SUBDIFFUSIVE MODEL OF RELEASED SUBSTANCE FROM A SPHERICAL MEDIUM*

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We study a process of released substance from a medium in the shape of sphere. In both the sphere and a surrounding medium occurs subdiffusion. Using linear partial differential equations with a fractional time derivative, we obtain concentration profiles and a time evolution of an amount of substance which released from the sphere, both in the limit of large values of time. We also briefly discuss the obtained results.

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1. Introduction

Process of subdiffusion can occur in media in which particles' movement is strongly hindered due to the internal structure of medium. Subdiffusion can be treated as a random walk process in which a mean square displacement of a particle $\langle(\Delta\vec{r})^2(t)\rangle$ fulfills the following relation [1]

$$\left\langle (\Delta\vec{r})^2\,(t)\right\rangle \sim t^{\alpha}\,, \tag{1}$$

where $\alpha \in (0,1)$ is a subdiffusion parameter. For $\alpha = 1$, we have a situation of normal diffusion. The examples of media in which the occurrence of subdiffusion has been experimentally confirmed are porous media [2] and gels [3, 4].

Subdiffusion can be described by means of a linear partial differential equation with a fractional time derivative [1]

$$\frac{\partial C\left(\vec{r},t\right)}{\partial t} = D_{\alpha}\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\nabla^2 C\left(\vec{r},t\right)\,, \tag{2}$$

where $C(\vec{r},t)$ is a concentration of the transported substance, D_{α} is a subdiffusion coefficient measured in the units of $\mathrm{m}^2/\mathrm{s}^{\alpha}$ and $d^{\alpha}f(t)/dt^{\alpha}$ denotes the Reimann–Liouville derivative which is defind for $\alpha > 0$ as [5]

$$\frac{d^{\alpha}f(t)}{dt^{\alpha}} = \frac{1}{\Gamma(n-\alpha)}\frac{d^n}{dt^n}\int\limits_0^t dt'\frac{f\left(t'\right)}{\left(t-t'\right)^{1+\alpha-n}}\,, \tag{3}$$

the integer number n fulfills the relation $n-1 < \alpha \leq n$.

The problem of released substance from various media is the area of interest for many domains of science, especially pharmacy. In particular, a released medicine from carrier seems to be an important problem in pharmacy. Certain results of recent experimental researches suggest that subdiffusion can occur when medicine is released from a carrier [6]. However, the majority of this researches is based on the experimental methods and, as far as we know, the problem of subdiffusive releasing substance from a medium has not been considered theoretically. In this paper, we present a theoretical model of released substance from carrier in the shape of sphere under assumption that transport in both the sphere and surrounding area is subdiffusive. In our model, we consider a particular case of released substance. Namely, we additionally assume that transport of substance is more hindered outside the sphere then inside it. In our model, this assumption takes the following form $\alpha > \beta$, where α denotes a subdiffusion parameter inside the sphere and β — outside. We suppose that the assumption about the easiest transport of substance inside the sphere is linked with expectations of fast released medicine from the carrier.

2. The system

We study a system containing a sphere which is surrounded with an unrestricted medium (see Fig. 1). In both parts of the system, subdiffusion occurs with the subdiffusion parameters α, β and subdiffusion coefficients D_α, D_β, respectively. We consider the process in the spherical coordinate system. We assume that this process is independent of the azimuthal angle θ and the polar angle φ. At the initial moment only the sphere is filled with a substance homogeneously thus, the problem is spherically symmetrical. In that case, we lose the angles θ and φ in the notation of functions' arguments and we denote $C(r,\theta,\varphi,t) \equiv C(r,t)$. The initial condition reads

$$C_1(r,0) = C_0 \,, \qquad C_2(r,0) = 0 \,, \tag{4}$$

where C_1 denotes a concentration inside the sphere (*i.e.* in the region $0 < r < R$, where R is a radius of the sphere) and C_2 denotes a concentration outside the sphere (*i.e.* for $r > R$).

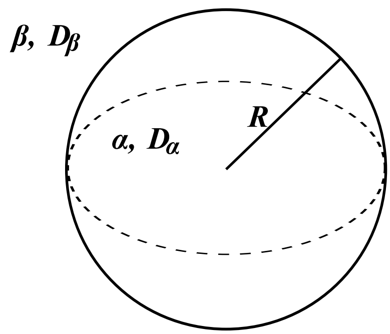

Fig. 1. The system under consideration.

Subdiffusion equations which describe the transport processes in the system under consideration are as follows

$$\frac{\partial C_1(r,t)}{\partial t} = D_\alpha \frac{\partial^{1-\alpha}}{dt^{1-\alpha}} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C_1(r,t)}{\partial r} \right) , \tag{5}$$

$$\frac{\partial C_2(r,t)}{\partial t} = D_\beta \frac{\partial^{1-\beta}}{dt^{1-\beta}} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C_2(r,t)}{\partial r} \right) . \tag{6}$$

We chose the following boundary conditions

$$C_1(R,t) = \kappa C_2(R,t) \,, \tag{7}$$

$$J_{r1}(R,t) = J_{r2}(R,t) \,, \tag{8}$$

$$C_2(+\infty,t) = 0 \,, \tag{9}$$

we also demand that $C_1(r,t)$ is finite for $0 \le r \le R$ and $t \ge 0$. The boundary condition (7) assumes that the ratio of concentrations C_1 to C_2 on both sides of the sphere surface is constant over time. The proportional coefficient κ can be assumed as a ratio of the sum of overlapping surfaces of pores at the sphere surface and the surrounding medium surface to the total surface of the sphere.

We solve the above equations by means of the Laplace transform method [7, 8]; the Laplace transform reads $\mathcal{L}\{f(t)\} \equiv \hat{f}(s) \equiv \int_0^\infty f(t)\exp(-st)dt$. The solutions to Eqs. (5) and (6) with the initial condition (4) and the boundary conditions (7)–(9) in the Laplace transform domain read

$$\hat{C}_1(r,s) = \frac{1}{M}\frac{C_0 D_\beta R}{s^\beta}\left(\frac{1}{R}+\delta\right)\frac{\sinh(\gamma r)}{r} + \frac{C_0}{s}\,, \tag{10}$$

$$\hat{C}_2(r,s) = \frac{1}{M}\frac{C_0 D_\alpha R}{s^\alpha}\left[\frac{1}{R}\sinh(\gamma R) - \gamma\cosh(\gamma R)\right]\frac{e^{-\delta(r-R)}}{r}\,, \tag{11}$$

where

$$\begin{aligned} M &= \kappa D_\alpha s^{1-\alpha}\left[\frac{1}{R}\sinh(\gamma R) - \gamma\cosh(\gamma R)\right] \\ &\quad -D_\beta s^{1-\beta}\left(\frac{1}{R}+\delta\right)\sinh(\gamma R)\,, \end{aligned} \tag{12}$$

and

$$\gamma = \frac{s^{\alpha/2}}{\sqrt{D_\alpha}}\,, \qquad \delta = \frac{s^{\beta/2}}{\sqrt{D_\beta}}\,. \tag{13}$$

In order to determine the inverse Laplace transform of Eqs. (10)–(13), we firstly calculate (10) and (11) in the limit of small values of s (which corresponds to large values of t). We get

$$\hat{C}_1(r,s) = \frac{C_0}{s} - \frac{C_0}{s}\left(1+\frac{Rs^{\beta/2}}{\sqrt{D_\beta}}\right)\left[1-\frac{Rs^{\beta/2}}{\sqrt{D_\beta}}+\frac{R^2 s^\beta}{D_\beta}\left(1-\frac{\kappa}{3}\right)\right]e^{-\frac{s^{\alpha/2}}{\sqrt{D_\alpha}}r}\,, \tag{14}$$

and

$$\begin{aligned} \hat{C}_2(r,s) &= \frac{C_0 R^3}{3D_\beta s^{1-\beta}}\left(1+\frac{R^2 s^\alpha}{10 D_\alpha}\right)\left[1-\frac{Rs^{\beta/2}}{\sqrt{D_\beta}}\right. \\ &\quad \left.+\frac{R^2 s^\beta}{D_\beta}\left(1-\frac{\kappa}{3}\right)\right]\frac{1}{r}e^{-\frac{s^{\beta/2}}{\sqrt{D_\beta}}(r-R)}\,. \end{aligned} \tag{15}$$

Next, using the following formula [8]

$$\mathcal{L}^{-1}\left\{s^{\nu}e^{-as^{\beta}}\right\} = f_{\nu,\beta}(t;a) \equiv \frac{1}{t^{1+\nu}}\sum_{k=0}^{\infty}\frac{1}{k!\Gamma(-k\beta-\nu)}\left(-\frac{a}{t^{\beta}}\right)^{k}, \qquad (16)$$

we obtain

$$\begin{aligned} C_1(x,t) &= C_0 - C_0\left[f_{-1,\alpha/2}\left(t;\frac{r}{\sqrt{D_\alpha}}\right) - \frac{R}{\sqrt{D_\beta}}f_{\beta/2-1,\alpha/2}\left(t;\frac{r}{\sqrt{D_\alpha}}\right)\right. \\ &\quad +\frac{R^2}{D_\beta}\left(1-\frac{\kappa}{3}\right)f_{\beta-1,\alpha/2}\left(t;\frac{r}{\sqrt{D_\alpha}}\right) + \frac{R}{\sqrt{D_\beta}}f_{\beta/2,\alpha/2}\left(t;\frac{r}{\sqrt{D_\alpha}}\right) \\ &\quad -\frac{R^2}{D_\beta}f_{\beta,\alpha/2}\left(t;\frac{r}{\sqrt{D_\alpha}}\right) \\ &\quad \left. +\frac{R^3}{D_\beta\sqrt{D_\beta}}\left(1-\frac{\kappa}{3}\right)f_{3\beta/2,\alpha/2}\left(t;\frac{r}{\sqrt{D_\alpha}}\right)\right], \qquad (17) \end{aligned}$$

$$\begin{aligned} C_2(x,t) &= \frac{C_0R^3}{3D_\beta}\frac{1}{r}\left[f_{\beta-1,\beta/2}\left(t;\frac{r-R}{\sqrt{D_\beta}}\right) - \frac{R}{\sqrt{D_\beta}}f_{(3/2)\beta-1,\beta/2}\left(t;\frac{r-R}{\sqrt{D_\beta}}\right)\right. \\ &\quad +\frac{R^2}{D_\beta}\left(1-\frac{\kappa}{3}\right)f_{2\beta-1,\beta/2}\left(t;\frac{r-R}{\sqrt{D_\beta}}\right) \\ &\quad +\frac{R^2}{10D_\alpha}f_{\alpha+\beta-1,\beta/2}\left(t;\frac{r-R}{\sqrt{D_\beta}}\right) \\ &\quad -\frac{R^3}{10D_\alpha\sqrt{D_\beta}}f_{\alpha+(3/2)\beta-1,\beta/2}\left(t;\frac{r-R}{\sqrt{D_\beta}}\right) \\ &\quad \left. +\frac{R^4}{10D_\alpha D_\beta}\left(1-\frac{\kappa}{3}\right)f_{\alpha+2\beta-1,\beta/2}\left(t;\frac{r-R}{\sqrt{D_\beta}}\right)\right]. \qquad (18) \end{aligned}$$

The example plots of the solutions (17) and (18) are presented in Fig. 2. The values of the parameters used in the calculation of the concentration profiles were $\kappa = 0.25$, $C_0 = 1.0$, $R = 2.5$, $\alpha = 0.7$, $D_\alpha = 2.4$, $\beta = 0.4$ and $D_\beta = 1.5$ (all quantities are given in arbitrary chosen units). The values of time are given in the legend of the figure. In Fig. 2 the sphere spreads over the range $(0, 2.5)$ and the surrounding medium exists for $r > 2.5$.

Time evolution of the amount of substance released from the sphere can be calculated from the following formula

$$W(t) = 4\pi\int_0^R r^2 C_1(r,t)\,dr\,. \qquad (19)$$

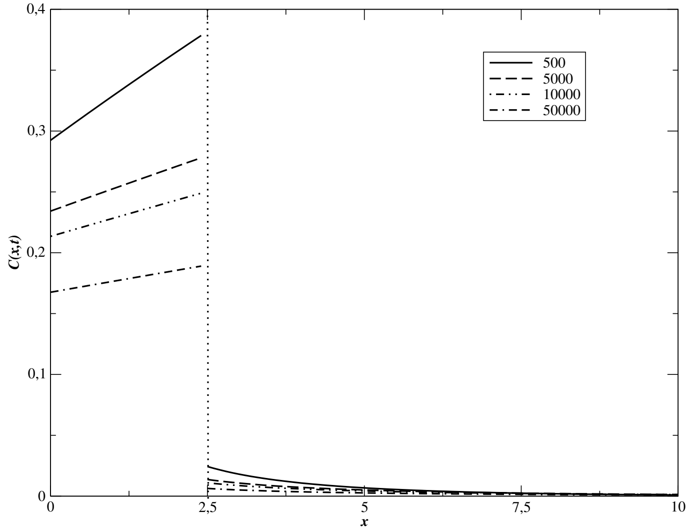

Fig. 2. The concentration profiles (17) and (18) obtained for different times given in the legend. The auxiliary dotted vertical line represents the surface of the sphere. The values of the rest of parameters are given in the text.

Keeping only leading terms of Eq. (19), we obtain

$$W(t) = \frac{4\pi R^3 C_0}{3} - \frac{4\pi R^2 \sqrt{D_\alpha} C_0}{D_\beta} \left(\frac{D_\beta t^{\alpha/2}}{\Gamma\left(\frac{\alpha}{2}+1\right)} - \frac{\kappa R^2 t^{(\alpha/2)-\beta}}{3\Gamma\left(\frac{\alpha}{2}-\beta+1\right)} \right) , \quad (20)$$

where $\Gamma(x)$ denotes the Gamma function.

3. Final remarks

We have found the concentration profiles (17) and (18) for the subdiffusive system composed of the sphere and surrounding medium under assumption that $\alpha > \beta$. It means that substance encounters more hindrance when is transported outside the sphere than inside it. The solutions have been obtained in the limit of large values of time. Moreover, we find the time evolution of an amount of substance released from the sphere (Eq. (20)). The model presented in this paper does not exclude the case of normal diffusion. For the case of normal diffusion, all formulae remain correct under condition that we substitute $\alpha = \beta = 1$.

The time evolution of amount of substance released from the sphere can be particularly useful in experimental determining of subdiffusive parameters characterizing the process. One of such experiments can be conducted by means of the laser interferometric method [6, 9–11].

In Fig. 2 we can notice that the boundary of the sphere acts as a partially reflecting wall causing an accumulation of the substance under the sphere surface. It is likely connected with a plenty of transport hindrance which substance occurs when leaving the sphere.

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