Modelling and parameter identification for a nonlinear time-delay system in microbial batch fermentation

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Abstract
Mathematical modelling and parameter identification of a microbial batch fermentation process is considered in this paper. In view of the existence of time delays, a nonlinear time-delay system is firstly proposed to formulate the fermentation process. Some important properties are also discussed. Taking the errors between the computational values and the experimental data as the cost function, a parameter identification model subject to continuous state constraints and parameter constraints is then presented. To seek the optimal time delay and the optimal kinetic parameters, an improved differential evolution algorithm in conjunction with the constraint transcription technique is developed. Finally, numerical results show that the model can describe the batch fermentation process reasonably.

1. Introduction

Time-delay systems are increasingly used in numerous application areas that include physiological kinetics, population dynamics, infectious diseases and so on [1]. Parameter identification problem is usually done by comparing the system output observed in practice with the system output predicted by the model, and then adjusting the parameters accordingly. Works on identification of time-delay systems have shown the complexity of the question [2]. Hence, the problem of identifying unknown parameters and time delays in time-delay systems has been extensively studied, see, for example, [3,4].

1,3-Propanediol (1,3-PD) is a valuable chemical intermediate that is suitable as a monomer for polycondensations to produce polyesters, polyethers and polyurethanes [5]. The fermentation of glycerol to 1,3-PD is particularly attractive in that the process is relatively easy and does not generate toxic byproducts. Glycerol can be converted to 1,3-PD by several microorganisms [6–8]. Among these, Klebsiella pneumoniae (K. pneumoniae) ferments glycerol to 1,3-PD in a high yield and productivity. The methods of glycerol bioconversion to 1,3-PD consist of batch, continuous and fed-batch cultures. Compared with continuous and fed-batch cultures, glycerol fermentation in batch culture can obtain the highest production concentration and molar yield 1,3-PD to glycerol [9]. As a result, there has been widely used in industrial fermentation process.

The widespread use of batch culture in 1,3-PD fermentation process has aroused an obvious interest in its modelling with a view to facilitating its design, control and optimization. The fermentation of glycerol by K. pneumoniae under anaerobic conditions is a complex bioprocess since the microbial growth is subjected to multiple inhibitions of substrate as well as products [10] and time delays exist in the process [11,12]. An excess kinetic model for substrate consumption and product formation was established in [13,14]. Later the model was improved so that it could describe substrate consumption and products formation in a large range of feed glycerol concentrations into medium [15]. The parameter identification problem based on this model and its optimization algorithm were investigated in [16,17]. A two-stage dynamical system to formulate...
the batch culture process was proposed in [18]. A nonlinear dynamical system describing the multistage cell growth in batch culture was presented by a modification at the specific rate of cell growth [19]. More recently, a nonlinear hybrid dynamical system including the transport modes of glycerol and 1,3-PD through the cell membrane was established [20]. Although the achieved results are interesting, time delays are ignored in the above researches.

In this paper, a novel mathematical model including time delay, i.e., nonlinear time-delay system, is proposed to describe the batch fermentations of glycerol by K. pneumoniae. Some important properties are also investigated. Taking the errors between the computational values and the experimental data, a parameter identification model subject to continuous state constraints is then presented to identify the delay argument and the kinetic parameters in the nonlinear time-delay system. The constraint transcription and smoothing techniques [21] are applied to dealing with the continuous state constraints in the parameter identification model. On this basis, an improved differential evolution algorithm is developed to solve the identification problem. Finally, comparisons between simulated and experimental results indicate that the model can be used to describe the batch fermentation process reasonably.

This paper is organized as follows. In the next section, Section 2, the nonlinear time-delay system in the batch fermentation process is presented. Section 3 gives the parameter identification problem. Section 4 illustrates the numerical results, while conclusions are provided in Section 5.

2. Nonlinear time-delay systems

In batch culture, a quantity of biomass and glycerol are added to the reactor only once and stirred uniformly under given conditions. During the process of the culture, the concentration of the glycerol decreases gradually and tends to zero finally. According to the fermentation process, we assume that.

(H1) Do not input or output the biomass, substrate and products in reactor during the batch fermentation process. (H2) The concentrations of reactants are uniform in reactor.

Although the uptake of nutrient by cells is an essential instantaneous process, cells have to undergo growth process before they produce products [22]. Thus, a time delay should be taken into account in modelling the fermentation process. Under the assumptions (H1) and (H2), mass balances of biomass, substrate and products in batch culture can be formulated as the following nonlinear time-delay system:

\[
\begin{align*}
\dot{x}_1(t) &= \mu x_1(t - \tau), \\
\dot{x}_2(t) &= -q_2 x_2(t), \\
\dot{x}_3(t) &= q_3 x_1(t - \tau), \quad t \in (0, T], \\
\dot{x}_4(t) &= q_4 x_1(t - \tau), \\
\dot{x}_5(t) &= q_5 x_1(t - \tau), \\
x(0) &= x_0,
\end{align*}
\]

(1)

where \(x(t) := (x_1(t), x_2(t), x_3(t), x_4(t), x_5(t))^T\) is the state vector whose components are, respectively, the concentrations of biomass, glycerol, 1,3-PD, acetate and ethanol in the reactor at time \(t\); \(x_0\) is a given initial state; \(T\) is the terminal moment of the batch culture and \(\tau\) is the delay argument. On the basis of previous work [15], the specific growth rate \(\mu\) of cells can be expressed as

\[
\mu = \begin{cases} 
\frac{\mu_m x_1(t)}{k_1 x_1(t) + k_2 Y_2} \prod_{i=2}^{5} \left(1 - \frac{x_i(t)}{x_i^*}\right), & \text{if } x_i < x_i^*, \\
0, & \text{otherwise},
\end{cases}
\]

(2)

where \(\mu_m\) is the maximum specific growth rate; \(k_1\) is the Monod saturation constant; \(x_i^*\) are the critical concentration for cells growth. The specific consumption rate of substrate \(q_2\) is

\[
q_2 = \frac{m_2 + \mu Y_2}{Y_2}
\]

(3)

In (3), \(m_2\) is the maintenance term of substrate consumption under substrate-limited conditions. \(Y_2\) is the maximum growth yield. The specific formation rates \(q_\ell, \ell = 3, 4\), of 1,3-PD and acetate are defined as

\[
q_\ell = -m_\ell + \mu Y_\ell,
\]

(4)

in which \(m_\ell\) are the maintenance terms of product formations under substrate-limited conditions; \(Y_\ell\) are the maximum product yields. The specific formation rates \(q_5\) of ethanol is defined as

\[
q_5 = m_5 + \mu Y_5,
\]

(5)

where \(m_5\) is the maintenance terms of ethanol formations under substrate-limited conditions; \(Y_5\) is the maximum ethanol yields.
Due to the introduction of time delay in the mathematical model, the values of kinetic parameters in the system (1) may be different from the previous ones in [15,16]. Hence, the time delay and \( x \) are required to be identified. Here, time delay \( \tau \) is assumed to be non-negative and bounded above by \( \bar{\tau} \), that is,

\[
\tau \in T := [0, \bar{\tau}].
\]  

Accordingly, the admissible set of the kinetic parameter vectors is defined as

\[
P := \prod_{i=1}^{10} [p_{ij}, p_{ij}^i],
\]

where \( p_{ij} = 0.5p_{ij}^i \) and \( p_{ij}^i = 1.5p_{ij}^i, i = 1, 2, \ldots, 10 \), are, respectively, the lower and the upper bounds of kinetic parameter and \( p^0 \) is the kinetic parameters in [15].

Now, define \( f(x(t), x(t - \tau), p) := (f_1(x(t), x(t - \tau), p), \ldots, f_5(x(t), x(t - \tau), p))^T \), in which \( f_i(x(t), x(t - \tau), p), i \in I_5 := \{1, 2, 3, 4, 5\} \) denotes the \( i \)th right item of the system (1). Then, the nonlinear time-delay system (1) can be rewritten as

\[
\begin{cases}
\dot{x}(t) = f(x(t), x(t - \tau), p), & t \in (0, T], \\
x(0) = x_0, & \\
x(t) = \phi(t), & t \in [-\bar{\tau}, 0],
\end{cases}
\]

where \( \phi(t) \in C^1([-\bar{\tau}, 0], R^5) \) is a given initial function, in which \( C^1([-\bar{\tau}, 0], R^5) \) is the Banach space of continuously differentiable functions mapping the interval \([-\bar{\tau}, 0]\) into \( R^5 \).

It should be noted that there exist critical concentrations, outside which cells cease to grow, of biomass, glycerol, 1,3-PD, acetate and ethanol. As a result, it is biologically meaningful to restrict the concentrations of biomass, glycerol and products in a set \( W \) defined as

\[
x^T(t) \in W := \prod_{i=1}^{5} [x_i, x_i^T].
\]

For the nonlinear time-delay system (8), some important properties are given in the following theorems.

**Theorem 1.** The function \( f : R_+^5 \times R_+^5 \times P \rightarrow R^5 \) in the system (8) satisfies the following conditions:

(a) \( f(\cdot, \cdot, \cdot) \) is lipschitz continuous in \( x, y \) and \( p \);

(b) There exists a constant \( K \geq 0 \) such that

\[
\|f(x, y, p)\| \leq K(1 + \|x\| + \|y\|),
\]

where \( \|\cdot\| \) denotes the Euclidean norm.

**Proof**

(a) This conclusion can be obtained by the expression of \( f \) in the system (1). 

(b) For each \((x, y, p) \in R_+^5 \times R_+^5 \times P\), we have

\[
|f_1(x, y, p)| \leq |y_1|,
\]

\[
|f_2(x, y, p)| \leq (|m_2| + \frac{1}{|Y_2|^2}) |x_2|,
\]

\[
|f_3(x, y, p)| \leq (|m_3| + |Y_3|) |y_1|, \quad \ell = 3, 4, 5.
\]

Let \( K = \max\left\{1, \frac{|m_2|}{|Y_2|^2}, |m_3| + |Y_3|, |m_4| + |Y_4|, |m_5| + |Y_5|\right\} \). Then,

\[
\|f(x, y, p)\| \leq (f_1^2 + f_2^2 + f_3^2 + f_4^2 + f_5^2)^{1/2} \leq K(1 + \|x\| + \|y\|).
\]

The proof is completed. \( \square \)

**Theorem 2.** For each \((\tau, p) \in T \times P\), the system (8) has a unique continuous solution, denoted by \( x(\cdot | \tau, p) \), on \([-\bar{\tau}, T]\). Furthermore, \( x(\cdot | \tau, p) \) satisfies that

\[
x(t, \tau, p) = x_0 + \int_0^t f(x(s, \tau, p), x(s - \tau| \tau, p), p)ds, \quad \forall t \in [0, T],
\]

and \( x(t \tau, p) = \phi(t), \forall t \in [-\bar{\tau}, 0] \).
Theorem 3. Given the initial function $\phi(t) \in C^1([\tau, 0], R^n)$ and the initial condition $x_0$, the solution $x(t|\tau, p)$ of the system (8) is uniformly bounded.

Proof. For each $(\tau, p) \in T \times P$, since $\phi(t)$ is continuous on $[-\tau, 0]$, there exists a real number $0 \leq M < +\infty$ such that $\sup\{\|\phi(t)\| | t \in [-\tau, 0]\} \leq M$.

Thus,

$$\|x(t|\tau, p)\| \leq M, \quad \forall t \in [-\tau, 0].$$

In view of Theorems 1 and 2, we obtain that

$$\|x(t|\tau, p)\| \leq \|x_0\| + \int_0^t \|f(x(s|\tau, p), x(s - \tau|\tau, p), p)\| ds \leq \|x_0\| + \int_0^t K(1 + \|x(s|\tau, p)\| + \|x(s - \tau|\tau, p)\|) ds,$$

$$\leq M + K \tau M + K \int_0^t (1 + 2\|x(s|\tau, p)\|) ds, \quad \forall t \in (0, T].$$

By Gronwall inequality, it follows that

$$\|x(t|\tau, p)\| \leq (M + K \tau M + KT) \exp(2KT), \quad \forall t \in (0, T].$$

Therefore,

$$\|x(t|\tau, p)\| \leq M, \quad \forall t \in [-\tau, T],$$

where $M := (M + K \tau M + KT) \exp(2KT)$. □

In view of theory of the delay-differential equations [23], the next theorem can be established.

Theorem 4. For all $t \in [0, T]$, the solution $x(t|\cdot, \cdot)$ of the system (8) is continuous on $T \times P$.

3. Parameter identification problems

The parameter identification problem for a time-delay system is generally to adjust values of the parameter and the delay so that the discrepancy between predicted and observed system output is as small as possible. In this section, we will investigate the parameter identification problem for the nonlinear time-delay system in batch fermentation process.

3.1. Parameter identification models

In the batch fermentation process, we have measured $n$ experimental data. The concentrations of biomass, glycerol, 1,3-PD, acetate and ethanol measured at the moment $t$, in the experiment are denoted by $z(t) := (z_1(t), z_2(t), z_3(t), z_4(t), z_5(t))^T, t \in \{1, 2, \ldots, n\}$, respectively. The identification problem is to choose an appropriate time delay $\tau$ and parameter vector $p$ such that the distinction between the system state $x(t|\tau, p)$ and the experiment data is minimized. Hence, the cost function can be defined by

$$J(\tau, p) := \sum_{i=1}^n \|x(t|\tau, p) - z(t_i)\|,$$

where $x(t|\tau, p)$ is the solution to the system (8) at time $t_i$.

Then, the parameter identification model (PIM) can be formulated as

$$(PIM) \quad \min_{(\tau, p)} J(\tau, p),$$

s.t. $x'(t|\tau, p) \in W, \quad t \in [0, T],$

$$\tau \times p \in T \times P.$$

Theorem 5. (PIM) has at least one optimal solution.

Proof. In view of Theorem 4, we know that the solution of the system (8) is continuous in $\tau$ and $p$. As a result, the cost function $J(\tau, p)$ is continuous in $\tau$ and $p$. Furthermore, define the set of feasible parameters

$$\mathcal{F} := \{(\tau, p) \in T \times P | x'(t|\tau, p) \in W, \quad \forall t \in [0, T]\}.$$
Since the sets $\mathcal{T}$ and $\mathcal{P}$ are closed according to their definitions, the set $\mathcal{F}$ is bounded. Moreover, let $\{(\tau^i, p^i)\}_{i=1}^\infty$ be any sequence in $\mathcal{F}$ and $(\bar{\tau}, \bar{p})$ be the corresponding limit. Then, due to the continuity of $x(t; \cdot)$ in $\tau$ and $p$, $x^i(t; \bar{\tau}, \bar{p}) \in W, \forall t \in [0, T]$. Consequently, $(\bar{\tau}, \bar{p}) \in \mathcal{F}$ and $\mathcal{F}$ is a closed set. Therefore, there exists at least one optimal solution for the identification problem. This completes the proof. □

3.2. Approximate problems

In essence, (PIM) is a constrained optimization problem. However, since the constraint (9) in (PIM) is a continuous state inequality constraint, (PIM) can be viewed as a semi-infinite programming problem. An efficient algorithm for solving optimization problems of this type is discussed in [21]. We will now briefly discuss the application of this algorithm to (PIM).

To begin with, let

$$
g_i(x(t;\tau, p)) := x_i' - x_i(t;\tau, p),$$

$$
g_{s,e}(x(t;\tau, p)) := x_i(t;\tau, p) - x_i, \quad e = 1, 2, \ldots, 5.$$

The condition $x^i(t;\tau, p) \in W$ is equivalently transcribed into

$$
G(\tau, p) = 0,
$$

where $G(\tau, p) := \sum_{i=1}^{l_1, l_2} \int_0^T \min(0, g_i(x(t;\tau, p)))dt$. However, the equality constraint (17) is non-differentiable at the points when $g_i = 0$. We replace (17) with

$$
\tilde{G}_{e,j}(\tau, p) := \gamma + \sum_{l=1}^{l_1, l_2} \int_0^T \varphi_{e}(g_i(x(s;\tau, p)))ds \geq 0,
$$

where $\epsilon > 0, \gamma > 0$ and

$$
\varphi_{e}(\eta) = \begin{cases} 
\eta, & \text{if } \eta < -\epsilon, \\
-(\eta - \epsilon)^2, & \text{if } -\epsilon \leq \eta \leq \epsilon, \\
0, & \text{if } \eta > \epsilon.
\end{cases}
$$

Thus, (PIM) can be approximated by a sequence of nonlinear programming problems $\{(\text{PIM}_{\epsilon,i})\}$ defined by replacing constraint (17) with (18). As is shown in [21], the following theorem indicates that the solution of the corresponding problem (PIM$_{\epsilon,i}$) will satisfy the continuous state inequality constraint (9).

**Theorem 6.** For each $\epsilon > 0$, there exists a $\gamma(\epsilon) > 0$ such that if (18) with $\gamma < \gamma(\epsilon)$ is satisfied for some $(\tau, p) \in \mathcal{T} \times \mathcal{P}$, then the original constraint (9) is also satisfied at $(\tau, p) \in \mathcal{T} \times \mathcal{P}$.

It is useful for constructing the optimization algorithm to provide the gradients information of constraint $\tilde{G}_{e,j}(\tau, p)$ with respect to each given delay and kinetic parameter. By the way, the traditional methods for computing the gradient of the constraint $G_{e,j}(\cdot, \cdot)$ involve integrating two systems of differential equations—the state system and the costate system—successively in different directions, which is difficult to implement in computation process [21]. In contrast, we will develop a new scheme for computing the gradients of the constraint $G_{e,j}(\cdot, \cdot)$ in the following theorems.

**Theorem 7.** For each $\epsilon > 0$ and $\gamma > 0$, the gradient of the constraint $\tilde{G}_{e,j}(\tau, p)$ defined in (18) with respect to $\tau$ is

$$
\frac{\partial \tilde{G}_{e,j}(\tau, p)}{\partial \tau} = \sum_{i=1}^{l_1, l_2} \int_0^T \frac{\partial \varphi_{e}(g_i(x(s;\tau, p)))}{\partial g_i} \frac{\partial g_i(x(s;\tau, p))}{\partial x} \xi(s)ds,
$$

where $\xi(s)$ is the solution of the following time-delay system:

$$
\dot{\xi}(s) = \frac{\partial f(x(s;\tau, p), x(s - \tau;\tau, p), p)}{\partial x} \xi(s) + \frac{\partial f(x(s;\tau, p), x(s - \tau;\tau, p), p)}{\partial x(s - \tau)} \xi(s - \tau) + \frac{\partial f(x(s;\tau, p), x(s - \tau;\tau, p), p)}{\partial x(s - \tau)} \int f(x(s;\tau, p), x(s - \tau;\tau, p), p) \forall s \in (0, T],
$$

with

$$
\xi(0) = 0,
$$

$$
\xi(s) = \frac{\partial \phi(s)}{\partial \tau}, \quad \forall s \in [-\tau, 0].
$$

**Proof.** For each $\epsilon > 0$, define

$$
\tau(\epsilon) = \tau + \epsilon \in [0, \bar{\tau}]
$$

Since...
For brevity, let \( x(t) \) and \( x(t; \epsilon) \), \( \forall \, t \in (0, T) \), denote, respectively, the solutions of the system (8) with \( p \in \mathcal{P} \). Clearly, we have
\[
x(t) = x_0 + \int_0^t f(x(s), x(s - \tau), p) \, ds, \quad \forall \, t \in [0, T]
\]
and
\[
x(t; \epsilon) = x_0 + \int_0^t f(x(s; \epsilon), x(s - \tau(\epsilon); \epsilon), p) \, ds, \quad \forall \, t \in [0, T].
\]
Consequently,
\[
\frac{\partial x(t)}{\partial \tau} = \int_0^t \left\{ \frac{\partial f(x(s), x(s - \tau), p)}{\partial x(s)} \frac{\partial x(s)}{\partial \tau} + \frac{\partial f(x(s), x(s - \tau), p)}{\partial (s - \tau)} \frac{\partial (s - \tau)}{\partial \tau} + \frac{\partial f(x(s), x(s - \tau), p)}{\partial x(s - \tau)} \right\} \, ds, \quad \forall \, t \in [0, T].
\]
Differentiating (21) with respect to time yields
\[
\frac{d}{dt} \left( \frac{\partial x(t)}{\partial \tau} \right) = \frac{\partial f(x(t), x(t - \tau), p)}{\partial x(t)} \frac{\partial x(t)}{\partial \tau} + \frac{\partial f(x(t), x(t - \tau), p)}{\partial (t - \tau)} \frac{\partial (t - \tau)}{\partial \tau} + \frac{\partial f(x(t), x(t - \tau), p)}{\partial x(t - \tau)} \frac{\partial x(t - \tau)}{\partial \tau} \, f(x(t), x(t - \tau), p), \quad \forall \, t \in [0, T].
\]
Furthermore,
\[
\frac{\partial x(0)}{\partial \tau} = \frac{\partial }{\partial \tau} (x_0) = 0,
\]
\[
\frac{\partial x(t)}{\partial \tau} = \frac{\partial g(t)}{\partial \tau}, \quad \forall \, t \in [-\tau, 0].
\]
Hence, define
\[
\zeta(t) = \frac{\partial x(t)}{\partial \tau}
\]
and differentiate \( \tilde{G}_{\epsilon, \gamma}(\tau, p) \) with respect to \( \tau \), we obtain the conclusion (20). The proof is completed. \( \square \)

**Theorem 8.** For each \( \epsilon > 0 \) and \( \gamma > 0 \), the gradient of the constraint \( \tilde{G}_{\epsilon, \gamma}(\tau, p) \) defined in (18) with respect to \( p \) is
\[
\frac{\partial \tilde{G}_{\epsilon, \gamma}(\tau, p)}{\partial p} = \sum_{i=1}^{10} \frac{\partial g_i(x(s|\tau, p))}{\partial \xi} \frac{\partial g(x(s|\tau, p))}{\partial \xi} \zeta(s) \, ds,
\]
where \( \zeta(s) \) is the solution of the following time-delay system:
\[
\zeta(s) = \frac{\partial f(x(s|\tau, p), x(s - \tau|\tau, p), p)}{\partial x(s)} \zeta(s) + \frac{\partial f(x(s|\tau, p), x(s - \tau|\tau, p), p)}{\partial x(s - \tau)} \zeta(s - \tau) + \frac{\partial f(x(s|\tau, p), x(s - \tau|\tau, p), p)}{\partial p}, \quad \forall \, s \in (0, T),
\]
with
\[
\zeta(0) = 0,
\]
\[
\zeta(s) = 0, \quad \forall \, s \in [-\tau, 0].
\]

**Proof.** The proof can be completed using the similar method given for Theorem 7. \( \square \)

### 3.3. Optimization algorithms

For each \( \epsilon \) and \( \gamma \), (PIM\(_{\epsilon, \gamma}\)) is obviously a mathematical programming in canonical form. However, determining the time delay \( \tau \) is very unusual since the delay influences the system state implicitly through the nonlinear time-delay system (8). To solve numerically (PIM\(_{\epsilon, \gamma}\)), various optimization routes, such as gradient-based algorithms [24], can be used. Nonetheless, all those techniques are only designed to find local optima. Furthermore, in solving (PIM\(_{\epsilon, \gamma}\)), the evaluation of candidate parameters is a computationally expensive operation because of solving the system (8). Consequently, finding the global optimum or a good suboptimal solution using traditional population based search algorithms such as genetic algorithm [25] is too consuming, or even impossible within the time available.

Differential evolution (DE), a recent optimization technique, is an exceptionally simple and easy to use evolution strategy, which is significantly fast and robust at numerical optimization and is more likely to find the true global optimum [26]. In particular, DE exhibited advantages in solving the optimization problem with high nonlinearity and high dimension [27]. As
for optimizing the computationally expensive cost functions with DE algorithm, many researchers have made some improvements on the original algorithm, see, for example [28,29]. Traditionally, these improved methods deal with unconstrained optimization problems. Nevertheless, what we need to solve is an optimization problem with both parameter bounds and state constraints, to which these improved methods cannot be applied directly. By the way, although there exist many constraint handling techniques in the evolutionary computation, see, for example [30,31], the treatment of continuous state constraints is rarely considered. In the sequel, we put forward an improved DE (IDE) algorithm to solve (PIM\textsubscript{ci}) including a handling technique for this type of constraints based on Theorems 7 and 8. For convenience, the optimization variables is denoted by \( \bm{v} = (\tau, \rho)^T \). The main steps of the IDE are as follows:

**Step 1.** Set the size of the population \( N \geq 4 \), the initial crossover probability \( CR(0) \in [0,1] \), the initial mutation factor \( F(0) \), the maximal and the minimal mutation factors \( F_{\text{max}} \) and \( F_{\text{min}} \), and the maximal iteration step \( T_{\text{max}} \).

**Step 2.** Initialize the population.

**Step 2.1.** Generate the initial parameters by

\[
\tau_i^0 = \tau_j^0 + r_j \times (\tau_j^u - \tau_j^l), \quad i = 1,2,\ldots,N; \quad j = 1,2,\ldots,D,
\]

where \( \tau_j^l \) and \( \tau_j^u \) are the lower and the upper bounds of the \( j \)th component for \( \tau \) which can be obtained by (6) and (7); \( r_j \) is a random number taken from \( [0,1] \); \( D \) is the dimension of \( \tau \).

**Step 2.2.** Check the value of \( G_{\text{ci}}(\tau^0) \). If \( G_{\text{ci}}(\tau^0) \geq 0 \), then the parameter is feasible. Otherwise, that is, \( G_{\text{ci}}(\tau^0) < 0 \), move the parameter towards the feasible region in the direction of \( \frac{\partial G_{\text{ci}}(\tau^0)}{\partial \tau^0} \) computed by Theorems 7 and 8 with Armijo line searches.

**Step 2.3.** Compute the \( j(\tau^0) \) by (16) and set \( k = 0 \).

**Step 3.** For the \( i \)th, \( i = 1,2,\ldots,N \), individual, execute the following operations:

**Step 3.1.** Random choose \( p_1, p_2 \) and \( p_3 \) (\( i \neq p_1 \neq p_2 \neq p_3 \)) from \( \{1,2,\ldots,N\} \) and generate the trial vector

\[
\tau_{ij}^k = \begin{cases} 
\tau_{ij}^0(k) + F(k + 1)(\tau_{ij}^0(k) - \tau_{ijk}^0(k)), & \text{if } r_{ij} \leq CR(k + 1) \text{ and } j = j, \\
\tau_{ij}^0(k), & \text{otherwise,}
\end{cases}
\]

where \( r_{ij} \) is a random number taken from \( [0,1] \); the crossover factor is regulated by the following adaptive strategy

\[
CR(k + 1) = \begin{cases} 
\tau, & \text{if } r_{ij} \leq R_{\tau}, \\
CR(k), & \text{otherwise.}
\end{cases}
\]

The mutation factor \( F(k + 1) \) is given by

\[
F(k + 1) = \begin{cases} 
F_{\text{min}} + r_k F_{\text{max}}, & \text{if } r_m \leq R_m, \\
F(k), & \text{otherwise.}
\end{cases}
\]

In (25) and (26), \( r, R_{\tau}, R_k \) and \( R_m \) are random numbers taken from \( [0,1] \); \( R_{\tau} \) and \( R_m \) are given constants.

**Step 3.2.** If \( \tau_{ij}^k + 1 \), \( j = 1,2,\ldots,D \), violates boundary constraints, then it is reflected back from the bound by the amount of violation:

\[
\tau_{ij}^k = \begin{cases} 
2\tau_{ij}^0 - \tau_{ij}^k(k + 1), & \text{if } \tau_{ij}^k(k + 1) < \tau_{ij}^0, \\
2\tau_{ij}^0 - \tau_{ij}^k(k + 1), & \text{if } \tau_{ij}^k(k + 1) > \tau_{ij}^0.
\end{cases}
\]

**Step 3.3.** Test the value of \( G_{\text{ci}}(\tau^k) \). If \( G_{\text{ci}}(\tau^k) \geq 0 \), then the parameter is feasible. Otherwise, move the parameter towards the feasible region in the direction of \( \frac{\partial G_{\text{ci}}(\tau^0)}{\partial \tau^0} \) computed by Theorems 7 and 8 with Armijo line searches.

**Step 3.4.** Compute \( j(\tau^k) \) by (16), and if \( j(\tau^k) < j(\tau^0) \), then set \( \tau^k = \tau^k(k + 1) \).

**Step 4.** If \( k \leq T_{\text{max}} \), then set \( k = k + 1 \) and go to Step 3. Otherwise output \( \bm{v} = \arg \min_{\in [1,2,\ldots,N]} j(\bm{v}(k)) \) and stop.

Combining the above IDE algorithm with Theorem 6, we can develop the following algorithm to solve the (PIM).

**Algorithm 1.**

**Step 1.** Choose initial values of \( \varepsilon > 0 \) and \( \gamma > 0 \).

**Step 2.** Solve Problem (PIM\textsubscript{ci}) using the IDE algorithm to give \( (\tau^*, p^*) \).

**Step 3.** Check feasibility of \( \tau^* \) for \( s \in [0, T], i = 1,2,\ldots,10 \).

**Step 4.** If \( (\tau^*, p^*) \) is feasible, go to Step 5. Otherwise, set \( \gamma = \varepsilon \gamma \). If \( \gamma < \gamma \), where \( \gamma \) is a prespecified positive constant, go to Step 6. Otherwise go to Step 2.

**Step 5.** Set \( \varepsilon = \varepsilon \gamma \). If \( \varepsilon > \varepsilon \), where \( \varepsilon \) is a prespecified positive constant, go to Step 2. Otherwise go to Step 6.

**Step 6.** Output \( (\tau^*, p^*) \) and stop.
4. Numerical results

Algorithm 1 was applied to seeking the optimal time delay and the optimal parameter vector in (PIM) and all computations were implemented in Matlab 7.10.0 (The Mathworks Inc.). We obtain that $\tau = 0.26h$ and $p^* = (0.994, 0.368, 3.24, 3.679, 0.491, 7.309, 0.0085, 76, 35.54, 14.78)^T$. Here, the involving time-delay systems is solved numerically using Matlab 7.10.0 and the intrinsic delay-differential equations (DDEs) with constant delays solver DDE23 which solved DDEs with explicit Runge–Kutta triples [32]. In particular, the relative error tolerance and the absolute error tolerance were set as $10^{-6}$ and $10^{-8}$, respectively. The initial function $\phi(t)$ is obtained by the cubic spline interpolation [33] of the measured data at the measurement time point prior to the zero time point. The initial state, the bound of time delay and the terminal time of fermentation are $x_0 = (0.102, 418.26087, 0.0, 0, 0, 0, 0, 0, 0, 0, 0)^T$, $\tau = 1h$ and $T = 6.92h$, respectively. The initial kinetic parameters and the critical concentrations are listed in Table 1. Moreover, in the IDE algorithm, $N, CR(0), F(0), F_{\text{max}}, F_{\text{min}}, R_c, R_m$, and $T_{\text{max}}$ are, respectively, 50, 0.5, 0.4, 0.9, 0.1, 0.3, 0.3, and 200. In addition, the smoothing and feasible parameters were initially selected as $\varepsilon = 0.1$ and $\gamma = 0.01$. The parameters $x$ and $\beta$ were chosen as 0.1 and 0.01 until the solution obtained was feasible for the original problem. The process terminated when $\varepsilon = 1.0 \times 10^{-8}$ and $\gamma = 1.0 \times 10^{-7}$. These parameters are derived empirically after numerous

<table>
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<tr>
<th>$\mu_m$</th>
<th>$k_1$</th>
<th>$m_2$</th>
<th>$m_3$</th>
<th>$m_4$</th>
<th>$m_5$</th>
<th>$Y_2$</th>
<th>$Y_3$</th>
<th>$Y_4$</th>
<th>$Y_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.67</td>
<td>0.28</td>
<td>2.2</td>
<td>2.69</td>
<td>0.97</td>
<td>5.26</td>
<td>0.0082</td>
<td>67.69</td>
<td>33.07</td>
<td>11.66</td>
</tr>
<tr>
<td>$x_1$</td>
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<td>$x_3$</td>
<td>$x_4$</td>
<td>$x_5$</td>
<td>$x_6$</td>
<td>$x_7$</td>
<td>$x_8$</td>
<td>$x_9$</td>
<td>$x_{10}$</td>
</tr>
<tr>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6</td>
<td>2039</td>
<td>939.5</td>
<td>1026</td>
<td>360.9</td>
</tr>
</tbody>
</table>

Table 1

The kinetic parameters and critical concentrations in the system (8) [15].

<table>
<thead>
<tr>
<th>$\ell$ = 1 (Biomass)</th>
<th>$e,%$ in this work</th>
<th>$e,%$ in [16]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\ell$ = 2 (Glycerol)</td>
<td>6.85</td>
<td>18.67</td>
</tr>
<tr>
<td>$\ell$ = 3 (1,3-PD)</td>
<td>3.41</td>
<td>6.71</td>
</tr>
<tr>
<td>$\ell$ = 4 (Acetate)</td>
<td>8.13</td>
<td>9.44</td>
</tr>
<tr>
<td>$\ell$ = 5 (Ethanol)</td>
<td>15.55</td>
<td>48.1</td>
</tr>
</tbody>
</table>

Table 2

The relative errors under the optimal time-delay and the optimal kinetic parameters.

Fig. 1. Concentrations change of biomass, glycerol, 1,3-PD, acetate and ethanol with respect to fermentation time.
experiments. For comparison, the relative errors between the computational values and the experimental data in this work and the ones in [16] are listed in Table 2, in which the relative errors are defined as

$$e_j = \frac{1}{n} \sum_{i=1}^{n} |y_i(t_i|t_i^*, p^*) - y_i(t_i)|,$$

$$\ell = 1, 2, \ldots, 5.$$  (28)

From Table 2, we can see that the relative errors are cut down greatly in comparison with the ones in [16]. Furthermore, the concentration changes computed by the optimal time delay and the optimal parameters are plotted in Fig. 1. The curves in Fig. 1 are also confirmed that the nonlinear time-delay system can describe the batch fermentation process reasonably.

5. Conclusions

In this paper, we proposed a nonlinear time-delay system to formulate the batch fermentation process. In order to establish the optimal time delay and the optimal parameters in the system, a parameter identification problem and its numerical solution approach were discussed. The numerical results showed the validity of the proposed model and the effectiveness of the developed numerical algorithm.

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