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Derivation and Solution of Space-Time Fractional Reaction-Convection-Diffusion Equation in Comb-Like Model

Israa M. Abdelsabour[1], Mohammed Sallah[1,2], Mohsen A. Zahran[1], Ahmed Elgarayhi[1]
[1] *Physics Department, Faculty of Science, Mansoura University, Mansoura 35516, Egypt*
[2] *Higher Institute for Engineering and Technology, New Damietta, Egypt*
Corresponding author: imsabour@mans.edu.eg

ABSTRACT : *The generalized equation of fractional reaction-diffusion exposed to an external force expressed as a velocity term was proposed, to explain the transport mechanism in a disordered system with the time-space variance. This work uses the Caputo derivation form to derive and solve the generalized fractional reaction-diffusion equation in terms of Mittage-Leffler and H-Fox functions. The solution is used to present some explanation of the anomalous diffusion phenomena in some disordered systems. For example, there is a sturdy index to show that for a system with doubled trappings, factional calculus provides some physical view of fractional dynamics like diffusion in the dendritic spine of the nervous system as an example of the diffusion process in biological systems.*

KEYWORDS:* *Anomalous diffusion; Comb-like model; Convection term; Fractional reaction-diffusion equation.

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I. INTRODUCTION

Diffusion is a passive transport process that results in a net movement of particles, without requiring bulk motion, from higher to lower concentrations. It exists in all states of matter on various time and space scales, which characterizes many physical, chemical, and biological phenomena, based on Fick's laws, or by taking into account a microscopic point of view in terms of the erratic motion of the suspended particles [1]. Diffusion can be described in terms of the mean-squared displacement (MSD) of the particle spreading $\langle x^2 \rangle \sim t$, where x is the distance traveled in time t, and this is known as normal diffusion (Brownian or Fickian). The standard normal diffusion described by the Gaussian distribution can be obtained from the usual Fokker-Planck equation with a constant diffusion coefficient and zero drift [2].

However, the disparity between anomalous diffusion and normal diffusion in terms of variance indicates a non-linear increase in time

$$\langle x^2 \rangle \sim t^{\gamma} \tag{1}$$

For this case, the MSD can be classified via anomalous diffusion exponent; the exponent γ can be either subdiffusion for $0 < \gamma < 1$ or super diffusion for $\gamma > 1$. In recent decades, the anomalous diffusion has been extensively studied in a variety of physical applications, e.g., the fluids transport in porous media [3], surface growth [4], numerical solution of the time-fractional reaction-advection diffusion equation in porous media [5], and the biological population's spatial diffusion [6]. A lot of examples can be found in Ref. [7,8]. To study anomalous diffusion extensions, the conventional Fokker-Planck equation has been used. For instance, the normal Fokker-Planck equation may achieve anomalous diffusion, but with a variable diffusion coefficient [9,10]. It is achieved also by subsuming nonlinear terms in the diffusion section, or external forces [11,12,13]. However, the fractional equations have been used in several approaches to analyzing anomalous diffusion and related phenomena [14,15]. Such interest in the absence and existence of external velocity or force fields has been extensively shown to be a compatible instrument for explaining anomalous transport processes [8,16,17].

Recently, the anomalous transport phenomenon on living biological cells have been revealed on the mesoscopic scale dynamics. Following the recent high-detailed simulation, this abnormal behavior found in living cells and the environments of artificially crowded regulation operates in the form described in Ref. [7,18].

Moreover, there is a swelling interest in studying the anomalous diffusion equation using fractional calculus, e.g., Elwakil et al. [19] have given a derivation for the fractional space-time diffusion equation using the comb-like structure as a draft model obtaining the solution for three different interesting cases. Zahran [20] described the equation with an integrodifferential form, defined the derivation of the generalized fractional reaction-diffusion equation, concerning time and space operators instead of the first-order derivative, the Riemann-Liouville derivative of fractional orders shall contain. Schot et al [21] found the solutions of a generalized diffusion equation that contains space-time fractional derivatives by taking an absorbent (or source) term and a linear external force into account. They were expressed in terms of the Fox H-function, and for some special cases, they are directly related to the Lévy distributions.

As a matter of fact, the ad-hoc representation of fractional operators should be carried with care and therefore this phenomenological approach of this type of differential equations should be solidly justified. Hence, this work suppresses the derivation and solution of the generalized fractional reaction convection diffusion equation using Caputo time-derivative of the order and space fractional derivative of order in a comb-like model. We have applied the co-moving technique that has yielded the general solution in the form of Mittage-Leffler and H-Fox Function.

II. FRACTIONAL REACTION-CONVECTION-DIFFUSION EQUATION

The comb model consists of a backbone along the horizontal axis and fingers or teeth along the perpendicular direction [22] (see Fig. (1) for a two-sided comb) [23]. To explain anomalous transport in percolating clusters, a comb model was implemented. [24,25] and it was considered a toy model for a porous medium used for low-dimensional percolation cluster exploration. [22,24]. The comb-like model has been used previously many times to derive well-known fractional differential equations, as fractional diffusion equation with or without external force. A matrix of diffusion coefficients describes the geometry of the comb, which means that the displacement in the x-direction is possible only along the structure axis, i.e., the diffusion happened at [22]. Zahran [20] derived the general fractional reaction-diffusion equation in an accurate way using the comb-like model as a background medium. Hence, the main motive of this work is assuming the anomalous diffusion along with the tooth of the structure, one can obtain the generalized form of the space-time fractional reaction-convection-diffusion equation for sake of completeness. This model can describe the transfer of the nerve signals in the dendritic spines, where the signal particles may be trapped. The trapping effect is caused by the fingers of the comb-like model. Consequently, the diffusion in the y-direction shall be considered in the convection term as it should be added to the x-direction diffusion.

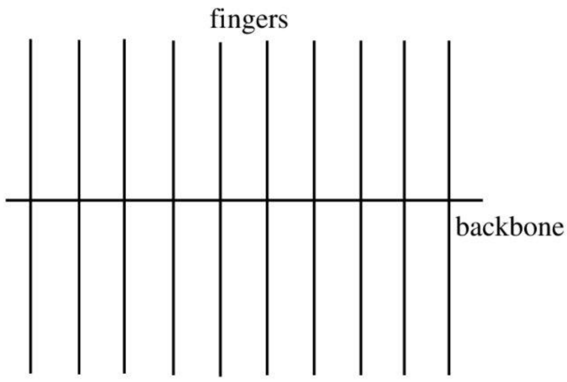

Fig.1. Two-sided comb-like model

In terms of the probability density function $P(x,y,t)$, the x-component of the current J along the backbone is given by

$$J_x = \delta(y)\left[v(x)P(x,y,t) - D_\alpha \frac{\partial^\mu}{\partial x^\mu} P(x,y,t)\right] \tag{2}$$

Moreover, the corresponding y-component of the current along with fingers (where the trapping may occur), has the form

$$J_y = -D(t)\frac{\partial}{\partial y} P(x,y,t) \tag{3}$$

The diffusion coefficient $D(t)$ is assumed as a function of time. From the continuity equation that follows

$$\frac{\partial}{\partial t} P(x,y,t) + \nabla \cdot J = -\delta(y)\psi(x,y,t) \tag{4}$$

where $\psi(x,y,t)$ corresponds to the reaction term. One shall get

$$\left[\frac{\partial}{\partial t}-D(t)\frac{\partial^2}{\partial y^2}\right]P(x,y,t)=\delta(y)\left\{D_\alpha\frac{\partial^\alpha}{\partial x^\alpha}P(x,y,t)-\frac{\partial}{\partial x}\left[v(x)P(x,y,t)\right]-\psi(x,y,t)\right\} \quad (5)$$

with $\alpha=\mu+1$. Assuming

$$D_\alpha\frac{\partial^\alpha}{\partial x^\alpha}P(x,y,t)-\frac{\partial}{\partial x}\left[v(x)P(x,y,t)\right]=\varphi(x,y,t) \quad (6)$$

yields

$$\left[\frac{\partial}{\partial t}-D(t)\frac{\partial^2}{\partial y^2}\right]P(x,y,t)=\delta(y)\left[\varphi(x,y,t)-\psi(x,y,t)\right] \quad (7)$$

The effective diffusion coefficient is believed to be $D(t)$, that has the following explicit time dependence [26] with the coefficient D_1

$$D(t)=D_1\beta t^{\beta-1} \quad (8)$$

with the exponent β that represents the diffusion type along with the structure of the comb. For $0<\beta<1$, the diffusion process is slower than normal diffusion and this denotes as sub-diffusion, while for $1<\beta<2$, the diffusion process is faster than normal diffusion and denotes as super-diffusion.

Finger diffusion is a fractional Brownian motion driven by the effective Fokker-Plank equation, and backbone diffusion is a fractal time process with a memory kernel, therefore The Green function is related to the homogeneous part of equation. (7) affected by the initial condition $G(y,0)=\delta(y)$ of has the form

$$G(y,t)=\frac{1}{\sqrt{\pi D_1 t^{\beta-1}}}\exp\left[\frac{-y^2}{4D_1 t^{\beta-1}}\right] \quad (9)$$

The general solution for equation (5) can be defined through the integration over the source term and for the different parameter values $t=t-t'$ as

$$P(x,0,t)=\int G(y-y',t-t')\left[\delta(y')\left\{D_\alpha\frac{\partial^\alpha}{\partial x^\alpha}P(x,y',t')-\frac{\partial}{\partial x}\left[v(x)P(x,y',t')\right]-\psi(x,y',t')\right\}dy'dt'\right] \quad (10)$$

Inserting equation (9) into equation (10) before integration over y (i.e. along with the main channel), the closed equation for the concentration of the particles along the main channel [27] is given by

$$P(x,t)={}_0D^{\gamma}_{t}\left\{D_\alpha\frac{\partial^\alpha}{\partial x^\alpha}P(x,t)-\frac{\partial}{\partial x}\left[v^*(x,\gamma)P(x,t)\right]-\psi(x,t)\right\} \quad (11)$$

under the following circumstance in terms of Gamma function $\Gamma(\gamma)$

$$v^*(x,\gamma)=\frac{V(x)\Gamma(\gamma)}{\sqrt{\pi D_1}} \quad , \quad \gamma=1-\frac{\beta}{2} \quad (12)$$

where the Caputo derivative ${}_0D_t^{\gamma}$, is defined as

$${}_0D_t^{\gamma}F(t)=\frac{1}{\Gamma(n-\alpha)}\int_0^t (t-t')^{n-\alpha-1}F(t')dt' \quad (13)$$

It is clear here that due to the trapping of the random walk particle along the y-direction, the integration of the fractional-order occurs. When the fractional derivative of Caputo is applied on both sides, it produces

$$\frac{\partial^\gamma}{\partial t^\gamma}P(x,t)=D_\alpha\frac{\partial^\alpha}{\partial x^\alpha}P(x,t)-\frac{\partial}{\partial x}\left[v(x)p(x,t)\right]-\psi(x,t) \quad (14)$$

III. ANALYTICAL SOLUTION OF THE FRACTIONAL DIFFUSION PROBLEM

Taking the special case that $D_\alpha=D_o$ and $V(x)=V_o$, the fractional reaction advection-diffusion equation can be studied if we convert the transport analysis from an external observer reference frame to a co-moving frame, as

$$\frac{\partial^\gamma}{\partial x^\gamma}P(x,t)=D_o\frac{\partial^\alpha}{\partial x^\alpha}P(x,t)-\psi(x,t) \quad (15)$$

At the origin $t=0$, we consider a point source so that the initial condition is given by $P(x,0)=\delta(x)$. Taking the Laplace transform of equation (15) gives

$$s^{\gamma} P(x,s) - s^{\gamma-1}\delta(x) = D_o \frac{\partial^{\alpha}}{\partial x^{\alpha}} P(x,s) - \psi(x,s) \tag{16}$$

We suppress the imaginary unit in Fourier space [8] as

$$\mathrm{F}\left\{ {}_0 D_x^{\alpha} F(x) \right\} = -\left|k\right|^{\alpha} F(x) \tag{17}$$

Then, equation (16) will have the from

$$P(k,s) = \frac{s^{\gamma-1}}{s^{\gamma} + D_0 \left|k\right|^{\alpha}} - \frac{\psi(k,s)}{s^{\gamma} + D_0 \left|k\right|^{\alpha}} \tag{18}$$

Taking the inverse Laplace and inverse Fourier to the above equation, respectively, will give the full solution. Accordingly, the general solution of the probability density function [28] can be expressed as

$$P(x,t) = \int_{-\infty}^{\infty} G_1(x-x',t) F(x')dx' + \int_0^t (t-t')^{\beta-1} \int_0^x \psi(x',t') G_2(x-x',t-t')dx'dt' \tag{19}$$

where

$$G_1(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(-ikx) E_{\gamma,1}\left(-D_0 \left|k\right|^{\alpha} t^{\gamma}\right) dk \tag{20}$$

Using the relation between Mittage-Leffler function and H–function

$$E_{\alpha,\beta}(z) = H_{1,2}^{1,1}\left[-z \left| \begin{matrix} (0,1) & \\ (0,1) & (1-\beta,\alpha) \end{matrix} \right. \right] \tag{21}$$

where H-function is defined by

$$H_{p,q}^{m,n}\left[z^{\alpha} \left| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right. \right] = \frac{1}{\alpha} H_{p,q}^{m,n}\left[z \left| \begin{matrix} (a_p, A_p/\alpha) \\ (b_q, B_q/\alpha) \end{matrix} \right. \right] \tag{22}$$

Taking the inverse Fourier cosine transform of the Fox H–function in the form [28]

$$\int_0^{\infty} t^{\rho-1} \mathrm{Cos}(kt) H_{p,q}^{m,n}\left[a t^{\mu} \left| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right. \right] dt = \frac{\pi}{k^{\rho}} H_{q+1,p+2}^{n+1,m}\left[\frac{k^{\mu}}{a} \left| \begin{matrix} (1-b_p, B_p) & \left(\frac{1+\rho}{2}, \frac{\mu}{2}\right) & \\ (\rho,\mu) & (1-a_p, A_p) & \left(\frac{1+\rho}{2}, \frac{\mu}{2}\right) \end{matrix} \right. \right] \tag{23}$$

Consequently, in terms of the Fox H–function, we get the analytical solution of the space-time fractional advection-reaction diffusion equation, as

$$G_1(x,t) = \frac{1}{\left|x-vt\right|\alpha} H_{3,3}^{2,1}\left[\frac{\left|x-vt\right|}{D_0^{1/\alpha} t^{\gamma/\alpha}} \left| \begin{matrix} (1,1/\alpha) & (1,\gamma/\alpha) & (1,1/2) \\ (1,1) & (1,1/\alpha) & (1,1/2) \end{matrix} \right. \right] \tag{24}$$

and

$$G_2(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(-ikx) E_{\gamma,\gamma}\left(-D_0 \left|k\right|^{\alpha} t^{\gamma}\right) dk \tag{25}$$

whose form can be expressed in terms of Fox H–function, as

$$G_2(x,t) = \frac{1}{\left|x-vt\right|\alpha} H_{3,3}^{2,1}\left[\frac{\left|x-vt\right|}{D_0^{1/\alpha} t^{\gamma/\alpha}} \left| \begin{matrix} (1,1/\alpha) & (\gamma,\gamma/\alpha) & (1,1/2) \\ (1,1) & (1,1/\alpha) & (1,1/2) \end{matrix} \right. \right] \tag{26}$$

IV. CONCLUSION

In a comb-like model, we have derived and analyzed the fractional reaction convection diffusion equation with Caputo time-derivative of the order γ and space fractional derivative of the order α . The random walker diffuses along the x-axis and on the y-axis, the trapping events occur. The diffusion along the x-direction is a process of fractal time that showed a mean-squared displacement $\left\langle x^2 \right\rangle \sim t^{\gamma}$ with the initial condition of Delta function $P(x,0) = \delta(x)$. Moreover, the y-direction diffusion is given by mean-squared displacement $\left\langle y^2 \right\rangle \sim t^{\beta}$, with order β related to order γ (see equation (12)). The main remark here is the direct connection between the integral fractional operators and the random disappearances or trappings along with the fingers of the structure. Also, we have introduced the co-moving technique in which the Laplace-Fourier technique can be applied to the resultant equation to give the solution in the form of Fox H–Function to get the solution described by the equations equation (19) – equation (26). The studied model can be used to describe some biophysical systems with trapping phenomena like the diffusion in the dendritic spine of neurons.

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