SCALING FORM OF CONCENTRATION PROFILES IN A SUBDIFFUSIVE MEMBRANE SYSTEM*

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We show that the concentration profiles in the subdiffusive system with a membrane, which separates a homogeneous solution from a pure solvent at an initial moment, has a general scaling form in the long time limit $C \sim t^\lambda F(\delta/t^\rho)$, where δ is a distance from the membrane surface. There is also derived the relation involving the subdiffusion parameters of the medium and the membrane with the scaling parameters λ and ρ, which are measured experimentally. The relation allows one to extract the subdiffusion parameters of the system from experimental data.

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1. Introduction

Subdiffusive systems can be study using the scaling method, which assumes that the concentration of a transported substance $C(x,t)$ is of the form

$$C(x,t) = t^\lambda F(z), \tag{1}$$

where

$$z \sim \frac{x - x_0}{t^\rho}, \tag{2}$$

x_0 is an arbitrary chosen point (here we consider the one-dimensional system). The parameters λ and ρ are controlled by subdiffusion parameters of the system. Since the parameters λ and ρ can be measured experimentally, it is possible to extract the values of subdiffusion parameters of the system from experimental data. This method was used already for subdiffusion in homogeneous systems [1, 2] and in the systems with chemical reactions [3].

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Recently the concentration of the form (1) was observed experimentally in the membrane subdiffusive system [4].

We study the subdiffusive system of two vessels separated by a thick membrane. At an initial moment one vessel contains a homogeneous solute whereas in the second one there is a pure solvent. Such a system has experimentally studied [4–7]. On the basis of theoretical model we show that the concentrations are given by the scaling functions (1) and (2). We also derive useful relations combining the subdiffusion parameters of the membrane and solvent with the parameters λ and ρ.

2. The method

Let us consider the one-dimensional system with a symmetrical membrane which is perpendicular to the x axis where $x = 0$ and $x = d$ are the positions of the membrane surfaces. In the regions $(-\infty, 0)$ and (d, ∞) there is a subdiffusion with the subdiffusion parameter α and subdiffusion coefficient D_α, inside the membrane a subdiffusion occurs with the parameters β and D_β. We assume that the transport of particles inside the membrane is more hindered than in the vessels, so $\alpha > \beta$.

The concentration is described by the subdiffusion equation with fractional Riemann–Liouville time derivative [8]

$$\frac{\partial C(x,t)}{\partial t} = D_\eta \frac{\partial^{1-\eta}}{\partial t^{1-\eta}} \frac{\partial^2 C(x,t)}{\partial x^2},$$

where $\eta = \alpha$ outside the membrane and $\eta = \beta$ inside it. To solve the subdiffusion equation we take the following boundary conditions:

$$J(0^-, t) = J(0^+, t), \tag{3}$$

$$C(0^-, t) = \lambda C(0^+, t), \tag{4}$$

$$J(d^-, t) = J(d^+, t), \tag{5}$$

$$\lambda C(d^-, t) = C(d^+, t), \tag{6}$$

where J denotes the subdiffusive flux [8], the dimensionless parameter λ controls the permeability of the membrane. We note that the boundary conditions (3)–(6) were already studied in the case of normal diffusion in membrane systems [9]. The initial condition we is chosen as:

$$C(x,0) = \begin{cases} C_0, & x < 0, \\ 0, & x > 0. \end{cases}$$

The solutions of the subdiffusion equations in terms of the Laplace transforms are

$$\hat{C}_1(x,s) = \frac{C_0}{s} - \frac{C_0}{s}e^{-\sqrt{s^\alpha/D_\alpha}(-x)}\left[\frac{1+\gamma-(1-\gamma)\,e^{-2\sqrt{s^\beta/D_\beta}d}}{(1+\gamma)^2-(1-\gamma)^2\,e^{-2\sqrt{s^\beta/D_\beta}d}}\right],\text{(7)}$$

$$\hat{C}_M(x,s) = \frac{C_0\gamma}{\lambda s}\left[\frac{(1+\gamma)\,e^{-\sqrt{s^\beta/D_\beta}(x)}+(1-\gamma)\,e^{-\sqrt{s^\beta/D_\beta}(2d-x)}}{(1+\gamma)^2-(1-\gamma)^2\,e^{-2\sqrt{s^\beta/D_\beta}d}}\right],\quad\text{(8)}$$

$$\hat{C}_2(x,s) = \frac{2C_0\gamma}{s}e^{-\sqrt{s^\alpha/D_\alpha}(x-d)-\sqrt{s^\beta/D_\beta}d}$$

$$\times\left[\frac{1}{(1+\gamma)^2-(1-\gamma)^2\,e^{-2\sqrt{s^\beta/D_\beta}d}}\right],\tag{9}$$

where $\gamma = \lambda\sqrt{D_\alpha/D_\beta}s^{(\beta-\alpha)/2}$, the indexes 1, M, and 2 are assigned to the regions $(-\infty,0)$, $(0,d)$, and (d,∞), respectively. To obtain the inverse Laplace transform L^{-1}, at first we find the series expansion of the functions (7)–(9) in terms of $s^\nu\,e^{-as^\beta}$, and next we use the following formula [10]

$$L^{-1}(s^\nu\,e^{-as^\mu}) = \frac{1}{t^{1+\nu}}F_{\nu,\mu}\left(\frac{a}{t^\mu}\right),\tag{10}$$

where

$$F_{\nu,\mu}\left(\frac{a}{t^\mu}\right) = -\frac{1}{\pi}\sum_{k=0}^{\infty}\frac{\sin\left[\pi\left(k\mu+\nu\right)\right]\Gamma\left(1+k\mu+\nu\right)}{k!}\left(-\frac{a}{t^\mu}\right)^k,$$

$a > 0$, $\mu > 0$, and the parameter ν is not limited.

Since the membrane used in experiments was not transparent for the laser beam and consequently the concentration profiles inside the membrane were not known, we focus in the following on the regions outside the membrane. To simplify the calculations we consider the above functions in the long time limit. According to the Tauberian theorem, the long time limit corresponds to the small values of the parameter s in the Laplace transform. For the subdiffusive system with relatively thin membrane described in the paper [11] the "long time" is evaluated to be longer than 100 seconds. Let us note that in considered system $\gamma \to \infty$ when $s \to 0$. The functions (7) and (9) in the limit of small s are

$$\hat{C}_1(x,s) = C_0\left[\frac{1}{s} - \frac{D_\beta}{\lambda\sqrt{D_\alpha}}s^{-1-\beta+\alpha/2}\,e^{-\sqrt{s^\alpha/D_\alpha}(-x)}\right],\tag{11}$$

$$\hat{C}_2(x,s) = \frac{C_0D_\beta}{\lambda\sqrt{D_\alpha}d}s^{-1-\beta+\alpha/2}\,e^{-\sqrt{s^\alpha/D_\alpha}(x-d)}.\tag{12}$$

Applying the formula (10) to Eqs. (11) and (12), we obtain

$$C_1(x,t) = C_0 \left[1 - \frac{D_\beta}{\lambda \sqrt{D_\alpha} d} t^{\beta - \alpha/2} F_{-1-\beta+\alpha/2,\alpha/2} \left(\frac{-x}{\sqrt{D_\alpha t^\alpha}} \right) \right], \quad (13)$$

$$C_2(x,t) = \frac{C_0 D_\beta}{\lambda \sqrt{D_\alpha} d} t^{\beta - \alpha/2} F_{-1-\beta+\alpha/2,\alpha/2} \left(\frac{x-d}{\sqrt{D_\alpha t^\alpha}} \right). \quad (14)$$

To illustrate the functions (13) and (14), there are shown few plots of the concentration profiles for different times in Fig. 1. Here $\alpha = 0.75$, $\beta = 0.5$, $D_\alpha = 1 \times 10^{-3}$, $D_\beta = 1 \times 10^{-4}$, $C_0 = 1$, $\lambda = 2$, and $d = 1$ (all quantities are in arbitrary units).
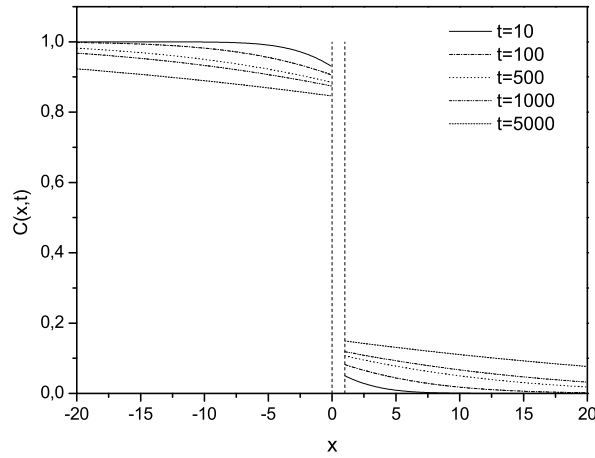

Fig. 1. The concentrations C for different times (in arbitrary unit). The dotted vertical lines represent the membrane surfaces.

In the study [4] it was found that the concentration profiles in the region (d, ∞) is given by the function (1) with the argument (2). The parameter ρ depends on the properties of subdiffusive medium outside the membrane and it is controlled by the subdiffusion parameter α whereas the parameter λ depends on the both of the subdiffusive parameters α and β. Comparing the function (14) with Eqs. (1) and (2), we obtain

$$\beta = \lambda + \rho, \quad (15)$$

and

$$\rho = \frac{\alpha}{2}. \quad (16)$$

Since the parameters λ and ρ are measured experimentally [4], we can get the subdiffusion parameter inside the membrane from Eq. (15).

3. Final remarks

We observe that the functions $C_0 - C_1(x,t)$ and $C_2(x,t)$ are of the same scaling form and they can be expressed by the function $t^{\beta-\alpha/2}F_{-1-\beta+\alpha/2,\alpha/2}\left(\delta/\sqrt{D_\alpha t^\alpha}\right)$, where δ is the distance from the membrane surface. Knowing the scaling form we derive the relations (15) and (16).

Presented procedure allows one to calculate the subdiffusion parameter inside the membrane. Our theoretical result fully coincides with the experimental one presented in [4], where it is reported that the concentration profiles obey the scaling function (1) for the system containing the membrane made of PEG 2000 located in the agarose gel solvent, with $\rho = 0.44 \pm 0.01$ and $\lambda = 0.17 \pm 0.01$. The first parameter was determined by means of the time evolution of near membrane layers, the second one was extracted from the time evolution of the concentration at the membrane surface $x = d$, which is $C_2(d,t) \sim t^{\beta-\alpha/2}$. Substituting these values to the relations (15) and (16), we obtain $\beta = 0.61 \pm 0.01$ for the membrane under considerations.

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