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Homotopy perturbation method to time-fractional diffusion equation with a moving boundary condition

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ABSTRACT

Homotopy perturbation method is successfully extended to solve time-fractional diffusion equation with a moving boundary condition and an approximate solution is obtained. The comparison with the exact solution shows that the approximate solution is sufficiently accurate for practical application in most cases.

1. Introduction

In recent years, the fractional derivative operators are of great interest for their being widely used as tools for dealing with complex systems [1–4]. A survey paper on the application of fractional derivatives in modern mechanics is given by Xu and Tan [5]. However, due to the highly nonlinearity of the moving boundary problem and difficulties of dealing with the fractional derivatives, fractional calculus has scarcely been applied to such problems. To the authors' knowledge, the first paper used fractional diffusion equation as the master equation of diffusion process in the release of a solute from a polymer matrix which is a typical moving boundary problem from the viewpoint of mathematics was given by Liu and Xu [6]. Li et al. [7,8] considered different types of time–space fractional models of the drug release devices and present exact solutions to the models.

The moving boundary problem is a special nonlinear problem which is difficult to get the exact solution [9]. Many approximate methods have been used to solve the moving boundary problems of integer order, e.g., the perturbation method [10–12], combination of variable method [13,14]. However, 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, and chain rules. As a result, many methods listed above are invalid in the fractional cases.

In this paper, the homotopy perturbation method is considered. The homotopy perturbation method which provides an analytical approximate solution was firstly presented by He [15–18] and applied to various nonlinear problems [19,20]. Odibat and Momani [21,22], Wang [23,24] applied the homotopy perturbation method to nonlinear fractional equations which have nonlinear terms in the equations. We extend the homotopy perturbation method to moving boundary problem encountered in drug release from polymer matrix.

The paper is organized as follows. In Section 2, a short introduction to the mathematical model of drug release and the definition and some properties of the Caputo fractional derivative operator are given. The solutions to the problem is presented in Section 3. The comparison of the approximate solution with the exact one is given in Section 4. Finally in Section 5, a summary and conclusion are obtained.

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2. Mathematical model and analysis

Here we consider the model given by Liu and Xu [6]. The initial drug loading and the concentration profile at time t are shown in Fig. 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 drug distributed in the matrix and the solubility of the drug in the tissue fluid, respectively. We will consider only the early stages of loss before the diffusion front moves to R and assume that $C_0 > C_s$. A condition of perfect sink is also assumed.

Accordingly, we have the governing equation and the posed conditions as follows:

$$ {}_0^C D_t^\alpha C(x,t) = \mathscr{D}\frac{\partial^2}{\partial x^2}C(x,t) \quad (0 < x < s(t),\ 0 < \alpha \leqslant 1,\ t > 0), \tag{1}$$
$$ C(x,t) = C_s \quad (x = s(t),\ t > 0), \tag{2}$$
$$ C(x,t) = 0 \quad (x = 0), \tag{3}$$
$$ (C_0 - C_s){}_0^C D_t^\alpha s(t) = \mathscr{D}\frac{\partial}{\partial x}C(x,t) \quad (x = s(t),\ t > 0), \tag{4}$$
$$ s(t) = 0 \quad (t = 0), \tag{5}$$

here $C(x,t)$ is the concentration of drug in the matrix. $\mathscr{D}$ is the diffusivity of drug in the matrix and assumed to be constant. The operator ${}_0^C D_t^\alpha$ appears in (1) is the Caputo fractional derivative defined as

$$ {}_0^C D_t^\alpha f(t) = {}_0^C D_t^{\alpha-n}[f^{(n)}(t)] \quad (n-1 < Re(\alpha) \leqslant n,\ n \in N), \tag{6}$$
$$ {}_0^C D_t^{-\alpha} f(t) = \int_0^t \frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)} f(\tau)d\tau \quad (\alpha > 0), \tag{7}$$

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

The properties of fractional derivative can be found in [1,2]. An important property used in the paper is

$$ {}_0^C D_t^\alpha t^\beta = \frac{\Gamma(1+\beta)}{\Gamma(1+\beta-\alpha)} t^{\beta-\alpha} \quad (0 \leqslant m \leqslant \alpha < m+1,\ \beta > m,\ m \in N). \tag{8}$$

The constraint of this relation can be removed if we treat ${}_0^C D_t^\alpha t^\beta$ as a Beta integral and consider the analytical continuation of the Gamma and Beta functions for the entire complex plane (see [1], Sections 1.1.3 and 1.1.4).

3. The approximate solution to the equations

By using reduced dimensionless variables defined as

$$ \xi = \frac{x}{R}, \quad \tau = \left(\frac{\mathscr{D}}{R^2}\right)^{\frac{1}{\alpha}} t, \quad \theta = \frac{C}{C_s}, \quad S(\tau) = \frac{s(\tau)}{R}, \tag{9}$$

the governing equation (1) subjected to the conditions (2)–(5) can be reduced to the respective dimensionless forms,

$$ {}_0^C D_\tau^\alpha \theta(\xi,\tau) = \frac{\partial^2}{\partial \xi^2}\theta(\xi,\tau) \quad (0 < \xi < S(\tau),\ \tau > 0), \tag{10}$$
$$ \theta(\xi,\tau) = 0 \quad (\xi = 0), \tag{11}$$
$$ \theta(\xi,\tau) = 1 \quad (\xi = S(\tau)), \tag{12}$$
$$ \frac{\partial}{\partial \xi}\theta(\xi,\tau) = \eta {}_0^C D_\tau^\alpha S(\tau) \quad (\xi = S(\tau)), \tag{13}$$
$$ S(0) = 0, \tag{14}$$

where $\eta = \frac{C_0 - C_s}{C_s}$.

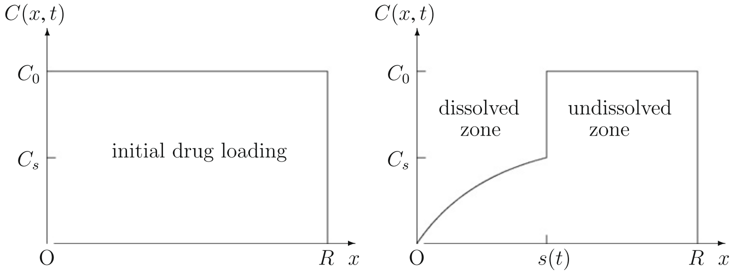

Fig. 1. Profile of concentration. The left one is the initial drug loading and the right one is the profile of concentration of the drug in the matrix at time t.

According to the homotopy perturbation method, we construct the following simple homotopy:

$$(1-p)\frac{\partial^2}{\partial\xi^2}\theta + p\left[\frac{\partial^2}{\partial\xi^2}\theta - {}_0^C D_\tau^\alpha \theta\right] = 0 \tag{15}$$

or

$$\frac{\partial^2}{\partial\xi^2}\theta - p{}_0^C D_\tau^\alpha \theta = 0, \tag{16}$$

where $p \in [0,1]$ is an embedding parameter. In case $p = 0$, (16) is an ordinary differential equation, $\frac{\partial^2}{\partial\xi^2}\theta = 0$, which is easy to solve; and when $p = 1$, (16) turns out to be the original one (10). The basic assumption is that the solutions can be written as a power series in p,

$$\theta = \sum_{n=0}^{\infty} p^n \theta_n, \quad S = \sum_{n=0}^{\infty} p^n S_n. \tag{17}$$

The approximate solution of the original equations can be obtained by setting $p = 1$, i.e.

$$\theta = \sum_{n=0}^{\infty} \theta_n, \quad S = \sum_{n=0}^{\infty} S_n. \tag{18}$$

Substituting (17) into (16), the following equation can be obtained:

$$\sum_{n=0}^{\infty} p^n \frac{\partial^2}{\partial\xi^2}\theta_n = \sum_{n=0}^{\infty} p^{n+1} {}_0^C D_\tau^\alpha \theta_n. \tag{19}$$

Accordingly, the boundary condition (12) becomes

$$\sum_{m=0}^{\infty} p^m \theta_m \left(\sum_{n=0}^{\infty} p^n S_n, \tau\right) = 1. \tag{20}$$

The perturbation parameter p is both explicit and implicit parameter. The implicit part relates to the variable S. In order to compare the coefficients of different powers of p, we need the explicit form of p. To do this, Taloy's series of θ_i is used. In a suitable neighborhood of a point (S_0, τ), $\theta_i(\xi, \tau)$ has a Taylor's series representation with respect to ξ

$$\theta_i(\xi,\tau) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n \theta_i}{\partial \xi^n}\bigg|_{(S_0,\tau)} (\xi - S_0)^n, \quad i = 0, 1, 2, \ldots$$

As a result, (20) becomes

$$\sum_{l=0}^{\infty}\sum_{m=0}^{\infty} \frac{p^l}{m!}\left(\sum_{n=1}^{\infty} p^n S_n\right)^m \frac{\partial^m}{\partial\xi^m}\theta_l = 1 \quad (\xi = S_0). \tag{21}$$

Similarly, boundary condition (13) becomes

$$\sum_{l=0}^{\infty}\sum_{m=0}^{\infty} \frac{p^l}{m!}\left(\sum_{n=1}^{\infty} p^n S_n\right)^m \frac{\partial^{m+1}}{\partial\xi^{m+1}}\theta_l = \eta \sum_{n=0}^{\infty} p^n {}_0^C D_\tau^\alpha S_n \quad (\xi = S_0). \tag{22}$$

Equating the terms with identical powers of p in (19), (21), (22), we can obtain a series of equations of the form

$$\begin{aligned}
p^0: \quad & \frac{\partial^2}{\partial\xi^2}\theta_0 = 0, \\
& \theta_0(0,\tau) = 0, \\
& \theta_0(S_0,\tau) = 1, \\
& \frac{\partial}{\partial\xi}\theta_0 = \eta {}_0^C D_\tau^\alpha S_0 \quad (\xi = S_0), \\
& S_0(0) = 0,
\end{aligned} \tag{23}$$

$$\begin{aligned}
p^1: \quad & \frac{\partial^2}{\partial\xi^2}\theta_1 = {}_0^C D_\tau^\alpha \theta_0, \\
& \theta_1(0,\tau) = 0, \\
& \theta_1(S_0,\tau) + S_1 \frac{\partial\theta_0}{\partial\xi} = 0 \quad (\xi = S_0),
\end{aligned} \tag{24}$$

$$\frac{\partial}{\partial\xi}\theta_1 + S_1\frac{\partial^2}{\partial\xi^2}\theta_0 = \eta_0{}^C D_\tau^\alpha S_1(\tau) \quad (\xi = S_0),$$
$$S_1(0) = 0,$$
$$\vdots$$

According to the first three equations of (23), we have

$$\theta_0 = S_0^{-1}\xi. \tag{25}$$

Substituting it into the fourth equation of (23), we have

$$S_0^{-1} = \eta_0{}^C D_\tau^\alpha S_0. \tag{26}$$

Considering the properties of fractional derivative (see Eq. (8)) and the initial condition of S_0, we can assume that

$$S_0 = a_0\tau^\gamma, \tag{27}$$

where a_0 and γ are constants to be determined. Employing Eq. (26), a_0 and γ can be obtained. After some computation, we have

$$\theta_0 = a_0^{-1}\tau^{-\gamma}\xi, \tag{28}$$

where

$$\gamma = \frac{\alpha}{2}, \quad a_0 = \left[\frac{\Gamma(1-\frac{\alpha}{2})}{\Gamma(1+\frac{\alpha}{2})\eta}\right]^{\frac{1}{2}}. \tag{29}$$

Substituting θ_0 and S_0 into Eqs. (24), the equations for θ_1 and S_1 are obtained. Using the method similar to the above process, we have

$$\theta_1 = a_1\xi^3\tau^{-\frac{3\alpha}{2}} - (a_1a_0^2 + a_2a_0^{-2})\xi\tau^{-\frac{\alpha}{2}}, \tag{30}$$
$$S_1 = a_2\tau^{\frac{\alpha}{2}}, \tag{31}$$

where

$$a_1 = \frac{\Gamma(1-\frac{\alpha}{2})a_0^{-1}}{6\Gamma(1-\frac{3\alpha}{2})}, \quad a_2 = \frac{2a_1a_0^2}{\eta\frac{\Gamma(1+\frac{\alpha}{2})}{\Gamma(1-\frac{\alpha}{2})} + a_0^{-2}}. \tag{32}$$

Sequentially, $\theta_2S_2, \theta_3S_3, \ldots$ can be obtained.

Substituting θ_0, θ_1, S_0, and S_1 into Eq. (18), the first order approximate solution can be written as

$$\theta = a_1\xi^3\tau^{-\frac{3\alpha}{2}} - (a_1a_0^2 + a_2a_0^{-2} - a_0^{-1})\xi\tau^{-\frac{\alpha}{2}}, \tag{33}$$
$$S = (a_0 + a_2)\tau^{\frac{\alpha}{2}}. \tag{34}$$

4. Comparison and analysis

In order to show the accuracy of the approximate solution, we compare it with the exact solution.

As a special case of the model in [8], We can see that

$$\theta = H\sum_{n=0}^{\infty}\frac{\left(\frac{\xi}{\tau^{\alpha/2}}\right)^{2n+1}}{(2n+1)!\Gamma(1-\frac{2n+1}{2}\alpha)} \tag{35}$$

and

$$S = \bar{p}\tau^{\alpha/2} \tag{36}$$

in which $\bar{p}$ and H satisfy

$$1 = H\sum_{n=0}^{\infty}\frac{\bar{p}^{2n+1}}{(2n+1)!\Gamma(1-\frac{2n+1}{2}\alpha)} \tag{37}$$

and

$$H\sum_{n=0}^{\infty}\frac{\bar{p}^{2n}}{(2n)!\Gamma(1-\frac{2n+1}{2}\alpha)} = \bar{p}\eta\frac{\Gamma(1+\alpha/2)}{\Gamma(1-\alpha/2)} \tag{38}$$

are exact solutions to (9)–(14).

Table 1
Comparison.

η	$\alpha = 0.5$			$\alpha = 0.75$			$\alpha = 1$		
	$\bar{p}$	$a_0 + a_2$	RE	$\bar{p}$	$a_0 + a_2$	RE	$\bar{p}$	$a_0 + a_2$	RE
0.5	1.8272	1.8947	0.0370	1.6216	1.6375	0.0098	1.6013	1.3333	0.1673
1	1.2423	1.2513	0.0072	1.2093	1.2141	0.0040	1.2402	1.1785	0.0497
3	0.6880	0.6883	0.0005	0.7222	0.7226	0.0005	0.7762	0.7711	0.0065
5	0.5279	0.5279	0.0000	0.5630	0.5631	0.0001	0.6129	0.6114	0.0025
7	0.4443	0.4443	0.0000	0.4771	0.4771	0.0000	0.5225	0.5218	0.0013
9	0.3909	0.3909	0.0000	0.4214	0.4214	0.0000	0.4631	0.4627	0.0009

In order to evaluate the accuracy of the approximate solution of $S(\tau)$, we compare the values of $\bar{p}$ and $a_0 + a_2$ for various values of η and α first. The result is listed in Table 1, where *RE* denotes the relative errors of the two solutions respectively. We can see that even if η is small (=0.5), the approximate solution is accurate enough ($RE = 3.7\%$) for practical use.

To show the accuracy of $\theta(\xi, \tau)$, we introduce the fractional release here. The amount of drug released per unit area at time t can be obtained using the following formula [13,14]:

$$M_t = C_0 s(t) - \int_0^{s(t)} C(x,t)\mathrm{d}x, \tag{39}$$

while the total amount of drug per unit area is given by $M_\infty = C_0 R$. Using the variables in Eq. (9), we can get the fractional release in a dimensionless form,

$$\frac{M_t}{M_\infty} = \delta(\tau) - \int_0^{S(\tau)} \frac{C_S}{C_0}\theta(\xi,\tau)\mathrm{d}\xi. \tag{40}$$

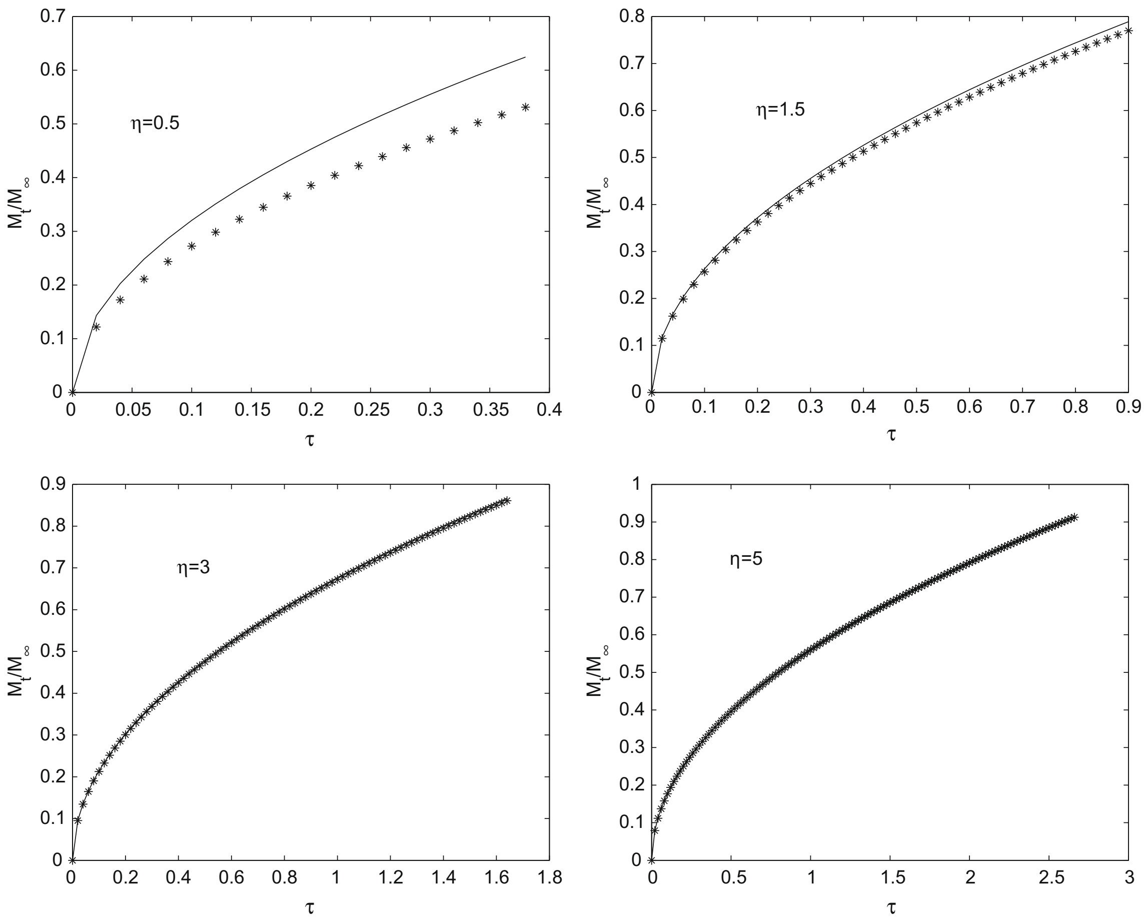

Fig. 2. The fractional release, — relates to the exact solutions, * relates to the approximate solutions, $\eta = \frac{C_0}{C_s} - 1$.

Employing (40), the fractional release with respect to $\{\theta, S\}$ is,

$$\frac{M_t}{M_\infty} = \left[a_0 + a_2 - \frac{a_1(a_0+a_2)^4}{4(\eta+1)} + \frac{a_1 a_0^2 + a_2 a_0^{-2} - a_0^{-1}}{2(\eta+1)}(a_0+a_2)^2\right]\tau^{\frac{\alpha}{2}}. \quad (41)$$

In Fig. 2, we give the profile of fractional release when $\alpha = 1$, in which case an exact form of the fractional release was obtained in Ref. [25]. For convenience of comparison, we give its dimensionless form here,

$$\frac{M_t}{M_\infty} = \frac{2}{\mathrm{erf}(\eta^*)(\eta+1)}\sqrt{\frac{\tau}{\pi}} \quad (42)$$

in which η^* satisfies:

$$\left(\frac{C_0}{C_s} - 1\right)\eta^*\sqrt{\pi}e^{\eta^{*2}}\mathrm{erf}(\eta^*) = 1, \quad (43)$$

where $\mathrm{erf}(\cdot)$ is the error function.

5. Summary and conclusions

In the paper, an approximate solution with high accuracy is obtained using the homotopy perturbation method. The following results can be obtained:

(1) When $\alpha = 1$, the model in [13,14,25] is recovered.
(2) As for the perturbation method, the explicit form of the parameters in the solution can be gotten by pen-and-paper calculations, while in [6–8], in order to get the explicit forms of the solutions, two equations like (37) and (38) must be solved, and in [25], the parameter is obtained by solving Eq. (43).
(3) From Table 1, we can see that for fixed α, the larger η, the smaller the relative error.

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