$$\bar{\rho}(r',s) = \bar{\Phi}(s) - \int_0^\infty \mathrm{d}r r^2[\varphi(r) - s\bar{\Phi}(s)]\bar{\mathcal{G}}(r,r';s) + \mathcal{R}^2 s\bar{\kappa}(s)\bar{\Phi}(s)\bar{\mathcal{G}}(\mathcal{R},r';s) \tag{8}$$

with the Green function obtained from the equation:

$$\mathcal{K}_\gamma s^{1-\gamma}\nabla^2\bar{\mathcal{G}}(r,r';s) - s\bar{\mathcal{G}}(r,r';s) = \frac{1}{r'^2}\delta(r-r') \tag{9}$$

with the boundary conditions:

$$\mathcal{K}_\gamma s^{1-\gamma}\frac{\partial}{\partial r}\bar{\mathcal{G}}(r,r';s)\Big|_{r=\mathcal{R}} = s\bar{\kappa}(s)\bar{\mathcal{G}}(\mathcal{R},r';s) \tag{10}$$

$$\bar{\mathcal{G}}(r,r';s)\Big|_{r=\infty} = 0 \tag{11}$$

By solving eq. (9), results the Green function given by the expression:

$$\bar{\mathcal{G}}(r,r';s) = -\frac{1}{2rr's\sqrt{\dfrac{\mathcal{K}_\gamma}{s^\gamma}}}\left(\mathrm{e}^{-\sqrt{\frac{s^\gamma}{\mathcal{K}_\gamma}}|r-r'|} - \mathrm{e}^{-\sqrt{\frac{s^\gamma}{\mathcal{K}_\gamma}}|r+r'-2R|}\right) - \\ -\frac{1}{rr'}\frac{\mathrm{e}^{-\sqrt{\frac{s^\gamma}{\mathcal{K}_\gamma}}|r+r'-2R|}}{s\sqrt{\dfrac{\mathcal{K}_\gamma}{s^\gamma}} + s\kappa(s) + \dfrac{\mathcal{K}_\gamma}{\mathcal{R}}s^{1-\gamma}} \tag{12}$$

Note that the effect of the surface on the solutions is given by the presence of the $\kappa(s)$, or $\kappa(t)$, in the last term of eq. (12). Depending on the choice of this function, the system can be physically characterized by an absorption, or adsorption – desorption, and a reaction process. In the last case, $\kappa(s)$ is related to the rate of the reaction process. For example, $\kappa(s) = \kappa'/(1 + s\tau)$ $[\kappa(t) = (\kappa'/\tau)\mathrm{e}^{-t/\tau}]$ is related to a Debye relaxation, connected a first order kinetic equation; $\kappa(s) = \kappa'/[(1 + (s\tau)^\delta]$ $\{\kappa(t) = (\kappa'/\tau)t^{\delta-1}E_{\delta,\delta}[-(t/\tau)^\delta]\}$ is connected to a fractional kinetic equation where memory effects are present, leading to a non-Debye relation. Among others, a typical choice for a reaction process is given the expression $\kappa(s) = \kappa'/s$. In addition, by using these results it is also possible to find the survival probability, $\mathcal{S}(t) = \int_{\mathcal{R}}^\infty \mathrm{d}r r^2\rho(r,t)$, which is connected to the quantity of substance present in the bulk. In fact, after some calculations with $\Phi(t) = 0$, one can obtain that:

$$\overline{\mathcal{S}}(s)=\frac{1}{s}\left(1-\mathcal{R}\int_{\mathcal{R}}^{\infty}\mathrm{d}\tilde{r}\tilde{r}\varphi(\tilde{r})\mathrm{e}^{-\sqrt{\frac{s^{\gamma}}{\mathcal{K}_{\gamma}}}(\tilde{r}-\mathcal{R})}\right)+$$
$$+\frac{\mathcal{R}+\sqrt{\frac{\mathcal{K}_{\gamma}}{s^{\gamma}}}}{s(1+\overline{\kappa}(s)s^{\gamma/2}\big/\sqrt{\mathcal{K}_{\gamma}}+\sqrt{\mathcal{K}_{\gamma}}\big/(\mathcal{R}\,s^{\gamma/2})}\int_{\mathcal{R}}^{\infty}\mathrm{d}\tilde{r}\tilde{r}\varphi(\tilde{r})\mathrm{e}^{-\sqrt{\frac{s^{\gamma}}{\mathcal{K}_{\gamma}}}(\tilde{r}-\mathcal{R})} \tag{13}$$

which, according to the choice of $\overline{\kappa}(s)$, may lead to different behaviors.

Let us consider the case of $\overline{\kappa}(s)=\kappa'/s^{\alpha}$, where for $\alpha\neq 1$ there is the introduction of memory effect, and for $\alpha = 0$ the usual Robin boundary condition is recovered, being related to a reaction process. By performing the inverse Laplace transform, one can obtain eq. (12) that can be written:

$$\mathcal{G}(r,r';t)=-\frac{1}{\sqrt{4K_{\gamma}t^{\alpha}rr'}}\left\{\mathrm{H}_{1,1}^{1,0}\left[\frac{|r-r'|}{\sqrt{K_{\gamma}t^{\gamma}}}\middle|\begin{matrix}\left(1-\frac{\gamma}{2},\frac{\gamma}{2}\right)\\(0,1)\end{matrix}\right]-\mathrm{H}_{1,1}^{1,0}\left[\frac{1}{\sqrt{K_{\gamma}t^{\gamma}}}|r+r'-2\mathcal{R}|\middle|\begin{matrix}\left(1-\frac{\gamma}{2},\frac{\gamma}{2}\right)\\(0,1)\end{matrix}\right]\right\}-$$
$$-\frac{1}{rr'}\int_{0}^{t'}\frac{\mathrm{d}t'}{\sqrt{t'^{\gamma}}}\Lambda(t-t')H_{1,1}^{1,0}\left[\frac{1}{\sqrt{K_{\gamma}t'^{\gamma}}}|r+r'-2R|\middle|\begin{matrix}\left(1-\gamma,\frac{\gamma}{2}\right)\\(0,1)\end{matrix}\right] \tag{14}$$

where

$$\Lambda(t)=\frac{1}{\kappa'}t^{\overline{\alpha}-1}E_{\overline{\alpha},\overline{\alpha}}\left(-\sqrt{\mathcal{K}_{\gamma}}\frac{t^{\overline{\alpha}}}{\kappa'}\right)+\frac{1}{\kappa'}\sum_{n=1}^{\infty}\frac{1}{n!}\left(-\frac{\mathcal{K}_{\gamma}}{\kappa'\mathcal{R}}t^{\gamma-\alpha}\right)^{n}t^{\overline{\alpha}-1}E_{\overline{\alpha},\overline{\alpha}+\frac{\gamma}{2}n}\left(-\sqrt{\mathcal{K}_{\gamma}}\frac{t^{\overline{\alpha}}}{\kappa'}\right) \tag{15}$$

with $\overline{\alpha}=\gamma/2-\alpha$ (fig. 2).

In this sense, eq. (8) is given by:

$$\rho(r',t)=\Phi(t)-\int_{\mathcal{R}}^{\infty}\mathrm{d}rr^{2}\varphi(r)G(r,r';t)+\frac{\partial}{\partial t}\int_{\mathcal{R}}^{\infty}\mathrm{d}rr^{2}\int_{0}^{t}\mathrm{d}t'\Phi(t-t')G(r,r';t')+$$
$$+\mathcal{R}^{2}\frac{\partial}{\partial t}\int_{0}^{t}\mathrm{d}t'\kappa(t-t')\int_{0}^{t'}\mathrm{d}\overline{t}\,\Phi(t'-\overline{t})G(\mathcal{R},r';\overline{t}) \tag{16}$$

For eq. (13):

$$\mathcal{S}(t)=1-\mathcal{R}\int_{\mathcal{R}}^{\infty}\mathrm{d}\tilde{r}\tilde{r}\varphi(\tilde{r})\,\mathrm{H}_{1,1}^{1,0}\left[\frac{\tilde{r}-\mathcal{R}}{\sqrt{\mathcal{K}_{\gamma}t^{\gamma}}}\middle|\begin{matrix}\left(1,\frac{\gamma}{2}\right)\\(0,1)\end{matrix}\right]+\mathcal{R}\int_{\mathcal{R}}^{\infty}\mathrm{d}\tilde{r}\tilde{r}\varphi(\tilde{r})\int_{0}^{t}\mathrm{d}t'\,\Psi(t-t')\mathrm{H}_{1,1}^{1,0}\left[\frac{\tilde{r}-\mathcal{R}}{\sqrt{\mathcal{K}_{\gamma}t'^{\gamma}}}\middle|\begin{matrix}\left(1,\frac{\gamma}{2}\right)\\(0,1)\end{matrix}\right] \tag{17}$$

where

$$\Psi(t)=\sqrt{\mathcal{K}_{\gamma}}\Lambda(t)+\frac{\mathcal{K}_{\gamma}}{\mathcal{R}\,\Gamma(\gamma)}\int_{0}^{t}\mathrm{d}t'\frac{\Lambda(t')}{(t-t')^{1-\gamma}} \tag{18}$$

Figure 3 illustrates the behavior of eq. (17) for different values of α in order to show how the surface influences the quantity present in the bulk. Note that depending on the value of the parameter α, the particles may be absorbed (black line) or adsorbed and after some time desorbed (dashed and dotted lines).

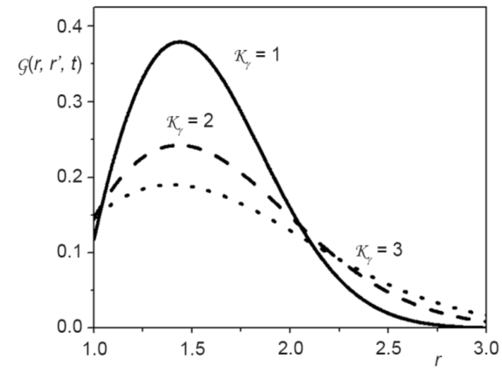

Figure 2. This figure illustrates the behavior of eq. (14) for different values of diffusion coefficient. Considering, for simplicity, $\kappa' = 1$, $\alpha = 1/2$, $t = 0.1$, $\mathcal{R} = 1$, and $\gamma = 1$ in arbitrary unities

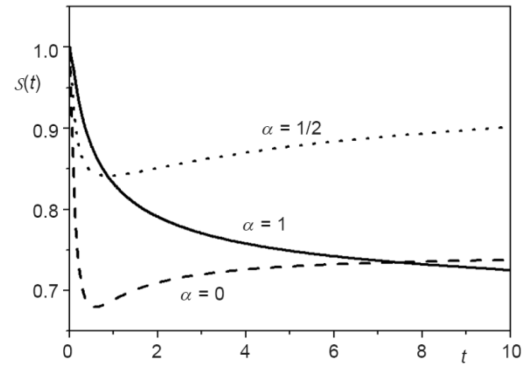

Figure 3. This figure illustrates the behavior of eq. (17) *vs.* t for different values of α. For simplicity, $\varphi(r) = (1/r^2)\delta(r - 3/2)$, $\kappa' = 1$, $\mathcal{K}_\gamma = 1$, $\mathcal{R} = 1$, and $\gamma = 1$ in arbitrary unities

Conclusions

The solutions for a fractional diffusion equation in the 3-D case with radial symmetry by taking integro-differential boundary conditions into account were investigated. The solutions obtained for this equation were expressed in terms of the Fox H functions and generalized Mittag-Leffler functions which are connected to an anomalous spreading. The survival probability was also found, showing shows that according to the choice of the function $\kappa(t)$ the surface may exhibit different behaviors such as absorption, adsorption, and desorption.

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Nomenclature

$\mathcal{D}_t^{1-\gamma}$ – fractional derivative of order $1-\gamma$, [–]
H – Fox function, [–]
$\mathcal{K}_{\gamma 0}$ – diffusion coefficient, [–]
r – distance, [–]
s – Laplace variable, [–]
t – time, [s]

Greek symbols

α – fractional derivative order, [–]
ρ – concentration, [–]

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