Research Article

An Optimal Method for Diffusion Parameters of Nonlinear Diffusion Problem of Drug Releasing in 2D-Disc Device by Separate Variable Method

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Received 14 November 2013; Revised 16 February 2014; Accepted 16 February 2014; Published 23 March 2014

Academic Editor: Vassilios C. Loukopoulos

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An optimization control model and the corresponding computational method drawing the diffusion parameters of the nonlinear problem for the drug releasing in the 2D-disc device were given in this paper. Firstly, based on the nonlinear diffusion equation of the drug releasing in the 2D-disc device, we used the linear diffusion problem to discrete the nonlinear diffusion problem with the discrete space and the discrete time. Then, by the separate variable method, the solution of the linear problem was given. Next, the least square method based on the separate variable idea (LSMSV) was used to estimate the nonlinear appropriate diffusion parameters. Finally, a numerical example was presented to show that the control model and the numerical method were valid for computing the diffusion coefficient of the nonlinear problem for the drug releasing in the 2D-disc device.

1. Introduction

In engineering fields, there exist many diffusion processes in many fields such as geomechanics engineering, biomedical science, civil engineering, water pollution, and soil engineering [1–5]. In order to simulate the diffusion processes to obtain their merits, it is important to draw the effective diffusiveness. There are many models for the simulation of the diffusion processes. Most of them are the nonlinear or linear models. For the linear models, most optimal control problems governed by the diffusion equations arose in many scientific and engineering applications such as the water pollution problems and the drug releasing fields [6–10]. There are many various techniques for the identification for the effective diffusiveness based on the linear models. These techniques are based on either empirical or semiempirical models from drug delivery mechanisms or on analytic solutions of the diffusion equation in 2D or in the special cases [6–8, 11, 12].

However, in the practice application, many diffusion processes are subjected to the nonlinear partial differential equations [6–12]. In order to illustrate the nonlinear diffusion processes in many fields, many nonlinear models are applied to estimate the properties. For many nonlinear diffusion fields, the diffusion coefficients are the functions of the diffusion concentration. Therefore, computing the diffusion parameters is mainly to determinate the parameters of the coefficient function called the diffusion parameters function. The diffusion parameter function of the concentration is considered as the main element to control the diffusion processes. Therefore, many researches were given to determine the parameter function to illustrate the diffusion processes. Many nonlinear optimal models drawing the diffusion parameters depended on both the lab technology and the shape of the container [9, 10, 12, 13]. In order to compute the diffusion parameters, many scientists and mathematicians provided some optimal methods to compute the diffusion parameters [9, 10, 12]. Most of them cost a lot of computing time and...
computing memory. Even some of them such as the different method or the finite element method cost more than one week [9, 14]. Therefore, in order to save the computing time and the computing memory, in our published papers, we had provided some numerical methods based on the separate variable method to compute the diffusion parameters of the linear process in the sphere device. For these reasons, in this paper, we will also propose a new numerical optimal method (the least square method based on the separate variable idea) to extract the diffusion parameters from the nonlinear diffusion problems.

The next two sections will give the nonlinear diffusion problem in the 2D-disc device based on the drug releasing property and the discrete method. Section 3 is devoted to providing the least square method based on the separate variable idea for the optimal control model of the nonlinear diffusion equation system governing the drug releasing process. In Section 4, the numerical example is presented to demonstrate the feasibility and the validity, the convergence process. In Section 4, the numerical example is presented to demonstrate the feasibility and the validity, the convergence process. In Section 3, the numerical example is presented to demonstrate the feasibility and the validity, the convergence process. In Section 4, the numerical example is presented to demonstrate the feasibility and the validity, the convergence process.

2. The Nonlinear Diffusion Problem in the 2D-Disc Device and the Discrete Linear Problem

The nonlinear diffusion process in 2D-disc device is governed by the following partial differential equation:

\[
\frac{\partial C(x, y, t)}{\partial t} - \nabla \cdot (D(C) \nabla C) = 0, \quad t > 0, \quad (x, y) \in \Omega,
\]

\[
\frac{\partial C(x, y, t)}{\partial n} = 0, \quad t > 0, \quad (x, y) \in \partial \Omega,
\]

\[
C(x, y, 0) = H(x, y), \quad (x, y) \in \Omega,
\]

where the drug concentration is uniform in the device and zero in liquid for the initial condition at \( t = 0 \); that is,

\[
H(x, y, 0) = \begin{cases} 
M_0 \frac{V_d}{V}, & (x, y) \in \Omega_1, \\
0, & (x, y) \in \Omega \setminus \Omega_1;
\end{cases}
\]

\( M_0 \) is the total mass of the diffusion material, \( V_d \) is the volume of \( \Omega_1 \), the diffusion coefficient \( D(C) \) is the function of the concentration, \( C(x, y, t) \) is the drug releasing concentration, \( \Omega_1 \) is the small disc containing the drug, and \( \Omega \) is the big disc containing the liquid shown in Figure 1.

In order to solve the nonlinear diffusion process by the separate variable method, it is necessary to use some linear equations to replace the nonlinear equation (1). The discretization process is given as follows.

**Time Discretization.** Setting \( \Delta t_i = t_{i+1} - t_i, i = 1, 2, \ldots, N \), the time \( [T_0, T_1] \) of the diffusion process is divided into many sections \( [t_i, t_{i+1}] \) and the concentration \( C_i \) is computed in \( [t_i, t_{i+1}] \).

**Space Discretization.** Setting \( \Delta r_j = r_{j+1} - r_j, j = 1, 2, \ldots, K - 1 \), \( R_1 = r_1 < r_2 < \cdots < r_K = R_2 \), the radius \( [R_1, R_2] \) is divided into many intervals and the diffusion concentration in the section of \([r_1, r_2], [r_2, r_3], \ldots, [r_{K-1}, r_K]\) is obtained. So the nonlinear equation system (1) can be changed into \((k-1) \times N\) linear equations.

Using the linear diffusion processes to replace the nonlinear diffusion process in the time, it is easy to obtain the following linear equation:

\[
\frac{\partial C_i}{\partial t} = D(C_{i-1})(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2}).
\]

Using the polar coordinate system to replace (3), the above equations can be changed as follows:

\[
\frac{\partial C_i}{\partial t} = D(C_{i-1})(\frac{\partial^2 C_i}{\partial r^2} + \frac{1}{r} \frac{\partial C_i}{\partial r}).
\]

From the above deduction, the nonlinear diffusion equation of the drug releasing in the section of \([t_i, t_{i+1}]\) and \([r_j, r_{j+1}]\) can be obtained as follows:

\[
\frac{\partial C_{ij}}{\partial t} = D(C_{i-1,j})(\frac{\partial^2 C_{ij}}{\partial r^2} + \frac{1}{r} \frac{\partial C_{ij}}{\partial r}),
\]

\( i = 1, 2, \ldots, N, \quad j = 1, 2, \ldots, K - 1 \).

Because the length of the time and the range of space by the discretion are very small, \( D(C_{i-1,j}) \) can be considered as a constant in \([t_i, t_{i+1}] \times [r_j, r_{j+1}]\).
In the section of \([t_i, t_{i+1}]\), the linear equations can be represented as follows:

\[
\frac{\partial C_{ij}}{\partial t} = D \left( C_{i-1,j} \right) \left( \frac{\partial^2 C_{ij}}{\partial r^2} + \frac{1}{r} \frac{\partial C_{ij}}{\partial r} \right), \quad t_i \leq t \leq t_{i+1},
\]

\[i = 1, \ldots, N, \quad 0 < r < r_{j+1}, \quad j = 1, \ldots, K - 1,
\]

\[
\frac{\partial C_{ij}}{\partial r} \bigg|_{r=r_{j+1}} = 0,
\]

\[
C_{ij}(r, t) = \begin{cases} M_{i-1,j} / V_{d_j}, & 0 < r < r_j, \\ 0, & r_j < r < r_{j+1}, \end{cases}
\]

where \(V_{d_j} = \pi(r_{j+1}^2 - r_j^2)\). Therefore, the concentrations \(C_{ij}\) of this equation in \([t_i, t_{i+1}] \times [r_j, r_{j+1}]\) can be obtained and get

\[
M_{ij} = \int_0^{2\pi} \int_{r_j}^{r_{j+1}} C_i(r, \theta, t) \, dr \, d\theta - \int_0^{2\pi} \int_{r_{j-1}}^{r_j} C_{i-1}(r, \theta, t) \, dr \, d\theta,
\]

\[i = 1, 2, \ldots, N, \quad j = 1, 2, \ldots, K.
\]

If \(i = 0\) and \(j = 1\), \(C_{00}(r, \theta, 0) = H(r, \theta, 0)\).

To solve \((K - 1) \times N\) linear equations, by the separation variable method, we can get the solutions of the nonlinear diffusion equation as follows:

\[
C_{ij} = \frac{M_{ij}}{V_{d_j}} + \sum_{n=1}^{\infty} \frac{2M_{ij}r_j}{\pi V_{d_j}r_j + \mu_n I_0(\mu_n)} I_1 \left( \frac{\mu_n}{r_{j+1}} \right) \left( \frac{r_j \mu_n}{r_{j+1}} \right) \left( \frac{1}{r_{j+1}} \right),
\]

\[
\times \exp \left( -D \left( C_{i-1,j} \right) \left( \frac{\mu_n}{r_{j+1}} \right)^2 \right) \left( \frac{\mu_n}{r_{j+1}} \right) \left( \frac{1}{r_{j+1}} \right),
\]

\[i = 1, 2, \ldots, N, \quad j = 1, 2, \ldots, K,
\]

\[
C_i = \sum_{j=1}^{N} C_{ij}(r, \theta, t), \quad r \in (r_j, r_{j+1}), \quad i = 1, 2, \ldots, K.
\]

Equation (9) can be changed into the following formula:

\[
C_i = \sum_{j=1}^{N} \sum_{l=1}^{K} \left( \frac{M_{ij}}{V_{d_j}} + \sum_{n=1}^{\infty} \frac{2M_{ij}r_j}{\pi V_{d_j}r_j + \mu_n I_0(\mu_n)} I_1 \left( \frac{\mu_n}{r_{j+1}} \right) \left( \frac{r_j \mu_n}{r_{j+1}} \right) \left( \frac{1}{r_{j+1}} \right) \right) \left( \frac{1}{r_{j+1}} \right) \left( \frac{1}{r_{j+1}} \right) \left( \frac{1}{r_{j+1}} \right),
\]

\[r \in (r_j, r_{j+1}), \quad i = 1, 2, \ldots, K - 1,
\]

where \(\mu_{n}^{(1)}(n = 1, 2, \ldots)\) are the positive roots of \(J_1(x)\) and \(\Gamma(m + 1) = m!\), \(m\) is the positive integer and

\[
J_1(\mu_n) = \sum_{m=0}^{\infty} \frac{(-1)^m}{\Gamma(m+1)\Gamma(m+2)} \left( \frac{\mu_n}{2} \right)^{2m+1},
\]

\[
J_0(\mu_n r / R_2) = \sum_{m=0}^{\infty} \frac{(-1)^m}{\Gamma(m+1)\Gamma(m+1)} \left( \frac{\mu_n r}{2R_2} \right)^{2m}.
\]

3. Control Problem Drawing Nonlinear Diffusion Parameters

**Problem 1.** Search the coefficient functions \(D(a_1, \ldots, a_L, C)\) to satisfy

\[
\min_{D>0} \left\{ (M_{T_1} - M_{T_1}^0)^2 + (M_{T_2} - M_{T_2}^0)^2 \right\},
\]

\[+ \cdots + (M_{T_e} - M_{T_e}^0)^2 \right\},
\]

where \(M_{T_1}, M_{T_2}, \ldots, M_{T_e}\) are the given experimental data and \(M_{T_1}, M_{T_2}, \ldots, M_{T_e}\) are the computed data by the following equations:

\[
M_{T_i} = \sum_{t \in T_i} M_{kj},
\]

4. Least Square Method Based on Separate Variable Method for Solving Optimal Control Problem

Let

\[
E(D) = (M_{T_1} - M_{T_1}^0)^2 + (M_{T_2} - M_{T_2}^0)^2
\]

\[+ \cdots + (M_{T_e} - M_{T_e}^0)^2 = (M - M^*)^T (M - M^*),
\]

where \(M = (M_{T_1}(a_1, \ldots, a_L), M_{T_2}(a_1, \ldots, a_L), \ldots, M_{T_e}(a_1, \ldots, a_L))^T\), and \(M^* = (M_{T_1}^0, M_{T_2}^0, M_{T_e}^0)^T\).

For an initial diffusion parameter point \(D(\alpha_1, \ldots, a_L)\), Problem 1 can be solved iteratively by the following deduction. If \(d_1, \ldots, d_k\) are the ith approximation and \(\delta d_1, \ldots, \delta d_k\) are the ith increment of \(a_1, \ldots, a_L\), respectively, in each step, an increment \(\delta D(\delta d_1, \ldots, \delta d_k)\) will be computed as follows. To minimize \(E(D) + \delta D(\delta d_1, \ldots, \delta d_k)\), let \(X = (x_1, \ldots, x_L) = (a_1, \ldots, a_L), f_{T_i}(X) = M_{T_i} - M_{T_i}^0, F(X) = E(D), \) so \(F(X) = E(X)\) and \(\delta D(\delta d_1, \ldots, \delta d_k) = \delta D(\delta d_1, \ldots, \delta d_k)\).

If set

\[
f_i(X) = M_{T_i} - M_{T_i}^0
\]

\[= \int_0^{2\pi} \int_{r_2}^{r_N} C_{T_i}(r, \theta, T_i) \, dr \, d\theta - M_{T_i}^0 \quad i = 1, 2, \ldots, e,
\]
where

$$C_{T_i} = \sum_{j=2}^{N} \sum_{i=1}^{\max(k,T_i)} C_{lj}(r, \theta, t), \quad r \in (r_j, r_{j+1}), \quad i = 1, 2, \ldots, e,$$

(16)

equation (15) can be written in the following form:

$$F(x) = \sum_{i=1}^{e} f_i^2(x). \quad (17)$$

To solve this problem, suppose $X_{(k)}$ is the kth approximation and let the function $f_j(X)$ be the Taylor expansion function at $X_{(k)}$; the minimal point $X_{(k+1)}$ and the $(k + 1)$th approximation can be computed by the iterative method. The iterative formula is deduced in detail as follows.

Set

$$\phi_i(X) = f_i(X_{(k)}) + \nabla f_i(X_{(k)})^T (X - X_{(k)})$$

$$= \nabla f_i(X_{(k)})^T X - [\nabla f_i(X_{(k)})^T X_i - f_i(X_{(k)})], \quad i = 1, 2, \ldots, e, \quad (18)$$

$$\phi(X) = \sum_{i=1}^{e} \phi_i^2(X). \quad (19)$$

We use $\phi(X)$ to replace $F(X)$ and compute the minimal point of $\phi(X)$ to estimate the function $F(X)$. The least square problem: $\min \phi(X)$ can be solved as follows. Set

$$A = \begin{bmatrix} \nabla f_1(X_{(k)})^T \\ \vdots \\ \nabla f_e(X_{(k)})^T \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(X_{(k)})}{\partial x_1} & \cdots & \frac{\partial f_1(X_{(k)})}{\partial x_L} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_e(X_{(k)})}{\partial x_1} & \cdots & \frac{\partial f_e(X_{(k)})}{\partial x_L} \end{bmatrix}, \quad (20)$$

$$B = \begin{bmatrix} \nabla f_1(X_{(k)})^T X_{(k)} - f_1(X_{(k)}) \\ \vdots \\ \nabla f_e(X_{(k)})^T X_{(k)} - f_e(X_{(k)}) \end{bmatrix} = AX_{(k)} - f_{(k)},$$

$$f_{(k)} = \begin{bmatrix} f_1(X_{(k)}) \\ f_2(X_{(k)}) \\ \vdots \\ f_e(X_{(k)}) \end{bmatrix},$$

$$\frac{\partial f_j(X_{(k)})}{\partial x_i} = r^2 \int_0^{r^2} \int_0^{2\pi} \sum_{j=1}^{N} \sum_{l=1}^{\max(k,T_i)} \frac{M_{lj}}{V_d} + \sum_{n=1}^{\infty} \frac{2M_l r_j}{V_d r_{j+1} b_0 (r_j)} \left( \frac{\mu_n}{r_{j+1}} \right)^{t_1} \times f_1 \left( \frac{\mu_n}{r_{j+1}} \right)$$

$$\times \exp \left( -D(X_{(k)}, C_{(j+1),i}) \right) \times \left( \frac{\mu_n}{r_{j+1}} \right)^2 t_1 j_0 \left( \frac{\mu_n}{r_{j+1}} \right)^2 t_1 d\theta dr. \quad (21)$$

Equation (19) can be written as

$$\phi(X) = (AX - B)^T (AX - B) = X^T A^T AX - 2B^T AX + B^T B. \quad (22)$$

In order to search the stable point of $\phi(X)$, set

$$\nabla \phi(X) = 2A^T AX - 2A^T B = 0. \quad (23)$$

Taking $A$ and $B$ into the above formula, there is

$$A^T AX = A^T (AX_{(k)} - f_{(k)}). \quad (24)$$

Moving the right $A^T AX_{(k)}$ to the left hand in the above equation, the following equation can be obtained:

$$A^T A (X - X_{(k)}) = -A^T f_{(k)}. \quad (25)$$

Obviously, this is a linear algebraic equation about the function value and the first order partial derivative $f_j(X_{(k)})$ at the point $X_{(k)}$. If matrix $A$ is the full column rank, $A^T A$ is a symmetry positive matrix. Therefore, there exists $(A^T A)^{-1}$. We can get the stable point of $\phi(X)$ by (19)

$$X_{(k+1)} = X_{(k)} - (A^T A)^{-1} A^T f_{(k)}. \quad (26)$$

Set $X_{(k+1)}$ as the $(k + 1)$th approximation of stable point $F(X)$.

Algorithm 2 (diffusion parameter of nonlinear process). Step 1. Give the initial point $X_{(1)} = (a_{1,1}, \ldots, a_{n,1})$ and set $t_1 = 0, M_1 = 0, k = 1, f_i(X_{(k)}) = 0$ and the control error $\varepsilon > 0$, go to Step 2.

Step 2. Compute the drug concentration $M_l(X_{(k)})$ and $C_{lj}(X_{(k)})$ at $t_i$ in $[r_j, r_{j+1}]$ by the formula (7) and (8), obtain the mass in all sections $[r_j, r_{j+1}]$ at the time $t_i$, and go to Step 3.
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Table 1: Diffusion qualities at the different times with diffusion parameters (0.0003 and 0.0003).

<table>
<thead>
<tr>
<th>Time (second)</th>
<th>M (second)</th>
<th>Time (second)</th>
<th>M (second)</th>
<th>M (second)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>160</td>
<td>50.0660</td>
<td>300</td>
</tr>
<tr>
<td>20</td>
<td>42.1695</td>
<td>180</td>
<td>52.2352</td>
<td>320</td>
</tr>
<tr>
<td>40</td>
<td>42.2755</td>
<td>200</td>
<td>54.4820</td>
<td>340</td>
</tr>
<tr>
<td>60</td>
<td>42.7675</td>
<td>220</td>
<td>56.6823</td>
<td>360</td>
</tr>
<tr>
<td>80</td>
<td>43.7504</td>
<td>240</td>
<td>58.8197</td>
<td>1000</td>
</tr>
<tr>
<td>100</td>
<td>45.5094</td>
<td>260</td>
<td>60.9205</td>
<td>2000</td>
</tr>
<tr>
<td>120</td>
<td>47.8335</td>
<td>280</td>
<td>62.9829</td>
<td>3000</td>
</tr>
</tbody>
</table>

Table 2: The different errors and optimization value based on initial value (0.0001 and 0.0001).

<table>
<thead>
<tr>
<th>Iterated number</th>
<th>Total error</th>
<th>$\delta a$</th>
<th>$\delta b$</th>
<th>Optimization value $(a, b)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.9804 × 10^{-4}</td>
<td>-3.0152 × 10^{-4}</td>
<td>1.1501 × 10^{-3}</td>
<td>(-2.0152 × 10^{-4}, 1.2502 × 10^{-3})</td>
</tr>
<tr>
<td>2</td>
<td>8.2626 × 10^{-4}</td>
<td>1.4436 × 10^{-5}</td>
<td>1.7564 × 10^{-4}</td>
<td>(-1.8708 × 10^{-4}, 1.4258 × 10^{-3})</td>
</tr>
<tr>
<td>3</td>
<td>2.9995 × 10^{-4}</td>
<td>1.3370 × 10^{-4}</td>
<td>-2.3741 × 10^{-4}</td>
<td>(-5.3387 × 10^{-4}, 1.1884 × 10^{-3})</td>
</tr>
<tr>
<td>4</td>
<td>9.03742 × 10^{-4}</td>
<td>1.5343 × 10^{-4}</td>
<td>-3.6483 × 10^{-4}</td>
<td>(1.0004 × 10^{-4}, 8.2360 × 10^{-4})</td>
</tr>
<tr>
<td>5</td>
<td>2.343 × 10^{-4}</td>
<td>1.1775 × 10^{-4}</td>
<td>-3.0877 × 10^{-4}</td>
<td>(2.1779 × 10^{-4}, 5.1482 × 10^{-4})</td>
</tr>
<tr>
<td>6</td>
<td>4.6960 × 10^{-4}</td>
<td>6.0218 × 10^{-5}</td>
<td>-1.693 × 10^{-4}</td>
<td>(2.7801 × 10^{-4}, 3.5290 × 10^{-4})</td>
</tr>
<tr>
<td>7</td>
<td>5.2935</td>
<td>1.7408 × 10^{-5}</td>
<td>-4.3911 × 10^{-5}</td>
<td>(2.9542 × 10^{-4}, 3.0898 × 10^{-4})</td>
</tr>
<tr>
<td>8</td>
<td>4.0114</td>
<td>3.1408 × 10^{-6}</td>
<td>-6.1503 × 10^{-6}</td>
<td>(2.9856 × 10^{-4}, 3.0283 × 10^{-4})</td>
</tr>
</tbody>
</table>

Step 3. Compute the mass $M_{T_i}(X(k))$, $i = 1, 2, \ldots, e$, at the outer container $\Omega \setminus \Omega_1$ by the formula (13); go to Step 4.

Step 4. According to the formula (15), compute $f(X(k)) = M_{T_i}(X(k)) - M_{T_i}^0$, get the vector: $f_k = \begin{bmatrix} f_i(X(k)^{[0]}_i) \\ f_j(X(k)^{[0]}_j) \end{bmatrix}$. Compute the first order partial derivative $a_i = \frac{\partial f_i(X(k))}{\partial x_i}$, $i = 1, 2, \ldots, e$, $j = 1, 2, \ldots, L$ by formula (21). Get the matrix $A_k = (a_j)_{k \times k}$ by the formula (20); go to Step 5.

Step 5. Compute $X_{(k+1)} = X(k) - (A^T A_k)^{-1} A^T f(k)$; go to Step 6.

Step 6. If $\|X_{(k+1)} - X(k)\|_2^2 \leq \varepsilon$, set $X^* = X_{(k+1)}$ and get the optimum coefficient $(a_1, \ldots, a_e) = X^*$, go to Step 7; otherwise, let $k = k + 1$, go to Step 2.

Step 7. Output the optimal diffusion $(a_1, \ldots, a_e)$ and stop the algorithm.

5. The Numerical Example

To investigate the feasibility and the validity of the proposed scheme, a numerical example is given in this section. The cylinder device for the drug releasing is divided into the large and small cylinder structures where the small container includes the drug and the large container is filled with the liquid. The radius of small and large cylinder devices are 0.4800 dm and 2.8399 dm, respectively, and there is 100 g of drug in small disc vessel. When $t = 0$, the inner concentration is 138.1553 g/dm² and the outer is 0 g/dm². After some diffusion process in a period of time, the inner and outer concentration will be equal and be 3.9468 g/dm²; it is

$$C(r, 0) = \frac{M^0}{\pi R_1^2} = 138.1553, \quad 0 < r < R_1,$$

$$C(r, T) = 3.9468 \quad 0 < r < R_2.$$  

In the numerical example, suppose $D(C) = aC + b$ where $a$ and $b$ are the unknown constants. We firstly suppose the given diffusion parameter $(a, b)$ to be $(0.0003, 0.0003)$ then compute the diffusion process to obtain the computed data as the experiment data of the concentration shown in Table 1. Next, the above optimal model and the optimal method to estimate the diffusion parameter based on the optimal control model with the separation variable method of the drug releasing in the 2D-disc device are used to illustrate the feasibility and the validity of the LMSV for the nonlinear diffusion process. The following formula is given to compute the total error in order to estimate the convergence rate:

$$\text{total error} (k) = \sum_{j=1}^{e} (M_{T_j} - M_{T_j}^0)^2,$$

Supposing the space interval to be 0.012 dm and the time interval 20 seconds; getting 25 terms in the Bessel function and by the least square method algorithm, the optimal points and their error values in each optimal step are given in the Table 2. In order to illustrate the convergence of the least square algorithm, the optimal increment $\delta a, \delta b$ and the optimal values $(a, b)$ of the diffusion parameter are depicted in Figures 2, 3 and 4.
In order to illustrate the convergence of the algorithm for diffusion parameter of nonlinear process by the least square method by separate variables (LSMSV), we discuss the convergence data as follows: from the second column in Table 2 and Figure 3, the increments $\delta a$ converges very fast because their values become from $-3.0152 \times 10^{-4}$ to $3.1408 \times 10^{-6}$ and from Table 2 and Figure 4 $\delta b$ varies from $1.1501 \times 10^{-3}$ to $-6.1503 \times 10^{-6}$. From the last column in Table 2, the optimized values $a, b$ also become very fast from $(-2.0152 \times 10^{-4}, 1.2502 \times 10^{-3})$ to $(2.9856 \times 10^{-4}, 3.0283 \times 10^{-3})$ by only eight iterated steps. Therefore, from Table 2 and the error value in Figures 2, 3 and 4, the data show the error and the increment $\delta a, \delta b$ convergent stately. It is easy to illustrate the convergence of the algorithm for diffusion parameter of nonlinear process by least square method by separate variables idea.

In order to test the convergent velocity, we obtain the computing time for the optimal parameters by the algorithm in the numerical examples. The computing time is 1 minute and 56 seconds by the algorithm for diffusion parameter of nonlinear process. In order to test the merits of the algorithm for diffusion parameter of nonlinear process by LSMSV, it is hard for us to use the algorithm in the paper [9] to compute the parameter values because the computed time is very long. In addition, from the computing processes, it is also easy to understand why the computing velocity becomes very high. Because the algorithm in this paper only computes some of the polynomial functions in each iteration to cost only less than 2 minutes, however, the algorithm in [9] needs to solve millions linear algebra equations in each iteration for the nonlinear diffusion process to cost more than one day. Therefore, from the computing convergent time and the computational theory, we can obtain the conclusion that the convergent velocity of algorithm for diffusion parameter of nonlinear process by LSMSV is very fast.

In order to estimate the validity of the algorithm for diffusion parameter of nonlinear process by LSMSV, the total error values between the experiment values and the computed values in this paper are shown in Figure 5 and the first column in Table 2. The optimal computed drug mass depending on the different optimal diffusion parameters and the experiment mass are depicted in Figure 6. From the first column in Table 2, the errors of the optimized values $a, b$ and the parameters are only $0.0156 \times 10^{-4}$ and $0.213 \times 10^{-4}$, the error between the optimal computed drug mass $100 \text{g}$ and the experiment mass data $97.1432 \text{g}$ is only $2.8568 \text{g}$, and the relative error of the mass is only $2.9\%$. The error result shows the algorithm for diffusion parameter of nonlinear process by LSMSV being valid to extract the diffusion parameter of the drug releasing in the disc devices for the nonlinear
The optimization of \(a, b\) × 10\(^{-3}\).

Figure 5: The optimization increments of \((a, b)\).

The optimization of \(a, b\).

Figure 6: Computed data in each iteration and experimental data.

6. Conclusion

In this paper, we propose an optimal method to extract the diffusion parameters of the nonlinear diffusion process of the drug releasing in the 2D-disc device based on the separation variable method with discrete time and discrete space. The numerical result given in the previous section demonstrates the feasibility and validity of this algorithm for diffusion parameter of nonlinear process by LSMSV. The effectiveness of this optimal control model to estimate the diffusion parameters for the nonlinear drug releasing in the 2D-disc device is also discussed. How to establish the theorem of the algorithm is our future work.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgments

This work is supported by National Natural Science Foundation of China (NSFC) Grants (no. 11072041 and 61202496), by State Key Laboratory of Simulation and Regulation of Water Cycle in River Basin (IWHRSKL201205), by State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology (GZI005), by China Postdoctoral Science Foundation (20100480944 and 2012T50692), and by Hunan Provincial Natural Science Foundation of China (13JJ3070, 13JJ2031).

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