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Modelling and parameter identification for a two-stage fractional dynamical system in microbial batch process*

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Abstract: In this paper, we consider mathematical modelling and parameter identification problem in bioconversion of glycerol to 1,3-propanediol by *Klebsiella pneumoniae*. In view of the dynamic behavior with memory and heredity and experimental results in batch culture, a two-stage fractional dynamical system with unknown fractional orders and unknown kinetic parameters is proposed to describe the fermentation process. For this system, some important properties of the solution are discussed. Then, taking the weighted least-squares error between the computational values and the experimental data as the performance index, a parameter identification model subject to continuous state inequality constraints is presented. An exact penalty method is introduced to transform the parameter identification problem into the one only with box constraints. On this basis, we develop a parallel Particle Swarm Optimization algorithm to find the optimal fractional orders and kinetic parameters. Finally, numerical results show that the model can reasonably describe the batch fermentation process, as well as the effectiveness of the developed algorithm.

Keywords: fractional dynamical system, parameter identification, parallel optimization, batch fermentation.

1 Introduction

Fractional calculus, also known as noninteger-order calculus in the literature, is a generalization of the ordinary calculus. From the perspective of mathematical classification it is a branch of mathematical analysis [5]. Fractional calculus has been widely used in numerous areas including control systems [1], bioengineering [21], viscoelasticmechanics [23], and image encryption [32]. However, its development was very slow before 1970. In 1970s, researchers discovered that a series of phenomena or processes, such as fractal geometry, power law phenomena, and memory processes, is closely related to fractional calculus. In particular, fractional differential equations (FDEs) are naturally related to system with memory and heredity, and this phenomenon is often reflected in the field of bioengineering [21, 30]. As a result, the applications of FDEs in complex biological system with memory and heredity have received particular attention during the past decades [11, 21, 30, 31]. It is

worth noting that there are two most popular fractional derivatives, i.e., the Caputo fractional derivative and the Riemann–Liouville fractional derivative. Compared with the initial value problem of FDEs in the Riemann–Liouville sense, differential equations in the Caputo sense are initialized by the integer-order derivatives, which enhances its practicability in mathematical modelling of real-world processes. Thus, FDEs in the Caputo sense will be considered in this paper.

1,3-propanediol (1,3-PD), a colorless, hygroscopic viscous liquid, is widely used in the production of polyester, polyurethane, and heterocyclic compounds [15]. There are two main routes to produce 1,3-PD: chemical synthesis and microbial fermentation. The latter one is becoming increasingly attractive in industrial 1,3-PD production since it has the advantages of mild conditions, few by-products, and environment friendly. 1,3-PD microbial production can be used one of three fermentation modes: batch culture, continuous culture, and fed-batch culture. In a batch culture, a quantity of microorganisms and substrate is poured into the reactor only once at the beginning of the process and nothing is added to, or removed from the reactor during the culture process. In a continuous culture, the substrate is continuously injected into the reactor at a certain rate. At the same time, the culture fluid is taken out at the same rate, and thus the volume of the fermentation broth in the reactor remains unchanged. The fed-batch culture process is implemented by switching between batch and feeding processes. Compared with the continuous and fed-batch cultures, the batch culture is rather simple to operate, and it can be regarded as a part of fed-batch culture. In particular, glycerol fermentation to 1,3-PD in batch culture can obtain the highest productivity and yield [9]. Therefore, in this paper, we will focus on the 1,3-PD batch production. For 1,3-PD batch production, extensive studies have been carried out in the literature. Mathematical models of glycerol fermentation by *Klebsiella pneumoniae* were proposed in [27,35]. On the basis of these models, various identification problems and optimization algorithms have been investigated in [18–20,39,40]. However, these parameter identification problems involve only one-stage systems. Recently, nonlinear multistage systems have been proposed to formulate the batch fermentation process in [6, 12, 37]. Nevertheless, all the dynamic systems mentioned above are based on the classical ordinary differential equations. As is well known, the physical and chemical properties of the fermentation process will lead to the existence of memory and hereditary behavior, and the fractional calculus can reasonably represent the behavioral systems with memory and heredity in [11, 30]. By the way, various forms of fractional differential equations and their practical applications have been discussed in [3,10,33]. Also, there are many successful numerical methods for solving the fractional optimal control problems; see, for example, [7, 16, 25]. More recently, a fractional dynamic system in batch culture and its parameter identification problem have been investigated in [24]. Although the fractional system in [24] can describe the first two stages (developmental phase and growth phase) of the batch culture well, the

simulation results in the stationary phase fail to meet the expectation. Hence, fractional dynamic system with only one stage cannot describe the whole batch fermentation process well.

In this paper, a two-stage fractional differential dynamical system in the sense of Caputo is proposed to formulate the batch fermentation process. For this system, some important properties of the solution are discussed. By taking the weighted least-squares error function as the cost function, we then present a parameter identification model subject to continuous state inequality constraints. To solve this parameter identification problem, an exact penalty method is used to transform the problem into the one only with box constraints. Furthermore, considering the fact that the number of fractional orders and kinetic parameters to be identified is very large, we develop a parallel Particle Swarm Optimization (PPSO) algorithm to solve the transformed problem. Numerical simulations show that the two-stage fractional dynamical system can reasonably describe the fermentation process, and the developed algorithm is applicable and effective.

The remaining of the paper is organized as follows. A two-stage fractional dynamical system of batch culture is established and some properties of the solution are discussed in Section 2. A parameter identification model is given in Section 3. A numerical solution approach based on the exact penalty method and PPSO algorithm is proposed in Section 4. Numerical simulations are given in Section 5. Conclusions are finally drawn in Section 6.

2 Two-stage fractional dynamical system and its properties in batch process

2.1 Fractional calculus

Before establishing the fractional fermentation model, some of the most popular definitions in fractional calculus will be introduced, and we refer the reader to book [2] for detail.

Definition 1. For a function $f \in L^1([a, b], \mathbb{R})$, the Riemann–Liouville fractional integral of order $\alpha > 0$ is defined by

$${}_a I_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t - \tau)^{\alpha-1} f(\tau) d\tau, \quad t \in [a, b],$$

where $L^1([a, b], \mathbb{R})$ is the set of Lebesgue measurable functions from $[a, b]$ to \mathbb{R} , and $\Gamma(\cdot)$ is the Gamma function

Definition 2. For a function f , if $f^{(m)} \in L^1([a, b], \mathbb{R})$, then the Caputo fractional derivative of order $\alpha > 0$ is defined by

$${}_a^C D_t^\alpha f(t) = \frac{1}{\Gamma(m-\alpha)} \int_a^t (t-\tau)^{(m-\alpha-1)} f^{(m)}(\tau) d\tau, \quad t \in [a, b],$$

where $m = [\alpha]$ is the smallest integer greater than or equal to α , and $f^{(m)}$ denotes the standard m -order derivative of function f .

Note that the Caputo fractional derivative of order $\alpha > 0$ can be converted to the one of order within range $(0, 1]$ [42]. Thus, for simplicity, we assume that $\alpha \in (0, 1]$ throughout the paper.

2.2 Two-stage fractional dynamical system in batch culture

At the beginning of the batch fermentation process, an appropriate number of substrates, i.e., biomass and glycerol, is added to the reactor, and no input or output is performed during the process. In particular, the memory and hereditary effects in enzyme reactions and microbial growth can be reasonably described by the characteristics of fractional calculus [11, 21, 30].

Based on the work [6, 24], we formulate the batch fermentation process as the following two-stage fractional differential equations:

$$\begin{aligned} {}_0^C D_t^{\alpha_1} x_1(t) &= c_1 x_1(t) x_2(t) - d_1 x_1(t), \\ {}_0^C D_t^{\alpha_2} x_2(t) &= -c_2 x_1(t) x_2(t) + d_2 x_1(t), \quad t \in [0, t_1], \\ {}_0^C D_t^{\alpha_i} x_i(t) &= c_i x_1(t) x_2(t) - d_i x_1(t), \quad i = 3, 4, 5, \end{aligned} \quad (1)$$

$$\begin{aligned} {}_{t_1}^C D_t^{\alpha_6} x_1(t) &= c_6 x_1(t) x_2(t) - d_6 x_1(t), \\ {}_{t_1}^C D_t^{\alpha_7} x_2(t) &= -c_7 x_1(t) x_2(t) + d_7 x_1(t), \quad t \in (t_1, T], \\ {}_{t_1}^C D_t^{\alpha_{i+5}} x_i(t) &= c_{(i+5)} x_1(t) x_2(t) - d_{(i+5)} x_1(t), \quad i = 3, 4, 5, \end{aligned} \quad (2)$$

where $x_i(t)$, $i = 1, 2, \dots, 5$, are, respectively, the concentrations of biomass, glycerol, 1,3-PD, ethanol, and acetate at time t ; $0 < \alpha_j \leq 1$, $j = 1, 2, \dots, 10$, are fractional orders; t_1 is a given switching time; T is a given terminal time of the fermentation process; c_k , $k = 1, 2, \dots, 10$, denote the kinetic parameters of biomass growth, glycerol consumption, 1,3-PD formation, ethanol formation, and acetate formation, respectively; and d_k , $k = 1, 2, \dots, 10$, denote the inhibitory effects of cell death on cell growth, glycerol consumption, 1,3-PD formation, ethanol formation, and acetate formation, respectively. For brevity, we define $\alpha^1 := (\alpha_1, \alpha_2, \dots, \alpha_5)^\top$, $\alpha^2 := (\alpha_6, \alpha_7, \dots, \alpha_{10})^\top$, $p := (c_1, c_2, \dots, c_{10}, d_1, d_2, \dots, d_{10})^\top$, and $x(t) := (x_1(t), x_2(t), \dots, x_5(t))^\top$. Moreover, denote the right-hand side of equations (1) and (2) by

$$f^1(x(t), p) := (f_1^1(x(t), p), f_2^1(x(t), p), \dots, f_5^1(x(t), p))^\top \quad (3)$$

and

$$f^2(x(t), p) := (f_1^2(x(t), p), f_2^2(x(t), p), \dots, f_5^2(x(t), p))^\top. \quad (4)$$

Then equations (1) and (2) can be rewritten as the following two-stage fractional dynamical system:

$${}_0^C D_t^{\alpha_1} x(t) = f^1(x(t), p), \quad t \in [0, t_1], \quad x(0) = x_0, \quad (5)$$

$${}_{t_1}^C D_t^{\alpha_2} x(t) = f^2(x(t), p), \quad t \in (t_1, T], \quad x(t_1^+) = x(t_1), \quad (6)$$

where $x_0 \in \mathbb{R}^5$ is a given initial state; and $x(t_1^+)$ is the right-hand limit of $x(t)$ at t_1 . Note that the two-stage dynamical system (5) and (6) is essentially similar to the short-memory fractional differential equations mentioned in [34], both of which make full use of the memory characteristics of the Caputo derivative in a given time horizon.

In system (5) and (6), the fractional orders and kinetic parameters need to be identified.

Thus, define the admissible set of fractional orders as

$$\mathcal{F} := \{(\alpha_1, \alpha_2, \dots, \alpha_{10})^\top \mid \alpha_j \in [\varepsilon, 1], j = 1, 2, \dots, 10\},$$

where $\varepsilon > 0$ is a given constant. Furthermore, define the admissible set of kinetic parameters as

$$\mathcal{P} := \{(c_1, c_2, \dots, c_{10}, d_1, d_2, \dots, d_{10})^\top \mid c_k \in [0, 1], d_k \in [0, 1], k = 1, 2, \dots, 10\}.$$

According to the biological significance, there are critical concentrations of biomass, glycerol, 1,3-PD, ethanol, and acetate in the batch fermentation process. Outside these critical concentrations, cells will cease to grow or even die. Therefore, define the admissible set W as

$$x(t) \in W := \prod_{i=1}^5 [x_{*i}, x_i^*], \quad t \in [0, T], \quad (7)$$

where $x_{*1} = 0.001 \text{ g L}^{-1}$, $x_{*i} = 0 \text{ mmol L}^{-1}$, $i = 2, 3, 4, 5$, are the lower concentration thresholds of biomass, glycerol, 1,3-PD, ethanol, and acetate for cell growth, respectively; and $x_1^* = 10 \text{ g L}^{-1}$, $x_2^* = 2039 \text{ mmol L}^{-1}$, $x_3^* = 939.5 \text{ mmol L}^{-1}$, $x_4^* = 360.9 \text{ mmol L}^{-1}$, and $x_5^* = 1026 \text{ mmol L}^{-1}$ are the corresponding upper concentration thresholds [24].

2.3 Properties of the two-stage fractional dynamical system

For system (5) and (6), some important properties will be discussed, e.g., the existence and uniqueness of the solution and the continuity of the solution with respect to fractional orders and kinetic parameters.

Property 1. For any $t \in [0, T]$, $x(t) \in W$, and $p \in \mathcal{P}$, f^ℓ , $\ell = 1, 2$, defined by (5) and (6) satisfy

1. f^ℓ are continuously differentiable with respect to $x(t)$ and p .

2. There exists a constant $M > 0$ such that, for any $t \in [0, T]$, $\|f^\ell(x(t), p)\| \leq M$ for all $(x(t), p) \in W \times \mathcal{P}$ where $\|\cdot\|$ is the Euclidean norm.

Proof. (i) According to the expressions of $f^\ell, \ell = 1, 2$, in (3) and (4), this conclusion can be obtained. (ii) The boundedness of f^ℓ can be verified by (1) and the compactness of W and \mathcal{P} .

Property 2. The functions $f^\ell : W \times \mathcal{P} \rightarrow \mathbb{R}^5, \ell = 1, 2$, defined by (3) and (4) are Lipschitz continuous, that is, for any $t \in [0, T], x^1(t), x^2(t) \in W$, and $p^1, p^2 \in \mathcal{P}$, there exists a constant $L > 0$ such that

$$\|f^\ell(x^1(t), p^1) - f^\ell(x^2(t), p^2)\| \leq L(\|x^1(t) - x^2(t)\| + \|p^1 - p^2\|).$$

Proof. By Property 1 and the differential mean value inequality [26] we have, for any $t \in [0, T], x^1(t), x^2(t) \in W$, and $p^1, p^2 \in \mathcal{P}$

$$\begin{aligned} & \|f^\ell(x^1(t), p^1) - f^\ell(x^2(t), p^2)\| \\ & \leq \|f^\ell(x^1(t), p^1) - f^\ell(x^2(t), p^1)\| + \|f^\ell(x^2(t), p^1) - f^\ell(x^2(t), p^2)\| \\ & \leq \left\| \frac{\partial f^\ell(x^1(t) + \theta_1(x^2(t) - x^1(t)), p^1)}{\partial x} \right\| \cdot \|x^1(t) - x^2(t)\| \\ & \quad + \left\| \frac{\partial f^\ell(x^2(t), p^1 + \theta_2(p^2 - p^1))}{\partial p} \right\| \cdot \|p^1 - p^2\|, \end{aligned} \quad (8)$$

where $\theta_1, \theta_2 \in (0, 1)$. Furthermore, by the compactness of W and \mathcal{P} there exists a constant $L > 0$ such that

$$\left\| \frac{\partial f^\ell(x^1(t) + \theta_1(x^2(t) - x^1(t)), p^1)}{\partial x} \right\| \leq L, \quad t \in [0, T], \ell = 1, 2, \quad (9)$$

$$\left\| \frac{\partial f^\ell(x^2(t), p^1 + \theta_2(p^2 - p^1))}{\partial p} \right\| \leq L, \quad t \in [0, T], \ell = 1, 2. \quad (10)$$

Combining (9), (10) with (8) gives

$$\|f^\ell(x^1(t), p^1) - f^\ell(x^2(t), p^2)\| \leq L(\|x^1(t) - x^2(t)\| + \|p^1 - p^2\|)$$

for any $t \in [0, T], x^1(t), x^2(t) \in W$, and $p^1, p^2 \in \mathcal{P}$.

Theorem 1. For each $(\alpha, p) \in \mathcal{F} \times \mathcal{P}$, the two-stage fractional system defined by (5) and (6) has a unique continuous solution $x(\cdot|\alpha, p)$. Moreover, $x_i(\cdot|\alpha, p), i = 1, 2, \dots, 5$, satisfy the following integral equations:

$$x_i(t|\alpha, p) = \begin{cases} x_i(0) + \frac{1}{\Gamma(\alpha_i^1)} \int_0^t (t - \tau)^{\alpha_i^1 - 1} f_i^1(x(\tau|\alpha, p), p) d\tau, & t \in [0, t_1], \\ x_i(t_1) + \frac{1}{\Gamma(\alpha_i^2)} \int_{t_1}^t (t - \tau)^{\alpha_i^2 - 1} f_i^2(x(\tau|\alpha, p), p) d\tau, & t \in (t_1, T]. \end{cases}$$

Proof. Using a similar proof as given for Theorem 3.4 in [42] with Properties 1 and 2, we can complete the proof.

Theorem 2. *The solution $x(\cdot|\alpha, p)$ of system (5) and (6) is continuous with respect to $(\alpha, p) \in \mathcal{F} \times \mathcal{P}$*

Proof. Case 1: $t \in [0, t_1]$

For any $(\alpha, p) \in \mathcal{F} \times \mathcal{P}$, there exists two real numbers η_1 and η_2 such that $\beta = \alpha + \eta_1 \in \mathcal{F}$, and $q = p + \eta_2 \in \mathcal{P}$. Furthermore,

$$\begin{aligned} & \|x(t|\alpha, p) - x(t|\beta, q)\| \\ &= \|x(t|\alpha, p) - x(t|\beta, p) + x(t|\beta, p) - x(t|\beta, q)\| \\ &\leq \|x(t|\alpha, p) - x(t|\beta, p)\| + \|x(t|\beta, p) - x(t|\beta, q)\|. \end{aligned} \quad (11)$$

According to Properties 1 and 2, the first part of inequality (11) can be rewritten as

$$\begin{aligned} & \|x_i(t|\alpha, p) - x_i(t|\beta, p)\| \\ &\leq \frac{L}{\Gamma(\alpha_i)} \cdot \left\| \int_0^t (t-s)^{\alpha_i-1} (x_i(s|\alpha, p) - x_i(s|\beta, p)) \, ds \right\| \\ &\quad + A_i^1(t), \quad i = 1, 2, \dots, 5, \end{aligned}$$

where

$$A_i^1(t) = \frac{M}{\Gamma(\alpha_i)} \cdot \left\| \int_0^t \left[1 - \frac{\Gamma(\alpha_i)}{\Gamma(\beta_i)} (t-s)^{\beta_i-\alpha_i} \right] (t-s)^{\alpha_i-1} \, ds \right\|.$$

By generalized Gronwall inequality in [36] we have

$$\begin{aligned} & \|x_i(t|\alpha, p) - x_i(t|\beta, p)\| \\ &\leq A_i^1(t) + \int_0^t \left[\sum_{m=1}^{\infty} \frac{L^m (t-s)^{m\alpha_i-1}}{\Gamma(m\alpha_i)} A_i^1(s) \right] \, ds, \quad i = 1, 2, \dots, 5. \end{aligned} \quad (12)$$

Furthermore, the second part of inequality (11) can be expressed as

$$\begin{aligned} & \|x_i(t|\beta, p) - x_i(t|\beta, q)\| \\ &\leq \frac{L}{\Gamma(\beta_i)} \cdot \left\| \int_0^t (t-s)^{\beta_i-1} (x_i(s|\beta, p) - x_i(s|\beta, q)) \, ds \right\| \\ &\quad + A_i^2(t), \quad i = 1, 2, \dots, 5, \end{aligned}$$

where

$$A_i^2(t) = L \cdot \left\| \int_0^t \frac{(t-s)^{\beta_i-1}}{\Gamma(\beta_i)} ds \right\| \cdot \|p_i - q_i\|.$$

Similarly, we have

$$\begin{aligned} & \|x_i(t|\beta, p) - x_i(t|\beta, q)\| \\ & \leq A_i^2(t) + \int_0^t \left[\sum_{m=1}^{\infty} \frac{L^m (t-s)^{m\beta_i-1}}{\Gamma(m\beta_i)} A_i^2(s) \right] ds, \quad i = 1, 2, \dots, 5. \end{aligned} \quad (13)$$

Note that $\beta \rightarrow \alpha$ and $q \rightarrow p$ as $\eta_1, \eta_2 \rightarrow 0$. Thus, from (12) and (13) we have $\|x_i(t|\alpha, p) - x_i(t|\beta, p)\| \rightarrow 0$ and $\|x_i(t|\beta, p) - x_i(t|\beta, q)\| \rightarrow 0$, $i = 1, 2, \dots, 5$, as $\eta_1, \eta_2 \rightarrow 0$, which imply $\|x(t|\alpha, p) - x(t|\beta, q)\| \rightarrow 0$ as $\eta_1, \eta_2 \rightarrow 0$.

Case 2: $t \in (t_1, T]$.

From Case 1, for $i = 1, 2, \dots, 5$, we have

$$\|x_i(t_1|\alpha, p) - x_i(t_1|\beta, p)\| \leq \epsilon_i^1, \quad \|x_i(t_1|\beta, p) - x_i(t_1|\beta, q)\| \leq \epsilon_i^2.$$

Then, using the similar proof as given for Case 1, we conclude

$$\begin{aligned} & \|x_i(t|\alpha, p) - x_i(t|\beta, p)\| \\ & \leq B_i^1(t) + \int_{t_1}^t \left[\sum_{m=1}^{\infty} \frac{L^m (t-s)^{m\alpha_i-1}}{\Gamma(m\alpha_i)} B_i^1(s) \right] ds, \quad i = 1, 2, \dots, 5, \end{aligned} \quad (14)$$

where

$$B_i^1(t) = \epsilon_i^1 + \frac{M}{\Gamma(\alpha_i)} \cdot \left\| \int_{t_1}^t \left[1 - \frac{\Gamma(\alpha_i)}{\Gamma(\beta_i)} (t-s)^{\beta_i-\alpha_i} \right] (t-s)^{\alpha_i-1} ds \right\|.$$

Similarly,

$$\begin{aligned} & \|x_i(t|\beta, p) - x_i(t|\beta, q)\| \\ & \leq B_i^2(t) + \int_{t_1}^t \left[\sum_{m=1}^{\infty} \frac{L^m (t-s)^{m\beta_i-1}}{\Gamma(m\beta_i)} B_i^2(s) \right] ds, \quad i = 1, 2, \dots, 5, \end{aligned} \quad (15)$$

where

$$B_i^2(t) = \epsilon_i^2 + L \cdot \left\| \int_{t_1}^t \frac{(t-s)^{\beta_i-1}}{\Gamma(\beta_i)} ds \right\| \cdot \|p_i - q_i\|.$$

Note that $\epsilon_i^1, \epsilon_i^2 \rightarrow 0$, $i = 1, 2, \dots, 5$, $\beta \rightarrow \alpha$, and $q \rightarrow p$ as $\eta_1, \eta_2 \rightarrow 0$. Thus, from (14) and (15) we have $\|x_i(t|\alpha, p) - x_i(t|\beta, p)\| \rightarrow 0$ and $\|x_i(t|\beta, p) - x_i(t|\beta, q)\| \rightarrow 0$, $i = 1, 2, \dots, 5$, as $\eta_1, \eta_2 \rightarrow 0$ which imply $\|x(t|\alpha, p) - x(t|\beta, q)\| \rightarrow 0$ as $\eta_1, \eta_2 \rightarrow 0$.

Based on Cases 1 and 2, we obtain that $\|x(t|\alpha, p) - x(t|\beta, q)\| \rightarrow 0, t \in [0, T]$ as $\eta_1, \eta_2 \rightarrow 0$, which completes the proof.

3 Parameter identification problem

Parameter identification is the problem of adjusting the values of parameter to make the predicted values of the system consistent with the experimental data as much as possible. In this section, we will discuss the parameter identification problem involving the two-stage fractional dynamical system.

In batch culture, we have N_s measured experimental data. Let $y^l = (y_1^l, y_2^l, \dots, y_5^l)^T$ be the measured concentrations of biomass, glycerol, 1,3-PD, ethanol, and acetate at the measured moment t_l , $l \in \{1, 2, \dots, N_s\}$. Furthermore, considering that the measured data at the later stage are more practical than the data measured in the initial stage, we propose the following weighted least-squares error function [14]:

$$J(\alpha, p) = \frac{1}{N_s} \sum_{i=1}^5 \sum_{l=1}^{N_s} t_l \frac{(x_i(t_l|\alpha, p) - y_i^l)^2}{(y_i^{\max})^2}, \quad (16)$$

where $x_i(t_l|\alpha, p)$ is the calculated value for the i th component at time t_l ; and $y_i^{\max} = \max_{l \in \{1, \dots, N_s\}} \{y_i^l\}$ is the maximum measured concentration of the i th component. Then the parameter identification model (PIM) in the batch culture can be stated as

(PIM) $\min J(\alpha, p)$ such that $x(t|\alpha, p) \in W, t \in [0, T], (\alpha, p) \in \mathcal{F} \times \mathcal{P}$

Theorem 3. For problem (PIM), there exists at least one optimal pair $(\alpha^*, p^*) \in \mathcal{F} \times \mathcal{P}$ such that

$$J(\alpha^*, p^*) \leq J(\alpha, p) \quad \forall (\alpha, p) \in \mathcal{F} \times \mathcal{P}. \quad (17)$$

Proof. By Theorem 2 the solution $x(\cdot|\alpha, p)$ of system (5) and (6) is continuous on $\mathcal{F} \times \mathcal{P}$. Then we define the feasible set of problem (PIM) as

$$V = \{(\alpha, p) \in \mathcal{F} \times \mathcal{P} \mid x(t|\alpha, p) \in W, t \in [0, T]\}.$$

Clearly, V is a nonempty set. According to the compactness of sets \mathcal{F} and \mathcal{P} is a bounded set. Let $\{(\alpha^q, p^q)\}_{q=1}^\infty \subseteq V$ denote any sequence, and let $(\alpha^q, p^q) \rightarrow (\bar{\alpha}, \bar{p})$ as $q \rightarrow \infty$. Based on Theorem 2 and the compactness of W , we have $x(t|\bar{\alpha}, \bar{p}) \in W$. Thus, $t \in [0, T]$, which indicates that the feasible set V is closed. Furthermore, since the cost function $J(\alpha, p)$ is also continuous on $\mathcal{F} \times \mathcal{P}$ by (16), we conclude that problem (PIM) has at least one optimal pair such that (17) holds. The proof is complete.

4 Numerical solution approach

Problem (PIM) is a parameter optimization problem subject to continuous state inequality constraints (7). In this section, a numerical solution approach will be developed based on an exact penalty method and a PPSO algorithm.

4.1 Exact penalty method

In solving problem (PIM), it is computationally difficult since continuous state inequality constraints (7) must hold at infinite number of points in $[0, T]$. Fortunately, constraints transcription techniques [8, 29] and exact penalty methods [17, 38] have been proposed to overcome these difficulties. In the exact penalty method [17], it only requires that the penalty parameter is large enough but finite, and its adjustable parameters are fewer. Thus, the exact penalty method [17] is applied to problem (PIM) to deal with continuous state inequality constraints (7).

Let

$$\begin{aligned} h_i(x(t|\alpha, p)) &:= x_i(t|\alpha, p) - x_i^*, \\ h_{i+5}(x(t|\alpha, p)) &:= x_{*i} - x(t|\alpha, p), \quad i = 1, 2, \dots, 5. \end{aligned}$$

Then the continuous state inequality constraints (7) can be equivalently converted to the following form:

$$H(\alpha, p) = 0,$$

where $H(\alpha, p) = \sum_{p=1}^{10} \int_0^T [\max\{h_p(x(t|\alpha, p)), 0\}]^2 dt$.

Let $\bar{\zeta} > 0$ be a given constant, and let $\zeta \in [0, \bar{\zeta}]$ be a new decision variable. The penalty function is defined as

$$\tilde{J}_\delta(\alpha, p, \zeta) := \begin{cases} J(\alpha, p) & \text{if } \zeta = 0, H(\alpha, p) = 0, \\ J(\alpha, p) + \zeta^{-\mu} H(\alpha, p) + \delta \zeta^\nu & \text{if } \zeta \in (0, \bar{\zeta}], \\ \infty & \text{if } \zeta = 0, H(\alpha, p) \neq 0, \end{cases} \quad (18)$$

where $\delta > 0$ is a penalty parameter; and μ and ν are two positive constants satisfying $1 \leq \nu \leq \mu$.

Then we can transform problem (PIM) into the penalty problem as follows:

$$(\text{PIM}_\delta) \quad \min_{(\alpha, p, \zeta) \in \mathcal{F} \times \mathcal{P} \times [0, \bar{\zeta}]} \tilde{J}_\delta(\alpha, p, \zeta).$$

Based on the derivation in [17], it is clear that \bar{J}_δ is an exact penalty function. As a result, the optimal solution of problem (PIM) can be obtained by solving a sequence of problem (PIM $_\delta$).

4.2 Optimization algorithm

For each $\delta > 0$, problem (PIM $_\delta$) is a parameter optimization problem. Various optimization methods can be selected to find the optimal fractional orders and kinetic parameters such as gradient-based algorithm [28]. Nevertheless, the gradient-based optimization method is easy to trap into the local optimum, which is obviously not desired. Furthermore, because there are a large number of parameters to be identified when solving problem (PIM $_\delta$), the time cost of estimating candidate parameters is quite expensive. As a result, we will develop a PPSO algorithm to solve problem (PIM $_\delta$) for each $\delta > 0$.

The Particle Swarm Optimization (PSO) algorithm, proposed by Professor Eberhart and Dr. Kennedy in 1995 [13], is a swarm cooperation-based random search algorithm developed by simulating the foraging behavior of birds in a group. In a standard PSO algorithm, each particle is regarded as a feasible solution to the optimization problem. Each particle has a current velocity and flies at that speed in a given space. In order to get the optimal solution of the optimization problem, each particle should fly to the globally optimized position through dynamically adjusting the flight speed by its own and the group's experiences. With the rapid growth of computing size, the serial PSO algorithm will produce high computational cost. Thus, some parallel PSO algorithms were developed in [22, 39, 41]. However, problem (PIM $_\delta$) is a penalty problem with penalty parameter δ . As a result, we propose the following PPSO algorithm to solve problem (PIM $_\delta$) for each δ . Here $\sigma = (\alpha_1, \dots, \alpha_{10}, c_1, \dots, c_{10}, d_1, \dots, d_{10}, \zeta)^T \in \mathbb{R}^{31}$ denotes the decision vector of problem (PIM $_\delta$).

Algorithm 1

Step 1. Allocate n_p slave processors. Initialize the total number of particles p_{size} . Compute the number of particles on each processor $n_s = p_{\text{size}}/n_p$. Initialize data and variables on the master processor.

1. Load experimental data $y_i^l, i = 1, 2, \dots, 5, l = 1, 2, \dots, N_\delta$.
2. Set the lower and upper bounds of the decision vector σ_{low} and σ_{upp} , the tolerance parameter ς , the cognitive and social parameters c_1 and c_2 , a sufficient large number Λ , and the maximal iteration K_{max} .
3. Set the global optimal solution $g_{\text{best}} = 0$, the global optimal fitness value $\bar{J}_\delta^{\min} := \Lambda$.
4. Set $q := 1$.

Step 2. Broadcast data and variables on master processor to all slave processors.

Step 3. Execute the following steps on each slave processor, and denote the identifier of each slave processor by τ ($\tau = 1, 2, \dots, n_p$).

1. Randomly initialize n_s decision vectors from the horizon $[\sigma_{\text{low}}, \sigma_{\text{upp}}]$, randomly initialize n_s velocities from the uniform distribution $U(0, 1)$, denote the decision vector and velocity of particles by $\sigma^{\tau,s}(q)$ and $v^{\tau,s}(q)$, $s = 1, 2, \dots, n_s$.
2. Set $\tilde{J}_\delta(pbest^{\tau,s}(q-1)) := \Lambda$, $s = 1, 2, \dots, n_s$.
3. Solve system (5) and (6), compute the cost function (18), update $\tilde{J}_\delta(pbest^{\tau,s}(q))$ and $pbest^{\tau,s}(q)$ by

$$\tilde{J}_\delta(pbest^{\tau,s}(q)) = \begin{cases} \tilde{J}_\delta(\sigma^{\tau,s}(q)) & \text{if } \tilde{J}_\delta(\sigma^{\tau,s}(q)) \leq \tilde{J}_\delta(pbest^{\tau,s}(q-1)), \\ \tilde{J}_\delta(pbest^{\tau,s}(q-1)) & \text{otherwise,} \end{cases}$$

$$pbest^{\tau,s}(q) = \begin{cases} \sigma^{\tau,s}(q) & \text{if } \tilde{J}_\delta(\sigma^{\tau,s}(q)) \leq \tilde{J}_\delta(pbest^{\tau,s}(q-1)), \\ pbest^{\tau,s}(q-1) & \text{otherwise.} \end{cases}$$

(iv) if $s < n_s$, then set $s := s + 1$ and go step 3 (iv). Otherwise, go to step 4.

Step 4. Gather $\tilde{J}_\delta(pbest^{\tau,s}(q))$, $pbest^{\tau,s}(q)$, $s = 1, 2, \dots, n_s$, from slave processor τ into the master processor.

Step 5. Assign the master processor to execute the following operations.

1. Choose the minimal values \tilde{J}_δ^{\min} and record $gbest$ as follows:

$$\tilde{J}_\delta^{\min} = \min_{\substack{\tau \in \{1, \dots, n_p\} \\ s \in \{1, \dots, n_s\}}} \tilde{J}_\delta(pbest^{\tau,s}(q)), \quad gbest = \arg \min_{\substack{\tau \in \{1, \dots, n_p\} \\ s \in \{1, \dots, n_s\}}} \tilde{J}_\delta(pbest^{\tau,s}(q)).$$

2 If $q \geq K_{\max}$ or $\tilde{J}_\delta^{\min} \leq \varsigma$, then take $\sigma_\delta^* = gbest$ and stop. Otherwise, set $q := q+1$, broadcast $gbest$ and q to all slave processors

Step 6. Execute the following procedure on each slave processor.

(i) Update particle velocities and positions by the following iterative formulas:

$$v_\kappa^{\tau,s}(q) = (-1 + c_1 \cdot r_{s,\kappa}^1) \cdot v_\kappa^{\tau,s}(q-1) + c_2 \cdot r_{s,\kappa}^2 \cdot (pbest_\kappa^{\tau,s}(q-1) - \sigma_\kappa^{\tau,s}(q-1)) + c_2 \cdot r_{s,\kappa}^3 \cdot (gbest_\kappa - \sigma_\kappa^{\tau,s}(q-1)),$$

$$\sigma_\kappa^{\tau,s}(q) = \sigma_\kappa^{\tau,s}(q-1) + \omega \cdot v_\kappa^{\tau,s}(q),$$

where $\tau = 1, 2, \dots, n_p$; $s = 1, 2, \dots, n_s$, $\kappa = 1, 2, \dots, 31$; $r_{s,\kappa}^1, r_{s,\kappa}^2, r_{s,\kappa}^3$ random numbers in $[0, 1]$; and $0.3 \cdot \exp(1/(1 + (q \cdot 0.7)/K_{\max}))$.

If $\sigma_\kappa^{\tau,s}(q)$ violates the bound constraint, then execute the following operations:

$$\sigma_\kappa^{\tau,s}(q) = \begin{cases} 2\sigma_{\text{low},\kappa} - \sigma_\kappa^{\tau,s}(q) & \text{if } \sigma_\kappa^{\tau,s}(q) < \sigma_{\text{low},\kappa}, \\ 2\sigma_{\text{upp},\kappa} - \sigma_\kappa^{\tau,s}(q) & \text{if } \sigma_\kappa^{\tau,s}(q) > \sigma_{\text{upp},\kappa}, \end{cases}$$

and go to step 3 (iii).

On the basis of Algorithm 1, we propose the following algorithm to solve problem (PIM).

Algorithm 2

Step 1. Choose initial values of $\delta > 0$, $\gamma > 1$, $\bar{\delta} > 0$, and $\bar{\zeta} > 0$.

Step 2. Solve problem (PIM $_{\delta}$) by Algorithm 1 to give $(\alpha_{\delta}^*, p_{\delta}^*, \zeta_{\delta}^*)$.

Step 3. If $\zeta_{\delta}^* > \bar{\zeta}$, then set $\delta := \gamma\delta$ and go to Step 4. Otherwise, take $(\alpha_{\delta}^*, p_{\delta}^*)$ as an optimal solution of problem (PIM) and stop.

Step 4. If $\delta > \bar{\delta}$, then stop and output abnormal exit. Otherwise, set $(\alpha, p, \zeta) := (\alpha_{\delta}^*, p_{\delta}^*, \bar{\zeta})$.

Remark 1. In Algorithm 2, δ is a penalty parameter; γ is an increment factor; $\bar{\delta}$ is a maximum penalty parameter; $\bar{\zeta}$ is an error tolerance. If Algorithm 2 is abnormally terminated in Step 4, the parameters μ and ν can be modified to resume Algorithm 2.

5 Numerical simulations

In the numerical simulation, Algorithm 2 is used to solve problem (PIM) to find the optimal fractional orders and kinetic parameters, and all computations are implemented in Matlab 2018a environment on a Intel Core i5-7400 (64-bit, 8GB RAM, 3.4GHz) machine. Here the two-stage fractional dynamical system is solved by the implicit trapezoidal product-integration rule [4], and the step-size for integration is taken as 2^{-8} . The initial state, the switching moment, and the terminal time are taken as $x_0 = (0.2245, 509.8913, 0, 0, 0)^T$, $t_1 = 5.75$ h, and $T = 7.75$ h, respectively [24]. In Algorithm 1, n_p , p_{size} , σ_{low} , σ_{upp} , ζ , c_1 , c_2 , λ , and K_{max} are, respectively, 2, 100, 0, 1, 10^{-3} , 2, 2, 10000, and 600. In Algorithm 2, the initial values of δ , γ , $\bar{\delta}$, and $\bar{\zeta}$ are, respectively, 5, 5, 10^3 , and 10^{-8} . The above parameters are determined on the basis of a large number of experiments.

Table 1

The optimal fractional orders and parameters in two-stage fractional dynamical system.

Fractional order	Value	Parameter	Value	Parameter	Value
α_1	0.9713	c_1	0.0016	d_1	0.1761
α_2	0.8813	c_2	0.1681	d_2	0.1017
α_3	0.7317	c_3	0.1031	d_3	0.2037
α_4	0.6223	c_4	0.0310	d_4	0.0385
α_5	0.8636	c_5	0.0380	d_5	0.3165
α_6	0.9876	c_6	0.0017	d_6	0.0009
α_7	0.8640	c_7	0.2065	d_7	0.2015
α_8	0.6996	c_8	0.1894	d_8	0.1161
α_9	0.9995	c_9	0.0621	d_9	0.0023
α_{10}	0.9760	c_{10}	0.0528	d_{10}	0.0008

Based on the obtained optimal fractional orders and kinetic parameters, we plot the concentrations of biomass, glycerol, 1,3-PD, ethanol, and acetate in Fig. 1. For comparison, the one-stage fractional dynamic system with fractional orders and kinetic parameters in [24] is

also solved. The obtained concentrations of biomass, glycerol, and 1,3-PD are also plotted in Fig. 1. From Fig. 1 we can see that, compared with the results in [24], our computed concentrations of biomass, glycerol, 1,3-PD, ethanol, and acetate can better describe the experimental data in [35]. In addition, Table 2 shows the relative errors between the calculated values and experimental data in this work, as well as relative errors in [24], where the relative errors are defined as

$$e_i = \frac{\sum_{l=1}^{N_s} |x_i(t_l|\alpha, p) - y_i^l|}{\sum_{l=1}^{N_s} y_i^l}, \quad i = 1, 2, 3, 4, 5.$$

From Table 2 it can be seen that the relative errors of the two-stage fractional model in this work are significantly smaller than those in [24]. This also confirms that our two-stage fractional dynamical system can reasonably describe the batch fermentation process. To further test the performance of our proposed PPSO algorithm, a serial PSO (SPSO) algorithm with the same parameters as in PPSO algorithm is also developed to solve problem (PIM₅). We perform 30 test runs in solving problem (PIM₅) with SPSO and PPSO algorithms. The obtained optimal costs, worst costs, average costs, and average iteration time are listed in Table 3. From Table 3 it can be seen that the optimal cost, the worst cost, the average cost, and the average iteration time obtained by our PPSO algorithm are all superior to those obtained by the SPSO algorithm. The convergence curves of the cost function by the PPSO and SPSO algorithms are also depicted in Fig. 2. From Fig. 2 we can see that the convergence of PPSO algorithm is faster than SPSO algorithm. From the above results we confirm that the developed PPSO algorithm is highly effective and efficient in solving problem (PIM).

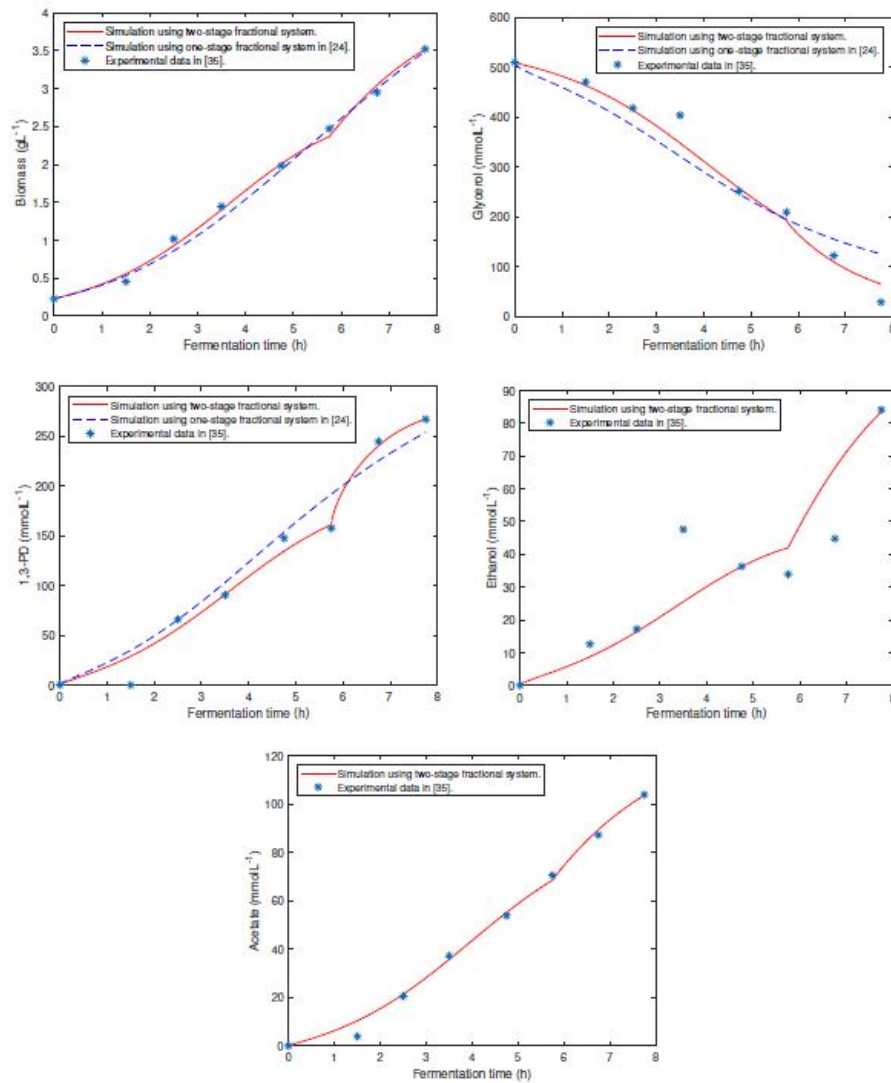


Figure 1
Concentration changes of substrates and products with respect to fermentation time.

Table 2
Relative errors

i	e_i in this work	e_i in [24]
1	3.3566%	3.7075%
2	5.6962%	12.4731%
3	6.2008%	12.4494%
4	20.6061%	—
5	3.8861%	—

Table 3
Computational results by using PPSO and SPSO algorithms

Algorithm	Optimal cost	Worst cost	Average cost	Average iteration time (s)
PPSO	0.1278	0.2086	0.1612	4.5083
SPSO	0.1380	0.2268	0.1797	9.4250

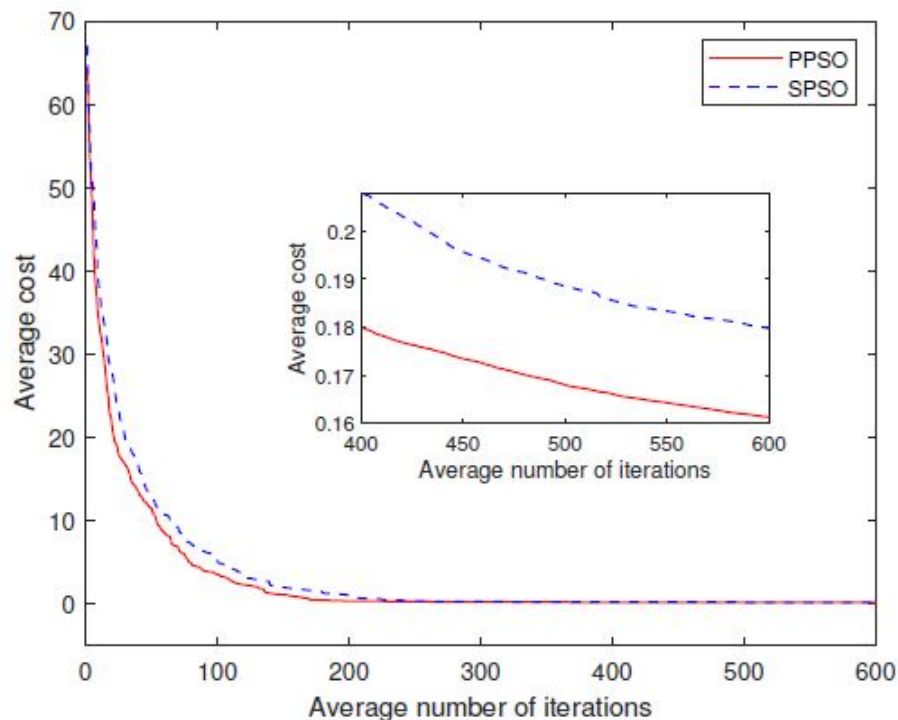


Figure 2
Convergence curves of PPSO and SPSO

6 Conclusions

In this paper, we have considered the parameter identification problem in batch process. A two-stage fractional dynamical system in the sense of Caputo is proposed to describe the batch process. Taking the error between the calculated values and the experimental data as the performance index, we present a parameter identification model subject to continuous state inequality constraints. By applying an exact penalty method the parameter identification problem is transformed into the one only with box constraints. A parallel Particle Swarm Optimization algorithm is developed to solve the resulting problem. Numerical results show that our proposed two-stage fractional dynamical system is reasonable and the proposed parallel algorithm is efficient. For further research, it will be of interest to investigate the optimal switching control problem involving the proposed two-stage fractional dynamical system.

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