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On the self-similar, early-time, anomalous diffusion in random networks — Approach by fractional calculus

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ABSTRACT

In a recent work, Zhang and Padrino (2017) derived an equation for diffusion in random networks consisting of junction pockets and connecting channels by applying the ensemble average method to the mass conservation principle. The resulting integro-differential equation was solved numerically using finite volumes for the test case of one-dimensional diffusion in the half-line. For early time, they found that the numerical predictions of pocket mass density depend on the similarity variable $xt^{-1/4}$, representing sub-diffusion. They argue that the sub-diffusive behavior is a consequence of the time needed to establish a linear concentration profile inside a channel. By theoretical analysis of the diffusion equation for small time, they confirmed this finding. Nevertheless, they did not present an exact solution for the small time limit to compare with. Here, starting with their small-time leading order diffusion equation in (x,t) space, we use elements of fractional calculus to cast it into a form for which an analytical solution has been obtained in the literature for the same boundary and initial conditions in terms of the Fox H-function (Schneider and Wyss, 1989). For ease of computation, we express the solution in terms of the Meijer G-function. We compare the exact solution with Zhang and Padrino's numerical predictions, resulting in excellent agreement, thereby validating their numerical approach.

1. Introduction

Diffusive transport is ubiquitous; it occurs in nature and in human-designed systems. Diffusion, in its ordinary or normal form, has received enormous attention from researchers and, as a result, is essentially well understood. The well-known distinctive attribute of ordinary diffusion is that the mean squared displacement of the transported agent evolves linearly with time. In recent decades, the focus in research on diffusion has shifted towards the study of the so-called anomalous diffusion. This process differs from ordinary diffusion in that the evolution of the mean squared displacement with time is slower (sub-diffusion) or faster (super-diffusion) [1–3]. Rather than being a rare event, anomalous diffusion has been observed and modeled in a wide variety of settings, such as in single-file particle diffusion [4–8]; charge carriers transport in amorphous semiconductors [9]; bead dynamics in a polymeric network [10,11]; bacterial motion [12]; transport in fractal geometries [13,14], in porous media [15,16], in random fractured networks [17], in turbulent plasmas [18], and in micelle systems [19] (for a comprehensive list of applications and some historical remarks, see [20]). What has been called “anomalous” is, in fact, a common occurrence [21].

A mathematical approach that has proven to be well suited to the theoretical analysis of anomalous diffusion is the fractional calculus and, in particular, the differential equations of fractional order [20]. In this case, the model differential equation is known as fractional diffusion equation [22,23]. Fractional calculus has been known for more than two centuries [24,25]; however, its application to modeling anomalous diffusion phenomena seems to be rather recent [20,23,26-28]. The fractional diffusion equation has been written as a somewhat heuristic extension of the ordinary diffusion equation to study anomalous diffusion [22,29-32]. On the other hand, it has arisen as the result of a rigorous application of the theory of continuous time random walks [20,31,33,34].

In a recent article, Zhang and Padrino [35] derived an equation for mass diffusion in a random network of junction pockets connected by tortuous channels of various lengths by applying the ensemble average method to the mass balance in the network. Random networks seem to be suitable idealizations of complex interactions of the most diverse nature. An example is the modeling of transport in porous media [36,37]. To attain closure, Zhang and Padrino [35] computed the flux in a single connecting channel assuming one-dimensional ordinary diffusion between the connected pockets. Given the isotropic probability density function $P(\boldsymbol{x},\boldsymbol{y},\ell)$ of having a pocket at $\boldsymbol{x}$ connected to another pocket at $\boldsymbol{y}$ by a channel of length ℓ, they obtained the

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following expression for the time evolution of pocket mass density $\rho_p(\boldsymbol{x},t)$:

$$\theta_p\frac{\partial\rho_p}{\partial t}+\int_{-\infty}^{t}K_m\left(\boldsymbol{x},\,t-\tau\right)\frac{\partial\rho_p(\boldsymbol{x},\,\tau)}{\partial\tau}d\tau=\nabla\cdot\left(D(\boldsymbol{x})\nabla\rho_p\right)+\nabla\cdot\int_{-\infty}^{t}K_D\left(\boldsymbol{x},\,t-\tau\right)\frac{\partial}{\partial\tau}\nabla\rho_p\left(\boldsymbol{x},\,\tau\right)d\tau, \tag{1}$$

where θ_p is the volume fraction of pockets, D is an effective diffusivity, and K_m and K_D are the mass and diffusivity kernels, respectively. These quantities are defined as

$$D(\boldsymbol{x})=\iint_0^\infty\frac{\overline{A}\,\widetilde{D}}{6\ell}r^2\widehat{P}\,(\boldsymbol{x},\,r,\,\ell)drd\ell, \tag{2}$$

$$K_m(\boldsymbol{x},\,t)=\iint_0^\infty\frac{2\overline{A}\,\widetilde{D}}{\ell}\left[K\left(\frac{\widetilde{D}\,t}{\ell^2}\right)-K\left(\frac{4\widetilde{D}\,t}{\ell^2}\right)\right]\widehat{P}\,(\boldsymbol{x},\,r,\,\ell)drd\ell, \tag{3}$$

$$K_D(\boldsymbol{x},\,t)=\iint_0^\infty\frac{\overline{A}\,\widetilde{D}}{6\ell}r^2K\left(\frac{4\widetilde{D}\,t}{\ell^2}\right)\widehat{P}\,(\boldsymbol{x},\,r,\,\ell)drd\ell, \tag{4}$$

where

$$K(u)=2\sum_{j=1}^{\infty}e^{-j^2\pi^2u}=\frac{1}{\sqrt{\pi u}}\left(1+2\sum_{j=1}^{\infty}e^{-j^2/u}\right)-1, \tag{5}$$

which arises from the Fourier series solution of normal (ordinary) diffusion in a single channel. Here, $P(\boldsymbol{x},\boldsymbol{y},\ell)=\widehat{P}\,(\boldsymbol{x},\,r,\,\ell)/(4\pi r^2)$ with $r=|\boldsymbol{y}-\boldsymbol{x}|$; $\overline{A}$ is the channel average cross sectional area, and $\widetilde{D}$ is the area-weighted average diffusivity inside the channel. The closed averaged integro-differential Eq. (1) contains time integrals representing history effects of mass diffusion. The details of the derivation of this equation can be found in [35]. It is noteworthy that they found the so-called dual-porosity model [38] to be equivalent to the leading order approximation of the integration kernel in their new model when the diffusion time scale inside the channels is small compared to the macroscopic time scale.

As a test problem, Zhang and Padrino considered one-dimensional diffusion in a random network occupying the half-line (semi-infinite domain) assuming that $\widehat{P}$ is also homogeneous and that all connecting channels have a fixed length ℓ_0. Specializing Eq. (1) for this case, the initial-boundary value problem considered in [35] can be stated as

$$\frac{\partial\rho_p}{\partial t}+4\frac{\theta_c}{\theta_p}\int_0^t\left[K(t-\tau)-K(4t-4\tau)\right]\frac{\partial\rho_p}{\partial\tau}d\tau=\frac{\partial^2\rho_p}{\partial x^2}+\frac{\partial^2}{\partial x^2}\int_0^t K(4t-4\tau)\frac{\partial\rho_p}{\partial\tau}d\tau, \tag{6}$$

for $x>0$ and $t>0$ and initial and boundary conditions

$$\rho_p(x,\,0^+)=0,\qquad x>0, \tag{7}$$

$$\rho_p(0^+,\,t)=1,\qquad \rho_p(+\infty,\,t)=0,\qquad t>0, \tag{8}$$

in dimensionless form. The problem was non-dimensionalized using $\ell_0\sqrt{\kappa_0\theta_c/\theta_p}$, $\ell_0^2/\widetilde{D}$, and ρ_0 as the length, time, and mass density scales, respectively, where ρ_0 is the pocket mass density on $x=0^+$, and parameter $\kappa_0=\pi/(8\mathscr{T}_0^2)$, with $\mathscr{T}_0$ being a reference tortuosity. This relation comes from the assumption that the probability density $\widehat{P}$ is modeled with the Maxwell-Boltzmann distribution and by relating its mean with $\mathscr{T}_0$. The model for the probability density function $\widehat{P}$ also brings in the volume fraction of channels, θ_c [35]. Zhang and Padrino proposed a numerical scheme consisting in casting the linear integro-differential equation (Eq. (1)) into a system of linear partial differential equations to which they applied the finite volume method and explicit time integration. After using this numerical approach to solve Eq. (6), they reported that for small time, for different values of the channel-to-pocket volume fraction ratio θ_c/θ_p, the pocket mass density becomes a function of the one variable $xt^{-1/4}$, hence showing a self-similar behavior. They confirmed this finding analytically by investigating the leading order balance in the diffusion equation in the limit of small time (see Appendix A.6 in their paper). Therefore, a point of constant pocket density changes its position according to $x\propto t^{1/4}$, corresponding to an anomalous, sub-diffusive process [21]. They explained this behavior by random walk theory. Assuming that each channel in the random network is formed by paths of random walks, they obtained the scaling of the straight distance between connected pockets with the one-fourth power of time by equating the total length of the path of the random walk traveled by tracer particles inside a channel with the characteristic diffusive length. From the point of view of continuum physics, they argued that the early-time sub-diffusion is caused by the amount of time required to establish a linear mass density profile inside the channels.

Although their asymptotic analysis predicted the early-time anomalous self-similar trend observed in the numerical results, they did not present an expression for the exact solution of the initial-boundary value problem considered for small time. The purpose of this note is to report on the exact solution for this limiting case within the framework of fractional calculus, and to compare its predictions with the numerical results in [35]. It should be remarked that the model derived and the numerical solution presented in [35] are not restricted to small times.

2. Analysis and results

On the basis of the conclusion by Zhang and Padrino [35], the leading order equation for pocket mass density diffusion in random networks for small time, resulting from the first and last terms of Eq. (6), may be written as

$$\frac{\partial\rho_p}{\partial t}=\frac{1}{2\sqrt{\pi}}\int_0^t(t-\tau)^{-\frac{1}{2}}\frac{\partial}{\partial\tau}\left(\frac{\partial^2\rho_p}{\partial x^2}\right)d\tau, \tag{9}$$

subjected to the initial and boundary conditions (7) and (8).

In this work, we use fractional calculus, in particular, the integrals and differential operators of fractional order, as the tool for the analysis. Several comprehensive monographs have been written on the fundamentals and applications of fractional calculus (e.g., [25,39-46]). The elements of fractional calculus invoked here, such as definitions and identities, are taken from the works of Gorenflo and Mainardi [24] and Mainardi et al. [47] unless otherwise noted.

We start by writing Eq. (9) in terms of fractional order time differential operators. For this purpose, we introduce the fractional derivative of order α, $0<\alpha\leqslant1$, in the Caputo sense, denoted as ${}_tD_*^\alpha$, and defined by

$${}_tD_*^\alpha f(t)=\begin{cases}\dfrac{1}{\Gamma(1-\alpha)}\displaystyle\int_0^t(t-\tau)^{-\alpha}\frac{df}{d\tau}(\tau)d\tau, & 0<\alpha<1,\\ \dfrac{df}{d\tau}, & \alpha=1,\end{cases} \tag{10}$$

where $\Gamma()$ denotes the Gamma function. With this definition, and letting $\mathscr{D}_\alpha=\Gamma(\alpha)/(2\sqrt{\pi})$, we can write Eq. (9) as

$$\frac{\partial\rho_p}{\partial t}=\mathscr{D}_\alpha\,{}_tD_*^{1-\alpha}\frac{\partial^2\rho_p}{\partial x^2}, \tag{11}$$

with $\alpha=1/2$. For the sake of the discussion, in what follows we shall consider the general case $0<\alpha<1$, except where noted otherwise.

Another widely used fractional operator is the fractional derivative of order α, $0<\alpha\leqslant1$, in the Riemann-Liouville sense, denoted as ${}_tD^\alpha$, and given by

$${}_tD^\alpha f(t)=\begin{cases}\dfrac{1}{\Gamma(1-\alpha)}\dfrac{d}{dt}\displaystyle\int_0^t(t-\tau)^{-\alpha}f(\tau)d\tau, & 0<\alpha<1,\\ \dfrac{df}{d\tau}, & \alpha=1.\end{cases} \tag{12}$$

It is customary to write ${}_tD^0=I$, the "identity" operator, so that ${}_tD^0f$