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Analytical solutions to the moving boundary problems with space–time-fractional derivatives in drug release devices

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Abstract
A mathematical model of a solute release from a planar polymer matrix is presented and the analytical solution in terms of the Fox H function is given. The equation of space–time-fractional diffusion and a generalized Fick's law are used in the paper. Three particular cases, the standard diffusion, the time-fractional and the space-fractional diffusions are discussed in detail. The model and the solution are the generalization of the previous works and include them as special cases.

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1. Introduction

It is well known that diffusion models play a very important role in biology, chemistry, and physics. The diffusion process is normally governed by Fick's first and second laws which lead to the ordinary diffusion equation in one dimension

$$\frac{\partial C(x,t)}{\partial t} = K\frac{\partial^2}{\partial x^2}C(x,t), \tag{1}$$

which has been extensively studied.

It has recently been shown that the solute movement in the heterogeneity media is usually anomalous and cannot be described by the standard diffusion equation. In the past two decades, anomalous diffusion has been widely researched by using the so-called fractional calculus [16, 17]. The fractional (space or time or space–time) diffusion equation is obtained from the standard diffusion equation by replacing the second-order space derivative with a Riesz or Riesz–Feller derivative of order $\alpha \in (0, 2]$, and the first-order time derivative with the

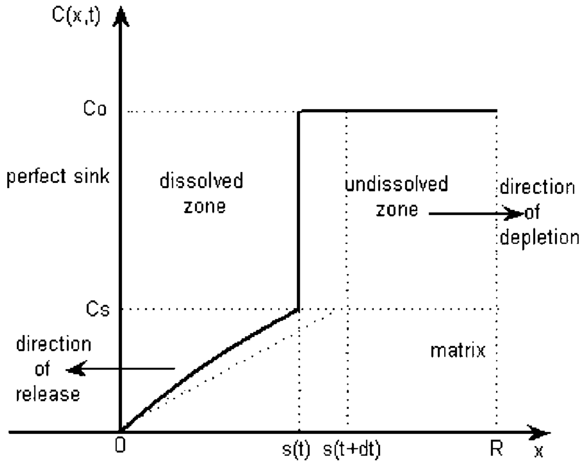

Figure 1. Profile of concentration.

Riemann–Liouville or the Caputo derivative of order $\beta \in (0, 1]$ (see [1–3] and the references therein). Different cases of Cauchy problems in a fixed domain have been considered, for example, the absorbing and reflecting boundaries in half-space and in a box [4], diffusion equation together with appropriate initial conditions [5].

Due to the high nonlinearity of moving boundary problems and the fact that many of the useful properties of ordinary derivative are not known to carry over analogously for the case of fractional derivative operator, such as a clear geometric or physical meaning, product rules, chain rules and so on, fractional calculus has scarcely been applied to such problems. Liu and Xu [6] were the first and only ones who introduced the time-fractional diffusion equation to the drug release process which is a moving boundary problem from the point of view of mathematics. They proved the well-known semi-empirical formula in the controlled drug release system given by Ritger and Peppas.

In this paper, we use the space–time-fractional diffusion equation to master the process of a solute release from a polymer matrix in which the initial solute loading is higher than the solubility. The mathematics model is proposed and the analytical solution is obtained. For convenience of practical use, we give the computable form of the solution in some particular cases. A diagram describing the diffusion front of the device is also given.

2. Mathematical model

A solute release from an undissolved monolithic polymeric matrix is considered and a condition of perfect sink is assumed.

The concentration profile at time t is shown in figure 1. Where R is the scale of the polymer matrix. Each matrix consists of two regions: the surface zone, $0 < x < s(t)$, in which all solute is dissolved, and the core, $s(t) < x < R$, which contains undissolved solute. The two zones are separated by the diffusion front, $x = s(t)$, which moves inward as time progresses. C_0 and C_s are the initial concentration of the solute distributed in the matrix and the solubility of the solute in the solvent, respectively. We will consider only the early stage of loss before the diffusion front moves to R and assume that $C_0 > C_s$.

We apply the space–time-fractional anomalous diffusion equation

$$ {}_0^cD_t^{\beta} C(x,t) = \mathscr{D}\nabla_x^{\alpha} C(x,t) \qquad (0 < \beta \leqslant 1 < \alpha \leqslant 2) \tag{2} $$

to the region $0 < x < s(t)$, and use the following boundary conditions:

$$x = 0, \qquad C = 0 \tag{3}$$

$$x = s(t), \qquad C = C_s. \tag{4}$$

and

$$(C_0 - C_s)\frac{\mathrm{d}s(t)}{\mathrm{d}t} = -F_l(x,t)|_{x=s(t)}, \tag{5}$$

where ${}_0^cD_t^\beta$ is the Caputo derivative defined by

$${}_0^cD_t^\beta f(t) = \frac{1}{\Gamma(m-\beta)}\int_0^t \frac{f^{(m)}(\tau)\,\mathrm{d}\tau}{(t-\tau)^{\beta+1-m}}, \qquad m-1 < \beta < m, \tag{6}$$

where $\Gamma(\cdot)$ is the gamma function. ∇_x^α is the Riesz derivative operator. By denoting the Fourier transform of a sufficiently well-behaved function $f(x)$, $\widehat{f(k)} = \mathscr{F}\{f(x);k\} = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx} f(x)\,\mathrm{d}x$, $k \in R$, the Riesz derivative of order α is defined by

$$\mathscr{F}\left\{\nabla_x^\alpha f(x);k\right\} = -|k|^\alpha \widehat{f(k)}. \tag{7}$$

$\mathscr{D}$ is the generalized diffusivity. Equation (3) is the perfect sink condition at the surface of matrix. Equation (5) is a condition for $x = s(t)$ which can be obtained using the conservation law of mass and $F_l(x,t)$ is the flux of diffusion. In the standard diffusion case,

$$F_l(x,t) = -K\frac{\partial}{\partial x}C(x,t), \tag{8}$$

which is the Fick's first law. Due to the non-local property of anomalous diffusion, following Chaves [7], Zannette [8] and Paradisi *et al* [9], we use the generalized non-local Fick's law,

$$F_l(x,t) = {}_0^cD_t^{1-\beta}\mathscr{F}^{-1}\left\{|k|^{\alpha-2}\mathscr{F}\left\{-\mathscr{D}\frac{\partial}{\partial x}C(x,t)\right\}\right\}, \tag{9}$$

to replace (8), where $\mathscr{F}^{-1}$ denotes the inverse Fourier transform.

The properties of the Caputo derivative can be found in [16, 17]. An important property used in the paper is

$${}_0^cD_t^a t^b = \frac{\Gamma(1+b)}{\Gamma(1+b-a)}t^{b-a} \qquad (0 \leqslant m \leqslant a < m+1, b > m, m \in N). \tag{10}$$

The constraint of this relation can be removed if we consider the analytical continuation of the gamma and beta functions for the entire complex plane (see [16], sections 1.1.3 and 1.1.4.).

3. The solution to the governing equation

By using reduced dimensionless variables defined as

$$\xi = \frac{x}{R}, \qquad \tau = \left(\frac{\mathscr{D}}{R^\alpha}\right)^{\frac{1}{\beta}} t, \qquad \theta = \frac{C}{C_s}, \qquad S(\tau) = \frac{s}{R}, \tag{11}$$

and the two relations (A.1)–(A.2) presented in the appendix, the governing equation (2) subjected to conditions (3)–(5) can be reduced to the respective dimensionless forms

$${}_0^cD_\tau^\beta\theta(\xi,\tau) = \nabla_\xi^\alpha\theta(\xi,\tau) \qquad (0 < \xi < S(\tau), \tau > 0), \tag{12}$$

$$\theta(\xi,\tau) = 0 \qquad (\xi = 0), \tag{13}$$

$$\theta(\xi,\tau)=1 \qquad (\xi=S(\tau)), \tag{14}$$

$$\eta\frac{\mathrm{d}S(\tau)}{\mathrm{d}\tau}=-F(\xi,\tau)|_{\xi=S(\tau)}, \tag{15}$$

$$S(0)=0, \tag{16}$$

where $\eta=\frac{C_0-C_s}{C_s}$ and $F(\xi,\tau)={}_0^cD_\tau^{1-\beta}\mathscr{F}^{-1}\left\{|k|^{\alpha-2}\mathscr{F}\left\{-\frac{\partial}{\partial\xi}\theta\right\}\right\}$ is the non-dimensional flux.

Since we consider only the early stage of loss before the diffusion front moves to R, the semi-infinite assumption can be used. As a result, we first consider equation (12) in the semi-infinite space which satisfies

$$\theta(0,\tau)=0 \tag{17}$$

and

$$\theta(\xi,0)=q=\text{const}. \tag{18}$$

As for the time-fractional diffusion, the above problem has been discussed by Schneider and Wyss [5] in detail. They gave the solution as

$$\theta=q\int_0^\infty \mathrm{d}y\{G(|\xi-y|,\tau)-G(|\xi+y|,\tau)\}, \tag{19}$$

in which $G(\xi,\tau)$ is the Green's function (or fundamental solution). It can also be written as

$$\theta(\xi,\tau)=q\int_0^\xi \mathrm{d}y\, G(\xi-y,\tau)+q\int_\xi^\infty \mathrm{d}y\, G(y-\xi,\tau)-q\int_0^\infty \mathrm{d}y\, G(\xi+y,\tau). \tag{20}$$

Substituting z for $\xi-y$, $y-\xi$, $\xi+y$, respectively, we obtain

$$\theta(\xi,\tau)=2q\int_0^\xi G(z,\tau)\,\mathrm{d}z. \tag{21}$$

For the space–time-fractional diffusion we considered, the solution has the same form as (21) except a difference of the Green's function. In Mainardi *et al*'s papers [10, 11], the Green's function for the Cauchy problem of space–time-fractional diffusion equation in terms of the Fox H function was given. The space-fractional derivative operator they used is the Riesz–Feller derivative. In this paper, we use the Riesz operator which is a special case of the Riesz–Feller operator as the space-fractional derivative operator. By using $G_{\alpha,\beta}(\xi,\tau)$ to denote the Green's function of our problem, we list the result we need in this paper here:

$$\begin{aligned}G_{\alpha,\beta}(\xi,\tau)&=\frac{1}{\alpha\xi}\frac{1}{2\pi\mathrm{i}}\int_{r-\mathrm{i}\infty}^{r+\mathrm{i}\infty}\frac{\Gamma\left(\frac{s}{\alpha}\right)\Gamma\left(1-\frac{s}{\alpha}\right)\Gamma(1-s)}{\Gamma\left(\frac{s}{2}\right)\Gamma\left(1-\frac{s}{2}\right)\Gamma\left(1-\frac{\beta s}{\alpha}\right)}\left(\frac{\xi}{\tau^\gamma}\right)^s\mathrm{d}s\\&=\frac{1}{\alpha\xi}H_{3,3}^{2,1}\left[\frac{|\xi|}{\tau^\gamma}\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,\frac{\beta}{\alpha})(1,\frac{1}{2})\\(1,\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\end{matrix}\right],\end{aligned} \tag{22}$$

where $\gamma=\frac{\beta}{\alpha}$ and $0<r<1$. The Fourier transform of $G_{\alpha,\beta}(\xi,\tau)$ is

$$\widehat{G_{\alpha,\beta}}(k,\tau)=E_\beta(-|k|^\alpha\tau^\beta), \tag{23}$$

where $E_\beta(\cdot)$ is the Mittag–Leffler function defined as

$$E_\beta(z)=\sum_{n=0}^\infty\frac{z^n}{\Gamma(\beta n+1)}, \qquad \beta>0, \quad Z\in \mathrm{C}. \tag{24}$$

From equation (21), the solution to the original problem (12)–(15) can be written as

$$\begin{aligned}\theta(\xi,\tau) &= 2q\int_0^{\xi}\frac{1}{\alpha\xi'}H_{3,3}^{2,1}\left[\frac{|\xi'|}{\tau^{\gamma}}\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,\frac{\beta}{\alpha})(1,\frac{1}{2})\\(1,\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\end{matrix}\right]\mathrm{d}\xi'\\ &= 2q\int_0^{\xi/\tau^{\gamma}}\frac{1}{\alpha z}H_{3,3}^{2,1}\left[z\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,\frac{\beta}{\alpha})(1,\frac{1}{2})\\(1,\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\end{matrix}\right]\mathrm{d}z\\ &= \frac{2q}{\alpha}\int_0^{\xi/\tau^{\gamma}}\frac{1}{2\pi\mathrm{i}}\int_{r-\mathrm{i}\infty}^{r+\mathrm{i}\infty}\frac{\Gamma\left(\frac{s}{\alpha}\right)\Gamma\left(1-\frac{s}{\alpha}\right)\Gamma(1-s)}{\Gamma\left(\frac{s}{2}\right)\Gamma\left(1-\frac{s}{2}\right)\Gamma\left(1-\frac{\beta s}{\alpha}\right)}z^{s-1}\,\mathrm{d}s\,\mathrm{d}z.\end{aligned}$$

Noting that $0<r<1$, z^{s-1} is an integrable function in $\left[0,\frac{\xi}{\tau^{\gamma}}\right]$, the order of integral can be exchanged. Consequently, we have

$$\theta(\xi,\tau)=\frac{2q}{\alpha}\frac{1}{2\pi\mathrm{i}}\int_{r-\mathrm{i}\infty}^{r+\mathrm{i}\infty}\frac{\Gamma\left(\frac{s}{\alpha}\right)\Gamma\left(1-\frac{s}{\alpha}\right)\Gamma(1-s)\Gamma(s)}{\Gamma\left(\frac{s}{2}\right)\Gamma\left(1-\frac{s}{2}\right)\Gamma\left(1-\frac{\beta s}{\alpha}\right)\Gamma(1+s)}\left(\frac{\xi}{\tau^{\gamma}}\right)^{s}\mathrm{d}s.$$

Since the contour separates the poles of $\Gamma\left(1-\frac{s}{\alpha}\right)$, $\Gamma(1-s)$ and $\Gamma\left(\frac{s}{\alpha}\right)$, $\Gamma(s)$, the integral above can be represented in terms of the Fox H function,

$$\theta(\xi,\tau)=\frac{2q}{\alpha}H_{4,4}^{2,2}\left[\frac{\xi}{\tau^{\gamma}}\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,1)(1,\frac{\beta}{\alpha})(1,\frac{1}{2})\\(1,\frac{1}{\alpha})(1,1)(0,1)(1,\frac{1}{2})\end{matrix}\right],\tag{25}$$

where q is a constant to be determined. Noting that the boundary condition (14) has to be satisfied for all the values of τ, $S(\tau)$ must be proportional to τ^{γ},

$$S(\tau)=p\tau^{\gamma},\tag{26}$$

where p is a constant to be determined.

Substituting (26) into (25), the first relationship between p and q can be obtained:

$$\frac{2q}{\alpha}H_{4,4}^{2,2}\left[p\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,1)(1,\frac{\beta}{\alpha})(1,\frac{1}{2})\\(1,\frac{1}{\alpha})(1,1)(0,1)(1,\frac{1}{2})\end{matrix}\right]=1.\tag{27}$$

In order to get another relationship between p and q, we must consider the flux. Using (21) and (23), we arrive at

$$\mathscr{F}\left\{-\frac{\partial\theta}{\partial\xi}\right\}=-2q\mathscr{F}\{G_{\alpha,\beta}(\xi,\tau)\}=-2qE_{\beta}(-|k|^{\alpha}\tau^{\beta}).\tag{28}$$

As a result,

$$F(\xi,\tau)=-2q\,{}_0^cD_{\tau}^{1-\beta}\mathscr{F}^{-1}\{E_{\beta}(-|k|^{\alpha}\tau^{\beta})|k|^{\alpha-2}\}.\tag{29}$$

Considering the properties of Mellin transform and

$$\mathscr{M}\{E_{\beta}(-z);s\}=\frac{\Gamma(s)\Gamma(1-s)}{\Gamma(1-\beta s)},\tag{30}$$

we have

$$\mathscr{M}\{E_{\beta}(-|k|^{\alpha}\tau^{\beta})|k|^{\alpha-2};s\}=\frac{1}{\alpha}\tau^{\frac{2\beta-\beta s}{\alpha}-\beta}\frac{\Gamma\left(\frac{\alpha-2}{\alpha}+\frac{s}{\alpha}\right)\Gamma\left(1+\frac{2-\alpha}{\alpha}-\frac{s}{\alpha}\right)}{\Gamma\left(1+\frac{2-\alpha}{\alpha}\beta-\frac{\beta s}{\alpha}\right)}.\tag{31}$$

Using the relationship between Fourier transform and Mellin transform [10],

$$I_c(x)=\frac{1}{\pi}\int_0^{\infty}f(k)\cos(kx)\,\mathrm{d}k,$$

$$I_c(x)=\frac{1}{\pi x}\frac{1}{2\pi\mathrm{i}}\int_{r-\mathrm{i}\infty}^{r+\mathrm{i}\infty}f^{*}(s)\Gamma(1-s)\sin\left(\frac{\pi x}{2}\right)x^{s}\,\mathrm{d}s,\qquad x>0,\quad 0<r<1,$$

where $I_c(x)$ is the inverse Fourier Cosine transform of $f(k)$ and $f^*(s)$ is the Mellin transform of $f(k)$, we can get the flux

$$
\begin{aligned}
F(\xi,\tau) &= {}_0^cD_\tau^{1-\beta}\frac{-2q}{\pi\xi}\frac{1}{2\pi\mathrm{i}}\int_{r-\mathrm{i}\infty}^{r+\mathrm{i}\infty}\mathscr{M}\{E_\beta(-|k|^\alpha\tau^\beta)|k|^{\alpha-2};s\}\Gamma(1-s)\sin\left(\frac{\pi s}{2}\right)\xi^s\,\mathrm{d}s\\
&= \frac{-2q\tau^{\frac{2\beta}{\alpha}-1}}{\alpha\xi}\frac{1}{2\pi\mathrm{i}}\int_{r-\mathrm{i}\infty}^{r+\mathrm{i}\infty}\mathcal{H}(s)\left(\frac{\xi}{\tau^\gamma}\right)^s\mathrm{d}s,
\end{aligned}
\tag{32}
$$

where

$$
\mathcal{H}(s) = \frac{\Gamma\left(\frac{\alpha-2}{\alpha}+\frac{s}{\alpha}\right)\Gamma\left(\frac{2}{\alpha}-\frac{s}{\alpha}\right)\Gamma(1-s)}{\Gamma\left(\frac{2\beta}{\alpha}-\frac{\beta}{\alpha}s\right)\Gamma\left(1-\frac{s}{2}\right)\Gamma\left(\frac{s}{2}\right)}. \tag{33}
$$

In the course of deriving (33), the complementary law of the gamma function

$$
\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin(\pi x)} \tag{34}
$$

and the formula of the Caputo derivative (10) are used. The flux can be expressed in terms of the H function:

$$
F(\xi,\tau) = -\frac{2q\tau^{2\gamma-1}}{\alpha\xi}H_{3,3}^{2,1}\left[\frac{\xi}{\tau^\gamma}\middle|\begin{matrix}(\frac{2}{\alpha},\frac{1}{\alpha})(\frac{2\beta}{\alpha},\frac{\beta}{\alpha})(1,\frac{1}{2})\\(\frac{2}{\alpha},\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\end{matrix}\right]. \tag{35}
$$

Therefore, from equations (15) and (26) the second equation of p, q is

$$
\eta p\gamma = \frac{2q}{\alpha p}H_{3,3}^{2,1}\left[p\middle|\begin{matrix}(\frac{2}{\alpha},\frac{1}{\alpha})(\frac{2\beta}{\alpha},\frac{\beta}{\alpha})(1,\frac{1}{2})\\(\frac{2}{\alpha},\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\end{matrix}\right]. \tag{36}
$$

Eliminating q in (27) and (36), we can obtain the equation of p:

$$
\eta p^2\gamma H_{4,4}^{2,2}\left[p\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,1)(1,\frac{\beta}{\alpha})(1,\frac{1}{2})\\(1,\frac{1}{\alpha})(1,1)(0,1)(1,\frac{1}{2})\end{matrix}\right] = H_{3,3}^{2,1}\left[p\middle|\begin{matrix}(\frac{2}{\alpha},\frac{1}{\alpha})(\frac{2\beta}{\alpha},\frac{\beta}{\alpha})(1,\frac{1}{2})\\(\frac{2}{\alpha},\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\end{matrix}\right]. \tag{37}
$$

In order to get the value of p, we must solve equation (37). However, computing routine for the H function is not available. Fortunately, in some special cases, the H function can be represented by convergent series which can be calculated.

4. Discussion on the solution

The standard diffusion equation, time-fractional and space-fractional diffusion equations are the three special cases which have been widely discussed. In this section, we consider our problem in these three cases.

Case 1. When $\beta = 1, \alpha = 2$ the governing equation (12) degenerates into the standard diffusion equation (1) and the generalized Fick's law (9) degenerates into the Fick's first law (8). In this case, the solution (25) becomes

$$
\begin{aligned}
\theta(\xi,\tau) &= qH_{4,4}^{2,2}\left[\frac{\xi}{\tau^{1/2}}\middle|\begin{matrix}(1,\frac{1}{2})(1,1)(1,\frac{1}{2})(1,\frac{1}{2})\\(1,\frac{1}{2})(1,1)(0,1)(1,\frac{1}{2})\end{matrix}\right] = qH_{2,2}^{1,1}\left[\frac{\xi}{\tau^{1/2}}\middle|\begin{matrix}(1,1)(1,\frac{1}{2})\\(1,1)(0,1)\end{matrix}\right]\\
&= q\sum_{k=0}^{\infty}\frac{(-1)^k\left(\frac{\xi}{\tau^{1/2}}\right)^{k+1}}{\Gamma\left(\frac{1}{2}-\frac{k}{2}\right)(k+1)!} = q\sum_{m=0}^{\infty}\frac{(-1)^{2m}\left(\frac{\xi}{\tau^{1/2}}\right)^{2m+1}}{\Gamma\left(\frac{1}{2}-m\right)(2m+1)!}\\
&= q\frac{2}{\sqrt{\pi}}\sum_{m=0}^{\infty}\frac{(-1)^m\left(\frac{\xi}{2\tau^{1/2}}\right)^{2m+1}}{m!(2m+1)} = q\,\mathrm{erf}\left(\frac{\xi}{2\tau^{1/2}}\right),
\end{aligned}
\tag{38}
$$

where erf$(\cdot)$ is the Error function. In the course of deriving (38), the expansion for the H function [18],

$$H_{p,q}^{m,n}(z) = \sum_{h=1}^{m}\sum_{k=0}^{\infty} \frac{\prod_{j=1,j\neq h}^{m}\Gamma\left(b_j - B_j\frac{b_h+k}{B_h}\right)\prod_{j=1}^{n}\Gamma\left(1-a_j+A_j\frac{b_h+k}{B_h}\right)}{\prod_{j=m+1}^{q}\Gamma\left(1-b_j+B_j\frac{b_h+k}{B_h}\right)\prod_{j=n+1}^{p}\Gamma\left(a_j-A_j\frac{b_h+k}{B_h}\right)}\frac{(-1)^k z^{(b_h+k)/B_h}}{k!B_h},$$

was used. Similarly, the non-dimensional flux becomes

$$\begin{aligned} F(\xi,\tau) &= -\frac{q}{\xi}H_{3,3}^{2,1}\left[\frac{\xi}{\tau^{\frac{1}{2}}}\middle|\begin{matrix}(1,\frac{1}{2})(1,\frac{1}{2})(1,\frac{1}{2})\\ (1,\frac{1}{2})(1,1)(1,\frac{1}{2})\end{matrix}\right]\\ &= -\frac{q}{\xi}H_{1,1}^{1,0}\left[\frac{\xi}{\tau^{\frac{1}{2}}}\middle|\begin{matrix}(1,\frac{1}{2})\\ (1,1)\end{matrix}\right]\\ &= -\frac{q}{\sqrt{\pi}}\exp\left(-\frac{\xi^2}{4\tau}\right)\tau^{-\frac{1}{2}}. \end{aligned} \tag{39}$$

Therefore, the equation of p is

$$\sqrt{\pi}\frac{p}{2}\mathrm{erf}\left(\frac{p}{2}\right)\exp\left(\frac{p^2}{4}\right) = \frac{C_s}{C_0 - C_s} \tag{40}$$

It is exactly the solution given by Paul and McSpadden [12].

Case 2. When $0 < \beta \leqslant 1$, $\alpha = 2$, (12) degenerates into the time-fractional diffusion equation. In this case,

$$\begin{aligned} \theta(\xi,\tau) &= qH_{4,4}^{2,2}\left[\frac{\xi}{\tau^{\beta/2}}\middle|\begin{matrix}(1,\frac{1}{2})(1,1)(1,\frac{\beta}{2})(1,\frac{1}{2})\\ (1,\frac{1}{2})(1,1)(0,1)(1,\frac{1}{2})\end{matrix}\right]\\ &= qH_{2,2}^{1,1}\left[\frac{\xi}{\tau^{\beta/2}}\middle|\begin{matrix}(1,1)(1,\frac{\beta}{2})\\ (1,1)(0,1)\end{matrix}\right]\\ &= q\sum_{n=0}^{\infty}\frac{(-1)^n}{\Gamma\left(1-\frac{\beta}{2}(1+n)\right)}\frac{\left(\frac{\xi}{\tau^{\beta/2}}\right)^{n+1}}{(n+1)!}, \end{aligned} \tag{41}$$

$$\begin{aligned} F(\xi,\tau) &= -\frac{q\tau^{\beta-1}}{\xi}H_{3,3}^{2,1}\left[\frac{\xi}{\tau^{\beta/2}}\middle|\begin{matrix}(1,\frac{1}{2})(\beta,\frac{\beta}{2})(1,\frac{1}{2})\\ (1,\frac{1}{2})(1,1)(1,\frac{1}{2})\end{matrix}\right]\\ &= -\frac{q\tau^{\beta-1}}{\xi}H_{1,1}^{1,0}\left[\frac{\xi}{\tau^{\beta/2}}\middle|\begin{matrix}(\beta,\frac{\beta}{2})\\ (1,1)\end{matrix}\right]\\ &= -\frac{q\tau^{\beta-1}}{\xi}\sum_{n=0}^{\infty}\frac{(-1)^n\left(\frac{\xi}{\tau^{\beta/2}}\right)^{n+1}}{\Gamma\left(\beta-\frac{\beta}{2}(1+n)\right)n!}. \end{aligned} \tag{42}$$

The equation of p becomes

$$\sum_{n=0}^{\infty}\frac{(-1)^n p^{n+1}}{\Gamma\left(\beta-\frac{\beta}{2}(1+n)\right)n!} = \eta p^2\frac{\beta}{2}\sum_{n=0}^{\infty}\frac{(-1)^n}{\Gamma\left(1-\frac{\beta}{2}(1+n)\right)}\frac{p^{n+1}}{(n+1)!}. \tag{43}$$

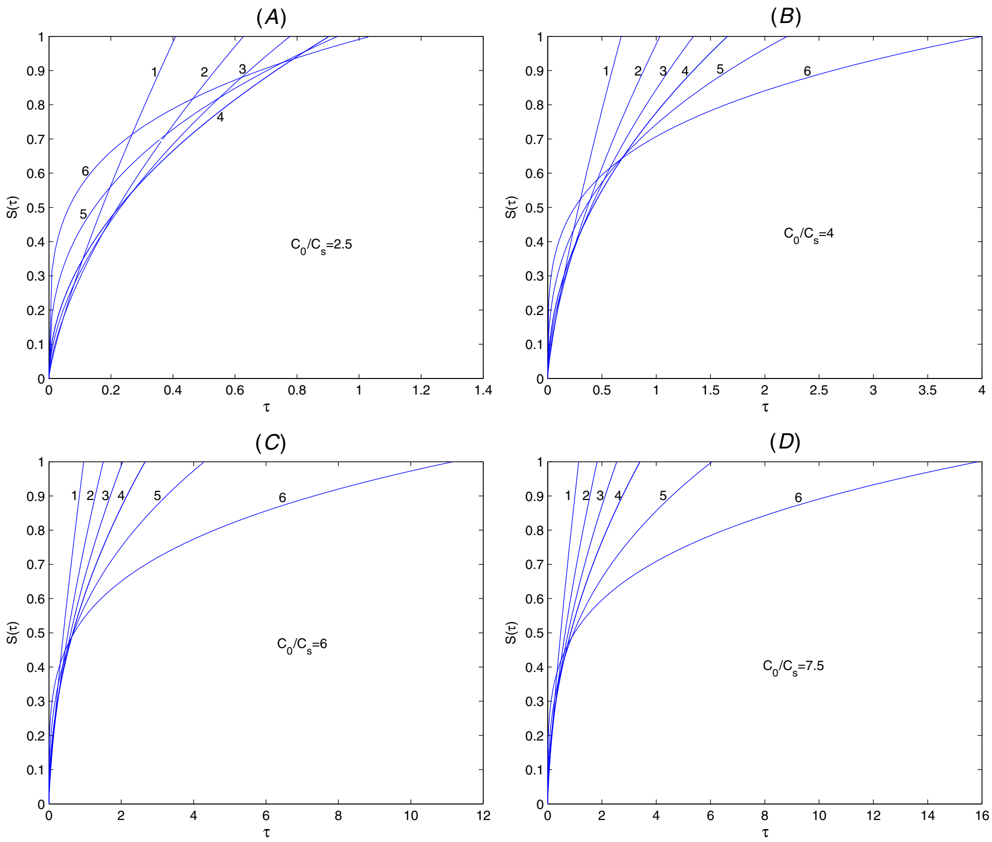

Figure 2. Non-dimensional diffusion front position $S(\tau)$ versus non-dimensional time at various solute loading levels. Curves 1–6 correspond to the cases that (α, β) equals to (1.25,1), (1.5,1), (1.75,1), (2,1), (2,0.75) and (2,0.5), respectively.

If applying the operator ${}_0^cD_\tau^{\beta-1}$ to both sides of (15) and using the properties of the Caputo derivative we can find that our solution is exactly the solution given by Liu and Xu [6].

Case 3. When $1 < \alpha \leqslant 2$, $\beta = 1$, (12) becomes the space-fractional diffusion equation. In this case,

$$\begin{aligned}\theta(\xi,\tau) &= \frac{2q}{\alpha} H_{4,4}^{2,2}\left[\frac{\xi}{\tau^{1/\alpha}}\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,1)(1,\frac{1}{\alpha})(1,\frac{1}{2})\\ (1,\frac{1}{\alpha})(1,1)(0,1)(1,\frac{1}{2})\end{matrix}\right]\\ &= \frac{2q}{\alpha} H_{3,3}^{1,2}\left[\frac{\xi}{\tau^{1/\alpha}}\middle|\begin{matrix}(1,\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\\ (1,1)(0,1)(1,\frac{1}{2})\end{matrix}\right]\\ &= \frac{2q}{\alpha\pi}\sum_{n=1}^{\infty}\left(\frac{-\xi}{\tau^{1/\alpha}}\right)^n \frac{\Gamma\left(\frac{n}{\alpha}\right)}{n!}\sin\left(-\frac{n}{2}\pi\right),\end{aligned} \tag{44}$$

$$F(\xi,\tau) = -\frac{2q\tau^{\frac{2}{\alpha}-1}}{\alpha\xi} H_{3,3}^{2,1}\left[\frac{\xi}{\tau^{1/\alpha}}\middle|\begin{matrix}(\frac{2}{\alpha},\frac{1}{\alpha})(\frac{2}{\alpha},\frac{1}{\alpha})(1,\frac{1}{2})\\ (\frac{2}{\alpha},\frac{1}{\alpha})(1,1)(1,\frac{1}{2})\end{matrix}\right]$$

$$= -\frac{2q\tau^{\frac{2}{\alpha}-1}}{\alpha\xi} H_{2,2}^{1,1}\left[\frac{\xi}{\tau^{1/\alpha}}\Bigg|_{(1,1)(1,\frac{1}{2})}^{(\frac{2}{\alpha},\frac{1}{\alpha})(1,\frac{1}{2})}\right]$$
$$= -\frac{2q\tau^{1/\alpha}}{\pi\alpha\xi}\sum_{n=1}^{\infty}\left(\frac{-\xi}{\tau^{1/\alpha}}\right)^{n}\frac{\Gamma\left(1-\frac{2}{\alpha}+\frac{n}{\alpha}\right)}{(n-1)!}\sin\left(-\frac{n}{2}\pi\right). \tag{45}$$

The equation of p becomes

$$\eta\frac{1}{\alpha}p^{2}\sum_{n=1}^{\infty}(-p)^{n}\frac{\Gamma\left(\frac{n}{\alpha}\right)}{n!}\sin\left(-\frac{n}{2}\pi\right) = \sum_{n=1}^{\infty}(-p)^{n}\frac{\Gamma\left(1-\frac{2}{\alpha}+\frac{n}{\alpha}\right)}{(n-1)!}\sin\left(-\frac{n}{2}\pi\right). \tag{46}$$

The non-dimensional diffusion front position $S(\tau)$ versus non-dimensional time τ at various solute loading levels is shown in figure 2. Curves 1–3 correspond to space-fractional diffusion models, curve 4 corresponds to the ordinary diffusion model, curves 5 and 6 correspond to time-fractional diffusion models. It is obvious that the time-fractional diffusion model and the space-fractional one describe sub-diffusion and super-diffusion, respectively. It is consistent with the conclusion of [1, 2]. As for the same curve, by comparing the four pictures in figure 2, we can see that the higher the initial solute loading level is, the longer the time to reach R for the diffusion front $s(t)$ needs. These conclusions show the fact that the models are well consistent with the truth.

5. Summary and conclusion

For the moving boundary problems, very few analytical solutions are available in closed form [19]. They are mainly for the one-dimensional cases of an infinite or semi-infinite region and are known as the similarity solution in the standard diffusion cases.

The scale invariant (or similarity solution) of the fractional diffusion equation has been considered in some cases [13–15]. The model in this paper is just a special case which has the similarity solution taking the form of the function of the single variable $\frac{\xi}{\tau^{\beta/\alpha}}$. In the cases when the matrix is cylindrical or spherical, the semi-infinite assumption cannot be used. The similarity solution may not exist because of the existence of the characteristic scale. Therefore, other skills must considered in these cases.

In researches on the controlled release drug delivery systems for which the release rate over time is pre-programmed into the device, the relevant mathematical models of drug releases from the polymer matrix are the most powerful tools. Therefore, the study of fractional calculus in moving boundary problems would be of great interest to both theoreticians and experimenters in the future.

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Appendix

In this section, we present some properties of the Caputo fractional derivative to show the derivation of the dimensionless form of (2) and (5).

If $t = A\tau$ ($A > 0$) and $f(t)$ is a function for which the Caputo fractional derivative ${}_0^cD_t^a f(t)$ of order a ($0 < a < 1$) exists, then, in accordance with the definition of the Caputo fractional derivative, we get the following relation:

$$\begin{aligned}
{}_0^cD_t^a f(t) &= \frac{1}{\Gamma(1-a)} \int_0^t \frac{\mathrm{d}f(s)/\mathrm{d}s}{(t-s)^a}\,\mathrm{d}s \\
&= \frac{1}{\Gamma(1-a)} \int_0^{A\tau} \frac{\mathrm{d}f(s)/\mathrm{d}s}{(A\tau-s)^a}\,\mathrm{d}s \\
&= \frac{1}{\Gamma(1-a)} \int_0^{\tau} \frac{\mathrm{d}f(As')/\mathrm{d}s'}{(A\tau-As')^a}\,\mathrm{d}s' \\
&= \frac{A^{-a}}{\Gamma(1-a)} \int_0^{\tau} \frac{\mathrm{d}f(As')/\mathrm{d}s'}{(\tau-s')^a}\,\mathrm{d}s' \\
&= A^{-a}\,{}_0^cD_\tau^a f(A\tau).
\end{aligned} \tag{A.1}$$

Similarly, if $x = B\xi$ and $B > 0$, we have the following relation for the Riesz fractional derivative ∇_x^b:

$$\begin{aligned}
\nabla_x^b g(x) &= \mathscr{F}^{-1}\{-|k|^b\widehat{g}(k)\} \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} -\mathrm{e}^{-\mathrm{i}kx}|k|^b\widehat{g}(k)\,\mathrm{d}k \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} -\mathrm{e}^{-\mathrm{i}kB\xi}|k|^b\widehat{g}(k)\,\mathrm{d}k \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} -\mathrm{e}^{-\mathrm{i}(kB)\xi}|kB|^b\widehat{g}(k)B^{-b-1}\,\mathrm{d}Bk.
\end{aligned}$$

Considering that

$$\begin{aligned}
\widehat{g}(k) &= \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx} g(x)\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(Bk)\xi} g(B\xi)B\,\mathrm{d}\xi \\
&= B\mathscr{F}\{g(B\xi);\, Bk\},
\end{aligned}$$

then we obtain

$$\nabla_x^b g(x) = B^{-b}\nabla_\xi^b g(B\xi). \tag{A.2}$$

References

[1] Metzler R and Klafter J 2000 *Phys. Rep.* **339** 1
[2] Metzler R and Klafter J 2004 *J. Phys. A: Math. Gen.* **37** 161
[3] Metzler R and Nonnenmacher T F 2002 *Chem. Phys.* **284** 67
[4] Metzler R and Klafter J 2000 *Physica* A **278** 107
[5] Schneider W R and Wyss W 1989 *J. Math. Phys* **30** 134
[6] Liu J Y and Xu M Y 2004 *Z. Angew. Math. Mech.* **84** 22
[7] Chaves A S 1998 *Phys. Lett.* A **239** 13
[8] Zanette D H 1998 *Physica* A **252** 159
[9] Paradisi P, Cesari R, Mainardi F and Tempieri F 2001 *Physica* A **293** 130
[10] Mainardi F, Luchko Y and Pagnini G 2001 *Frac. Calc. Appl. Anal.* **4** 153
[11] Mainardi F, Pagnini G and Saxena R K 2005 *J. Comput. Appl. Math.* **178** 321
[12] Paul D R and McSpadden S K 1976 *J. Membr. Sci.* **1** 33
[13] Buckwar E and Luchko Y 1998 *J. Math. Anal. Appl.* **227** 81

[14] Gorenflo R, Luchko Y and Mainardi F 2000 *J. Comput. Appl. Math.* **118** 175
[15] Xu M Y and Tan W C 2001 *Sci. China Ser.* A **44** 1387
[16] Podlubny I 1999 *Fractional Differential Equations* (New York: Academic)
[17] Kilbas A A, Srivastava H M and Trujillo J J 2006 *Theory and Applications of Fractional Differential Equations* (Amsterdam: Elsevier)
[18] Mathai A M and Saxena R K 1978 *The H Function with Applications in Statistics and Other Disciplines* (New Delhi: Wiley Eastern Ltd)
[19] Crank J 1987 *Free and Moving Boundary Problems* (Oxford: Clarendon)