
Araştırma Makalesi / Research Article

A Numerical Method for Solving the Mathematical Model of Controlled Drug Release

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Abstract

Over the past few decades, significant medical advances have been made in the area of drug delivery with the development of controlled release dosage forms. Controlled release formulations bring scientists in different fields to work together with the common aim of realizing more and more effective products. For this purpose, the use of mathematical modeling turns out to be very useful as this approach enables, in the best case, the prediction of release kinetics before the release systems are realized. In this article, we have introduced a Taylor collocation method, which is based on collocation method for solving initial-boundary value problem describing the Fick's second law.

Keywords: Controlled drug release, Fick's second law, fractional differential equation, collocation method

Kontrollü İlaç Salım Matematiksel Modelinin Çözümleri için Nümerik Yöntemler

Özet

Son birkaç yıldır kontrollü ilaç salım dozaj formlarındaki gelişmeler ile birlikte, ilaç salım alanında önemli medikal ilerlemeler sağlanmıştır. Kontrollü ilaç salım formülasyonları, daha da etkili ürünler geliştirmek amacıyla çeşitli alanlardaki bilim adamlarını birlikte çalışmak üzere biraraya getirmiştir. Bu amaçla, bu yaklaşım, matematiksel modelleme kullanımının önemini ortaya koymakta daha da önemlisi, salım sistemleri gerçekleştirilmeden önce salım kinetiği tahmini yapılabilmektedir. Bu çalışmada ikinci Fick kanununu tanımlayan başlangıç sınır değer probleminin nümerik çözümü için sıralama yöntemini temel alan Taylor sıralama yöntemi verilmiştir.

Anahtar Kelimeler: Kontrollü ilaç salımı, İkinci Fick kanunu, kesirli türevli diferansiyel denklem, sıralama yöntemi

1. Introduction

With advances in biotechnology, genomics and combinatorial chemistry, a wide variety of new, more potent and specific therapeutics are being created. Controlled release drug delivery systems are being developed to address many of the difficulties associated with traditional methods of administration. Controlled release systems are systems that release the drug in a controlled fashion to maintain an appropriate concentration for a long period of time. Such systems offer several potential advantages over traditional methods of administration. First, drug release rates can be tailored to the needs of a specific application; for example, providing a constant rate of delivery or pulsatile release. Second, controlled release systems provide protection of drugs, especially proteins, that are otherwise rapidly destroyed by the body. Finally, controlled release systems can increase patient comfort and compliance by replacing frequent (e.g., daily) doses with infrequent (once per month or less) injection.

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The modeling of drug release from delivery systems is important for our understanding and elucidation of the transport mechanisms and allows the prediction of the effect of the device design parameters on the drug release rate. Furthermore, given the significant advances in computer simulation technology, numerical modeling is increasingly becoming an integral part of research and development in this area. Although extensive experimental studies have been carried out in this field in the recent years, modeling of these systems is currently lacking. Numerical modeling relies on careful representation of the physical situation, and it requires a thorough understanding of drug release kinetics, as well as mathematical expressions and modeling tools.

Despite the complexity of the phenomena involved in drug release mechanisms, the mathematical models commonly used to describe the kinetics of drug release from a large variety of devices. Some efforts have been made in recent years to analyze release systems[1-5]. One of the important mathematical model is Fick's second law[6] which is a partial differential equation (PDE). Fick's second law states that the rate of change in concentration in a volume within the diffusional field is proportional to the rate of change in spatial concentration gradient at that point in the field and is expressed as:

$$\frac{\partial C}{\partial t} = L \frac{\partial^2 C}{\partial^2 x} \tag{1}$$

where C is the concentration for dissolved drug per unit volume, L is the diffusion coefficient, x denotes the direction normal to the membrane.

In this article, we present the experimental approach for solving Eq.(1) with fractional calculus and collocation method. This propose, Eq.(1) is reduced to differential equation with fractional term, then fractional differential equation is solved by the generalized Taylor series i.e.

$$y_N(t) = \sum_{i=0}^N \frac{(t-a)^{i\alpha}}{\Gamma(i\alpha+1)} (D_a^{i\alpha} y(t))(a) \tag{2}$$

where $0 < \alpha \leq 1$. In recently, collocation method has become very useful technique for solving equations[7-13]. This method transform each part of equation into matrix form and using the collocation points as

$$t_i = \frac{i}{N}, i = 0, 1, \dots, N \tag{3}$$

and we get the nonlinear algebraic equation. Solving this equation, we obtain the coefficients of the generalized Taylor series and so we obtain the approximate solutions for various N . All computations are performed on the computer algebraic system Maple 13 in this paper.

2. Basic Definitions

Almost most of the mathematical theory applicable to the study of non-integer order calculus was developed through the end of 19th century [14,16]. The fractional differential equations (FDEs) have received considerable interest in recent years. FDEs have shown to be adequate models for various physical phenomena in areas like damping laws, diffusion processes, etc. For example, the nonlinear oscillation of earthquake can be modeled with fractional derivatives[17], the fluid-dynamic traffic model with fractional derivatives[18], psychology[19], modeling of viscoelastic dampers[20-22], self-similar protein dynamics[23], bioengineering[24] and others. In this section, we first give some basic definitions and then present properties of fractional calculus[15].

Definition 2.1 The Riemann-Liouville fractional derivative of order α with respect to the variable t and with the starting point at $t = a$ is

$${}_a D_t^\alpha f(t) = \begin{cases} \frac{1}{\Gamma(-\alpha+m+1)} \frac{d^{m+1}}{dt^{m+1}} \int_a^t (t-\tau)^{m-\alpha} f(\tau) d\tau, & 0 \leq m \leq \alpha < m+1 \\ \frac{d^m f(t)}{dt^m} & , \alpha = m+1 \in N \end{cases}$$

Definition 2.2 The Riemann-Liouville fractional integral of order α is

$${}_a D_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} f(\tau) d\tau, p > 0$$

Definition 2.3 The fractional derivative of $f(t)$ by means of Caputo sense is defined as

$$D^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} f^{(n)}(\tau) d\tau$$

for $n-1 < \alpha \leq n$, $n \in \mathbb{N}$, $t > 0$, $f \in C_{-1}^n$.

Theorem 1. (Generalized Taylor Formula) [14] Suppose that $D_a^{k\alpha} f(t) \in C(a, b)$ for $k = 0, 1, \dots, n+1$ where $0 < \alpha \leq 1$, then we have

$$f(t) = \sum_{i=0}^n \frac{(t-a)^{i\alpha}}{\Gamma(i\alpha+1)} (D_a^{i\alpha} f(t))(a) + \frac{(D_a^{(n+1)} f)(\xi)}{\Gamma((n+1)\alpha+1)} (t-a)^{(n+1)\alpha}$$

with $a \leq \xi \leq t$, $\forall t \in (a, b]$, where

$$D_a^{n\alpha} = D_a^\alpha . D_a^\alpha . D_a^\alpha \dots D_a^\alpha \quad (n \text{ times}).$$

3. Converting to a Nonlinear FDE

Let us consider the initial conditions[15]

$$\frac{\partial u}{\partial x}(t, 0) = \lambda u^4(t), \quad u(t, \infty) = u(0, x) = u_0 \tag{4}$$

We are interest in $C(0, t)$ for $t > 0$. It is obtained for $\frac{\partial u}{\partial x}(0, t)$ a representation via fractional derivative of $C(x, t)$ with respect to time t [15] as:

$$\frac{\partial C}{\partial x}(t, 0) = D_a^{1/2} (C_0 - C(t, 0)).$$

Then it is obtained the following one-dimensional initial-value problem for the non-linear fractional differential equation:

$$D_a^{1/2} y(t) - L\lambda(C_0 - y(t))^4 = 0, \quad t > 0 \tag{5}$$

$$y(0) = C_0 \tag{6}$$

where $y(t) = C_0 - C(0, t)$.

Next sections, we seek the approximate solution of Eq.(5) with initial condition Eq.(6).

4. Fundamental Relations

In this section, we consider the one-dimensional initial-value problem for the non-linear fractional differential equation Eq.(5). We use the generalized Taylor collocation method to find the truncated generalized Taylor series expansions of each term in expression at $t=c$ and their matrix representations for solving α -th order linear fractional part and nonlinear part. We first consider the solution $y_N(t)$ of Eq. (5) defined by a truncated generalized Taylor series (2). Then, we have the matrix form of the solution $y_N(t)$

$$[y_N(t)] = \mathbf{T}(t)\mathbf{A} = \mathbf{X}\mathbf{M}_0\mathbf{A} \tag{7}$$

where

$$\mathbf{X} = \begin{bmatrix} 1 & (t-c)^\alpha & (t-c)^{2\alpha} & \dots & (t-c)^{N\alpha} \end{bmatrix}$$

$$\mathbf{M}_0 = \begin{bmatrix} \frac{1}{\Gamma(1)} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\Gamma(\alpha+1)} & 0 & \dots & 0 \\ 0 & 0 & \frac{1}{\Gamma(2\alpha+1)} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \frac{1}{\Gamma(N\alpha+1)} \end{bmatrix} \quad \mathbf{A} = \begin{bmatrix} D_a^{0\alpha} y(c) \\ D_a^{1\alpha} y(c) \\ D_a^{2\alpha} y(c) \\ \vdots \\ D_a^{N\alpha} y(c) \end{bmatrix}$$

Similarly, the matrix representation of the function $D_a^\alpha y_N(t)$ become

$$D_a^\alpha y_N(t) = D_a^\alpha \mathbf{X} \mathbf{M}_0 \mathbf{A}$$

where, we compute the $D_a^\alpha \mathbf{X}$, then

$$\begin{aligned} D_a^\alpha \mathbf{X} &= \begin{bmatrix} D_a^\alpha 1 & D_a^\alpha (t-c)^\alpha & D_a^\alpha (t-c)^{2\alpha} & \dots & D_a^\alpha (t-c)^{N\alpha} \end{bmatrix} \\ &= \begin{bmatrix} 0 & \frac{\Gamma(\alpha+1)}{\Gamma(1)} & \frac{\Gamma(2\alpha+1)}{\Gamma(\alpha+1)} (t-c)^\alpha & \dots & \frac{\Gamma(N\alpha+1)}{\Gamma((N-1)\alpha+1)} (t-c)^{(N-1)\alpha} \end{bmatrix} \\ &= \mathbf{X} \mathbf{M}_1 \end{aligned}$$

where

$$\mathbf{M}_1 = \begin{bmatrix} 0 & \frac{\Gamma(\alpha+1)}{\Gamma(1)} & 0 & \dots & 0 \\ 0 & 0 & \frac{\Gamma(2\alpha+1)}{\Gamma(\alpha+1)} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \frac{\Gamma(N\alpha+1)}{\Gamma((N-1)\alpha+1)} \\ 0 & 0 & 0 & \dots & 0 \end{bmatrix}$$

Then, so the matrix representation of fractional differential part as

$$D_*^\alpha y_N(t) = \mathbf{X} \mathbf{M}_1 \mathbf{M}_0 \mathbf{A} \tag{8}$$

Moreover, since [9,24]

$$\mathbf{Y}^m = \mathbf{Y}^{m-1} \overline{\mathbf{Y}} \tag{9}$$

where

$$\mathbf{Y}^{m-1}(t) = \begin{bmatrix} y_N^{m-1}(t) \\ y_N^{m-1}(t) \\ \vdots \\ y_N^{m-1}(t) \end{bmatrix}, \quad \overline{\mathbf{Y}}(t) = \begin{bmatrix} y_N(t) & 0 & \dots & 0 \\ 0 & y_N(t) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & y_N(t) \end{bmatrix}$$

And using collocation points in Eq.(3)

$$\overline{\mathbf{Y}} = \overline{\mathbf{T}} \overline{\mathbf{A}} \tag{10}$$

where

$$\overline{\mathbf{T}}(t) = \begin{bmatrix} \mathbf{T}(t) & 0 & \dots & 0 \\ 0 & \mathbf{T}(t) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mathbf{T}(t) \end{bmatrix}, \quad \overline{\mathbf{A}} = \begin{bmatrix} \mathbf{A} & 0 & \dots & 0 \\ 0 & \mathbf{A} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mathbf{A} \end{bmatrix}$$

Then, we construct the following relation

$$y_N^2(t_i) = y_N(t_i) y_N(t_i) = (\overline{\mathbf{T}} \overline{\mathbf{A}}) \mathbf{X}(t_i) \mathbf{M}_0 \mathbf{A} \tag{11}$$

$$y_N^3(t_i) = y_N^2(t_i)y_N(t_i) = (\bar{\mathbf{T}}\bar{\mathbf{A}})^2 \mathbf{X}(t_i)\mathbf{M}_0\mathbf{A} \tag{12}$$

$$y_N^4(t_i) = y_N^3(t_i)y_N(t_i) = (\bar{\mathbf{T}}\bar{\mathbf{A}})^3 \mathbf{X}(t_i)\mathbf{M}_0\mathbf{A} \tag{13}$$

Finally, we obtained matrix representation of the condition in Eq.(6) as

$$\mathbf{U}_0 = \mathbf{X}(0)\mathbf{M}_0\mathbf{A} = [1 \quad 0 \quad 0 \quad \dots \quad 0] = [\mathbf{C}_0] \tag{14}$$

4. Solution of the Problem

In this section, we consider the Eq.(3) with condition Eq.(4). Then, we can write the Eq.(5) as:

$$D_a^{1/2} y(t) + 4L\lambda C_0^3 y(t) - 6L\lambda C_0^2 y^2(t) + 4L\lambda C_0 y^3(t) - L\lambda y^4(t) = L\lambda C_0^4 \tag{15}$$

Then, using Eq.(8), Eqs.(11),(12),(13) and collocation points in Eq.(3), we can write

$$\left(\mathbf{X}\mathbf{M}_1\mathbf{M}_0 + 4L\lambda C_0^3 \mathbf{X}(t_i)\mathbf{M}_0 - 6L\lambda C_0^2 (\bar{\mathbf{T}}\bar{\mathbf{A}})\mathbf{X}(t_i)\mathbf{M}_0 + 4L\lambda C_0 (\bar{\mathbf{T}}\bar{\mathbf{A}})^2 \mathbf{X}(t_i)\mathbf{M}_0 - L\lambda (\bar{\mathbf{T}}\bar{\mathbf{A}})^3 \mathbf{X}(t_i)\mathbf{M}_0 \right) \mathbf{A} = L\lambda C_0^4 \tag{16}$$

or briefly the fundamental matrix equation of Eq.(16) as

$$\left(\mathbf{X}\mathbf{M}_1\mathbf{M}_0 + 4L\lambda C_0^3 \mathbf{X}\mathbf{M}_0 - 6L\lambda C_0^2 (\bar{\mathbf{T}}\bar{\mathbf{A}})\mathbf{X}\mathbf{M}_0 + 4L\lambda C_0 (\bar{\mathbf{T}}\bar{\mathbf{A}})^2 \mathbf{X}\mathbf{M}_0 - L\lambda C_0 (\bar{\mathbf{T}}\bar{\mathbf{A}})^3 \mathbf{X}\mathbf{M}_0 \right) \mathbf{A} = \mathbf{F} \tag{17}$$

where

$$\mathbf{X} = \begin{bmatrix} 1 & (t_0 - c)^\alpha & (t_0 - c)^{2\alpha} & \dots & (t_0 - c)^{N\alpha} \\ 1 & (t_1 - c)^\alpha & (t_1 - c)^{2\alpha} & \dots & (t_1 - c)^{N\alpha} \\ 1 & (t_2 - c)^\alpha & (t_2 - c)^{2\alpha} & \dots & (t_2 - c)^{N\alpha} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & (t_N - c)^\alpha & (t_N - c)^{2\alpha} & \dots & (t_N - c)^{N\alpha} \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} L\lambda C_0^4 \\ L\lambda C_0^4 \\ L\lambda C_0^4 \\ \vdots \\ L\lambda C_0^4 \end{bmatrix} \quad \bar{\mathbf{T}} = \begin{bmatrix} T(t_0) & 0 & 0 & \dots & 0 \\ 0 & T(t_1) & 0 & \dots & 0 \\ 0 & 0 & T(t_2) & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & T(t_N) \end{bmatrix}$$

Hence, the fundamental matrix equation (17) corresponding to Eq. (5) can be written in the form

$$\mathbf{W}\mathbf{A} = \mathbf{F} \text{ or } [\mathbf{W};\mathbf{F}], \quad \mathbf{W} = [w_{i,j}], \quad i, j = 0,1,\dots,N \tag{18}$$

where

$$\mathbf{W} = \mathbf{X}\mathbf{M}_1\mathbf{M}_0 - (\bar{\mathbf{T}}\bar{\mathbf{A}})^3 \mathbf{X}\mathbf{M}_0.$$

To obtain the solution of Eq. (5) under conditions (6), by replacing the row matrices (14) by the first 1 rows of the matrix (18) and we have the new augmented matrix:

$$[\tilde{\mathbf{W}}; \tilde{\mathbf{F}}] = \begin{bmatrix} 1 & 0 & \dots & 0 & ; & C_0 \\ w_{10} & w_{11} & \dots & w_{1N} & ; & L\lambda C_0^4 \\ \vdots & \vdots & \ddots & \vdots & ; & \vdots \\ w_{N-20} & w_{N-21} & \dots & w_{N-2N} & ; & L\lambda C_0^4 \\ w_{N-10} & w_{N-11} & \dots & w_{N-1N} & ; & L\lambda C_0^4 \\ w_{N0} & w_{N1} & \dots & w_{NN} & ; & L\lambda C_0^4 \end{bmatrix} \tag{19}$$

So, we obtained to a system of $(N + 1)$ nonlinear algebraic equations with unknown generalized Taylor coefficients.

We can easily check the accuracy of the method. Since the truncated fractional Taylor series (2) is an approximate solution of Eq.(5), when the solution $y_N(t)$ and its derivatives are substituted in Eq.(5), the resulting equation must be satisfied approximately; that is, for $t = t_q \in [0,1]$, $q = 0,1,2,\dots$

$$E_N(t_q) = \left| D_*^\alpha y_N(t_q) - L\lambda(C_0 - y_N(t_q))^4 \right| \cong 0 \tag{20}$$

5. Numerical results

We take the values of $L = 0.00169 \text{ cm}^2 / \text{hour}$, $\lambda = 1$, $C_0 = 10 \text{ mg} / \text{cm}^3$ in Ref. [6]. Then, we display the numerical results are shown in Fig. 1. Fick's second law assumes that all drug dissolves, but that does not apply in the real world, there are always some drug particles left behind. The flux is greatest at the beginning which is logical as the drug amount in the matrix is at maximum at the beginning and then decreases as t gets bigger and the drug releases.

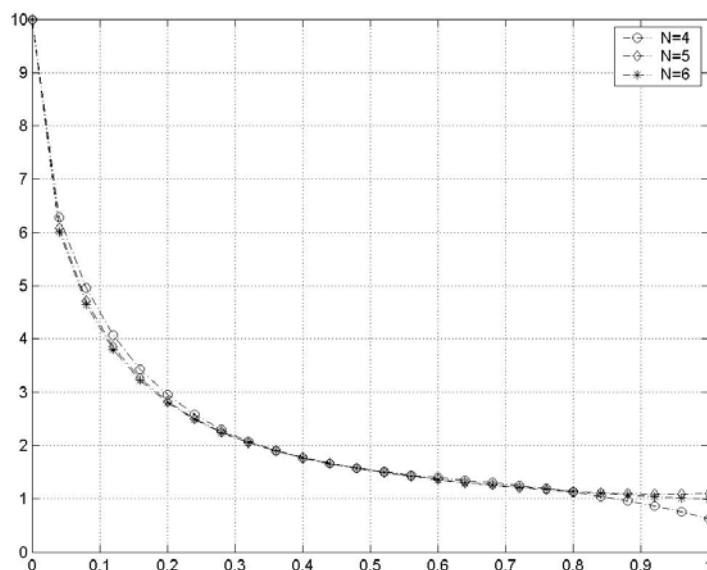


Figure 1. Flux through bottom boundary as function of time

6. Conclusion

The fractional differential equation has an important role in calculus theory and applications in physics and engineering. Fick's second law presents more general and useful equation in resolving most diffusion problems. In this study, the mathematical model of Fick's second law which is the one-dimensional initial-value problem for the non-linear fractional differential equation is solved approximately with the fractional Taylor series using the collocation points. This method transforms non-linear fractional differential equation into a matrix equations. The desired approximate solutions can be determined by solving the resulting system, which can be effectively computed using symbolic computing codes on Maple 13. Numerical solutions of example display in figures and numerical results is discuss. The modeling of drug release from delivery systems is important for our understanding and elucidation of the transport mechanisms and allows the prediction of the effect of the device design parameters on the drug release rate. Mathematical models explain to the path to predict the fundamental theory of controlled release drug product design. The model can definitely ensure batch to batch uniformity and the success of the intended therapy with the expected quality, safety and efficacy of the product. The model can have the control over all critical parameters, which will lead to predictability & reproducibility of the drug release profile of a dosage form. It can also significantly facilitate the optimization of existing product as well as the development of new products. In addition to the prevention from excessive experimentation, it will not only help to bring down the cost but also save the time.

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