



OPTIMAL CONTROL OF MICROBIAL FERMENTATION IN BATCH CULTURE USING PARTICLE SWARM ALGORITHM*

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Abstract: We propose an optimal control formulation of the batch culture of glycerol bio-dissimilation to 1,3-propanediol (1,3-PD) in industrial production, a gradient-based optimization algorithm is developed to solve the problem. Since the algorithm needs to solve state and costate differential equations simultaneously, and the solution may be trapped at a local one, in this paper, based on the theory of swarm intelligence algorithm, together with the time-scaling transformation and smoothing technique, we propose a modified particle swarm algorithm to solve the optimal control problem. Numerical results show that by employing the optimal control strategy, the concentration of 1,3-PD at the terminal time is higher compared with the previous results.

Key words: *batch culture, optimal control, multistage nonlinear dynamical system, swarm intelligence algorithm.*

Mathematics Subject Classification: *49J15, 49M37, 65K10.*

1 Introduction

1,3-propanediol (1,3-PD) is an important chemical raw material that can be used as a monomer to synthesize polyesters and polyurethanes. Microbial fermentation has provided a new perspective to produce bulk chemicals such as 1,3-PD. The process can be carried out under relatively mild conditions and can rely on renewable resources. It is environmentally friendly and its operation is simple. For these reasons, microbial fermentation of 1,3-PD has received considerable attention [29, 34, 35], for which batch and fed-batch fermentation are common strategies being adopted. In addition, co-fermentation, two-stage fermentation, continuous fermentation, repeated batch/fed-batch fermentation and nonsterile fermentation strategies have also been studied extensively [3, 8, 9, 11, 17, 24, 25].

Compared with continuous and fed-batch cultures, glycerol fermentation in batch culture trends to obtain the highest production concentration and molar yield 1,3-PD to glycerol [23]. Thus, nonlinear dynamical systems arising in batch culture have been adopted in recent years [1, 2, 10, 22]. In the batch culture of glycerol bio-dissimilation to 1,3-PD, the aim of adding glycerol is to obtain as much 1,3-PD as possible. Modeling the fermentation

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process can help establish strategy to improve the productivity. To formulate the fermentation process, a mathematical model is used in the optimization of bioprocess (see [4] and references therein). In [16], a novel mathematical model is proposed to describe the concentration changes of extracellular and intracellular substances. The parameter identification and robustness analysis of nonlinear multi-stage enzyme-catalytic dynamical system in batch culture are investigated in [6, 32, 33]. In [1, 26, 27], an excess kinetic model for substrate consumption and product formation are established and the parameter identification and the optimal control of the constructed models are investigated.

In this paper, we proposed an optimal control formulation for the microbial fermentation in batch culture, where the yield intensity of 1,3-PD at the terminal time, which is yet to be determined, is maximized subject to some specified to some specified continuous inequality constraints. The construction and analysis of efficient algorithms for state constrained optimal control problems is still a considerable challenge. It is motivated by the idea to exploit the global solution of the optimal control problem. Together with the time-scaling transformation and smoothing technique, an algorithm is proposed to solve the optimal control problem. This is done in the spirit of particle swarm optimization (PSO) algorithm, but modified in a way that fits into our particular requirements. Traditionally, the original PSO method deals with unconstrained optimization problems. However, an optimization problem with both control bounds and state constraints cannot be applied directly. Moreover, if an updated particle doesn't satisfy the constraints in the procedure, the information of the previous computation for this particle will be wasted. So, in this paper, the gradients of constraints are utilized and a reflection strategy is introduced to handle this situation. Numerical results show that by employing the optimal control strategy, the concentration of 1,3-PD at the terminal time is higher when compared with the previous results.

Our paper is organized as follows. In Section 2, a nonlinear dynamical system of batch culture is reviewed. In Section 3, we propose an optimal control model and some properties of the nonlinear dynamical system are discussed. Then, using the time-scaling technique and smoothing method, the approximate problems are presented and the main theorems about the gradient information are derived in Section 4. In Section 5, we develop a modified PSO algorithm to solve the optimal control model. The numerical results are illustrated in Section 6. Finally, conclusions are provided in Section 7.

2 Nonlinear Dynamical System

In practical experiments, we assume the following conditions to be satisfied.

- (A1) There is no medium pumped inside or outside of the reactor in the process of batch fermentation.
- (A2) The concentration of reactants are uniform in the reactor.

On the basis of our previous work (see [27]) and assumptions A1 and A2, mass balances of biomass, substrate and products in batch culture can be formulated as the following nonlinear dynamical system:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t)), \quad t \in [0, t_f], \quad (2.1)$$

$$\mathbf{x}(0) = \xi, \quad (2.2)$$

where

$$\begin{aligned} \mathbf{f}(t, \mathbf{x}(t)) &:= [f_1(t, \mathbf{x}(t)), f_2(t, \mathbf{x}(t)), f_3(t, \mathbf{x}(t)), f_4(t, \mathbf{x}(t)), f_5(t, \mathbf{x}(t))]^\top \\ &:= [\mu(t)x_1(t), -q_2(t)x_1(t), q_3(t)x_1(t), q_4(t)x_1(t), q_5(t)x_1(t)]^\top. \end{aligned}$$

Here, $x_1(t)$, $x_2(t)$, $x_3(t)$, $x_4(t)$ and $x_5(t)$ are biomass, glycerol, 1,3-PD, acetate and ethanol concentrations at time t in the reactor, respectively; $\xi := [\xi_1, \xi_2, \xi_3, \xi_4, \xi_5]^\top$ denotes the initial state vector; t_f is the terminal time of the fermentation process; $\mathbf{x}(t) := [x_1(t), x_2(t), x_3(t), x_4(t), x_5(t)]^\top \in R_+^5$ is known as the state vector. The specific growth rate of cells μ , specific consumption rate of substrate q_2 and specific formation rate of products q_i , $i = 3, 4, 5$, are expressed by the following equations [27].

$$\mu(t) = \mu_m \exp\left(\frac{-(t - t_m)^2}{2t_l^2}\right) \prod_{i=2}^5 \left(1 - \frac{x_i}{x_i^*}\right), \tag{2.3}$$

$$q_2(t) = m_2 + \frac{\mu}{Y_2}, \tag{2.4}$$

$$q_i(t) = m_i + \mu Y_i, \quad i = 3, 4, 5, \tag{2.5}$$

where μ_m is the maximum specific growth rate; t_l is the starting moment of lag growth phase and t_m is the time when μ reaches the maximum; m_i , $i = 2, 3, 4, 5$, are, respectively, the maintenance terms of substrate consumption and product formation under substrate-limited conditions; Y_2 is the maximum growth yield; and Y_i , $i = 3, 4, 5$, are the maximum product yields; x^{*i} , $i = 1, 2, 3, 4, 5$, are, respectively, the critical concentrations of biomass, glycerol, 1,3-PD, acetate and ethanol for cell growth. These values are well-defined in [26] and given in Section 6.

In a batch culture, the grow rate of bacteria is controlled only by their ability to utilize some component of their environment. Thus, the initial concentrations of biomass, glycerol and the terminal time can be treated as control variables. Let $u := [u_1, u_2, u_3]^\top := [\xi_1, \xi_2, t_f]^\top \in R_+^3$ be the control vector. The solution of system (2.1)-(2.2) with respect to control vector is defined by $\mathbf{x}(\cdot; u)$.

Based on the factual fermentation, there exist critical concentrations of biomass, glycerol, 1,3-PD, acetate and ethanol, outside which cells cease to grow. Hence, it is biologically meaningful to restrict the concentrations of biomass, glycerol, products to a admissible set W . The control vector also should be restricted to a admissible control set U . The definitions are respectively as follows:

$$W := \left\{ \mathbf{x}(t; \mathbf{u}) \in \prod_{i=1}^5 [x_{*i}, x_i^*] \mid \forall t \in I = [0, t_f], \quad \mathbf{u} \in U \right\}, \tag{2.6}$$

$$U := \prod_{i=1}^3 [u_{*i}, u_i^*], \tag{2.7}$$

where x_{*i} , $i = 1, 2, 3, 4, 5$, are, respectively, the lowest allowable concentrations of biomass, glycerol, 1,3-PD, acetate and ethanol for cell growth. u_{*i} , u_i^* , $i = 1, 2, 3$, are, respectively, the critical values of the initial concentrations of biomass, glycerol and the terminal time. Let $C_b([0, T], R^5)$ denote the space of continuous bounded functions on $[0, T]$ with values in R^5 , equipped with the sup norm topology, that is, for $z \in C_b([0, T], R^5)$, $\|z\|_c = \sup\{\|z(t)\|, t \in [0, T]\}$, where $\|\cdot\|$ is the Euclidean norm, $t_f \in [0, T]$.

Similar to these described in [21], we have the main properties as follows:

Property 1. $\mathbf{f}(t, \mathbf{x}(t))$ is Lipschitz in x on W .

Property 2. There exist positive constants a and b , such that $\|\mathbf{f}(t, \mathbf{x}(t))\| \leq a\|\mathbf{x}\| + b$.

Property 3. For fixed $\mathbf{u} \in U$, there exists a unique solution $x(\cdot; \mathbf{u})$ to system (2.1)-(2.2) and it is continuous in \mathbf{u} on U .

3 Optimal Control Problem

The control objective in microbial fermentation is to maximize the yield intensity of 1,3-PD. Thus, we want to choose the control variables to minimize the following objective function:

$$J(\mathbf{u}) := -\frac{\mathbf{e}_3^\top \mathbf{x}(u_3; \mathbf{u})}{u_3}, \quad (3.1)$$

where $\mathbf{e}_3 := [0, 0, 1, 0, 0]^\top$ for the convenience of notation.

Our optimal control problem (OCP) can be stated formally as follows: given the dynamic system (2.1)-(2.2), find an admissible control $\mathbf{u} \in U$ such that the yield intensity of 1,3-PD at the terminal time (3.1) is minimized subject to the constraints (2.6)-(2.7).

Note that, the terminal time u_3 of OCP is a control variable, existing optimal control software cannot be used directly to solve this type of problem. To overcome this difficulty, we use the well-known time-scaling transformation technique to convert the OCP to a equivalent fixed terminal time optimal control problem on a new time horizon.

The time-scaling transformation works by introducing a new time variable $s \in [0, 1]$ and relating s to t through the equation $t = \mu(s)$, where μ is the so-called time-scaling function defined by [13, 19]. In this paper, the specific form of $\mu(s)$ is given as follows:

$$\mu(s) := t_f s, \quad s \in [0, 1]. \quad (3.2)$$

Then the original nonlinear dynamical system (2.1)-(2.2) can be converted into an equivalent form as follows:

$$\dot{\tilde{\mathbf{x}}}(s) = t_f \tilde{\mathbf{f}}(s, \tilde{\mathbf{x}}(s)), \quad (3.3)$$

$$\tilde{\mathbf{x}}(0) = \xi, \quad (3.4)$$

where

$$\tilde{\mathbf{x}}(s) = \mathbf{x}(t_f s),$$

$$\tilde{\mathbf{f}}(t, \mathbf{x}(s)) = t_f (\tilde{\mu}(s) \tilde{\mathbf{x}}_1(s), -\tilde{q}_2(s) \tilde{\mathbf{x}}_1(s), \tilde{q}_3(s) \tilde{\mathbf{x}}_1(s), \tilde{q}_4(s) \tilde{\mathbf{x}}_1(s), \tilde{q}_5(s) \tilde{\mathbf{x}}_1(s))^\top,$$

$$\tilde{\mu}(s) = \mu(t_f s),$$

$$\tilde{q}_i(s) = q_i(t_f s), \quad i = 2, 3, 4, 5.$$

Thus, after applying the time-scaling transformation, the Problem OCP is equivalent to the following standard fixed terminal time optimal control Problem OCP'.

$$\begin{aligned} \text{(OCP')} : \quad & \inf_{\mathbf{u} \in U} J(\mathbf{u}) = -\frac{\mathbf{e}_3^\top \tilde{\mathbf{x}}(1; \mathbf{u})}{u_3} \\ & \text{s.t. } \tilde{\mathbf{x}}(s; \mathbf{u}) \in W, \quad s \in [0, 1]. \end{aligned}$$

4 Approximate Problems

Problem OCP' is in fact an optimization problem subject to a dynamical system and continuous state constraints, it is a constrained dynamical optimization problem with functional inequality. In this section, the constraint transcription method and local smoothing technique [5, 19, 20] will be applied to the Problem OCP'.

In Problem OCP', the essential difficulty lies in that we need to judge whether or not the system state is in the admissible set W for each $s \in [0, 1]$. Essentially, it is semi-infinite dimensional dynamical constraints [14, 30, 31]. So, in order to overcome the difficulty, we need to further transform this kind of constraints. Similar to those done in [15], for each $s \in [0, 1]$ and $i = 1, 2, 3, 4, 5$, we let

$$g_i(\tilde{\mathbf{x}}(s; \mathbf{u})) := \tilde{\mathbf{x}}_i(s; \mathbf{u}) - x_i^*, \tag{4.1}$$

$$g_{i+5}(\tilde{\mathbf{x}}(s; \mathbf{u})) := x_{*i} - \tilde{\mathbf{x}}_i(s; \mathbf{u}), \tag{4.2}$$

and

$$G(\mathbf{u}) := \sum_{i=1}^{10} \int_0^1 \max\{0, g_i(\tilde{\mathbf{x}}(s; \mathbf{u}))\} ds. \tag{4.3}$$

Then, for each $s \in [0, 1]$, the constraints $\tilde{\mathbf{x}}(s; \mathbf{u}) \in W$ is equivalently transcribed into $G(\mathbf{u}) = 0$. However, $G(\mathbf{u})$ is non-smooth in \mathbf{u} on U . Consequently, standard optimization routines would have difficulties in dealing with this type of equality constraints. The following smoothing technique is adopted to replace the non-smooth item $\max\{0, g_i(\tilde{\mathbf{x}}(s; \mathbf{u}))\}$ by defining following functions:

$$\hat{g}_{i,\epsilon}(\tilde{\mathbf{x}}(s; \mathbf{u})) := \begin{cases} 0, & \text{if } g_i(\tilde{\mathbf{x}}(s; \mathbf{u})) < -\epsilon, \\ \frac{(g_i(\tilde{\mathbf{x}}(s; \mathbf{u})) + \epsilon)^2}{4\epsilon}, & \text{if } -\epsilon \leq g_i(\tilde{\mathbf{x}}(s; \mathbf{u})) \leq \epsilon, \\ g_i(\tilde{\mathbf{x}}(s; \mathbf{u})), & \text{if } g_i(\tilde{\mathbf{x}}(s; \mathbf{u})) > \epsilon, \end{cases}$$

and

$$\hat{G}_\epsilon(\mathbf{u}) := \sum_{i=1}^{10} \int_0^1 \hat{g}_{i,\epsilon}(s; \mathbf{u}) ds, \tag{4.4}$$

where $\epsilon > 0$ is an adjustable parameter controlling the accuracy of the approximation.

Note that $\hat{G}_\epsilon(\mathbf{u})$ is a smooth function in \mathbf{u} . The equality constraint $G(\mathbf{u}) = 0$ can now be approximated by

$$\hat{G}_\epsilon(\mathbf{u}) = 0. \tag{4.5}$$

In fact, (4.5) can be further slackened to the following inequality constraint in the actual computation procedure.

$$\bar{G}_{\epsilon,\gamma}(\mathbf{u}) := \hat{G}_\epsilon(\mathbf{u}) - \gamma \geq 0, \tag{4.6}$$

where $\gamma > 0$ is an adjustable parameter controlling the feasibility of constraint (4.6).

Then, similar with [12, 19], the gradient formula for constraint functions with respect to the control parameters are given in the next theorem.

Theorem 4.1 For each $\epsilon > 0, \gamma > 0$, the derivatives of the constraint functions $\bar{G}_{\epsilon,\gamma}(\mathbf{u})$ with respect to the parameters are

$$\frac{\partial \bar{G}_{\epsilon,\gamma}(\mathbf{u})}{\partial u_j} = \int_0^1 \frac{\partial H(\tilde{\mathbf{x}}(s; \mathbf{u}), \mathbf{u}, \boldsymbol{\lambda}(s))}{\partial u_j} ds, \quad j = 1, 2, 3, \tag{4.7}$$

where

$$H(\tilde{\mathbf{x}}(s; \mathbf{u}), \mathbf{u}, \boldsymbol{\lambda}(s)) = \sum_{i=1}^{10} \int_0^1 \hat{g}_{i,\epsilon}(\tilde{\mathbf{x}}(s; \mathbf{u})) ds + \boldsymbol{\lambda}^\top(s) \tilde{f}(s, \tilde{\mathbf{x}}(s; \mathbf{u})), \quad (4.8)$$

and $\boldsymbol{\lambda}(s) = [\lambda_1(s), \lambda_2(s), \dots, \lambda_5(s)]^\top$ is the solution of the costate system

$$\dot{\boldsymbol{\lambda}}(s) = -\frac{\partial H(\tilde{\mathbf{x}}(s; \mathbf{u}), \mathbf{u}, \boldsymbol{\lambda}(s))^\top}{\partial x}. \quad (4.9)$$

with the terminal condition $\boldsymbol{\lambda}(1) = (0, 0, 0, 0, 0)^\top$.

Let $D_{\epsilon,\gamma} := \{\mathbf{u} | \tilde{\mathbf{x}}(\cdot; \mathbf{u}) \in W \text{ and } \tilde{G}_{\epsilon,\gamma}(\mathbf{u}) \geq 0\}$. Then, OCP' can be approximated by the following Problem OCP $_{\epsilon,\gamma}$,

$$\begin{aligned} (\text{OCP})_{\epsilon,\gamma} : \quad \min J(\mathbf{u}) &:= -\frac{e_3^\top \tilde{\mathbf{x}}(1; \mathbf{u})}{u_3} \\ \text{s.t. } \mathbf{u} &\in D_{\epsilon,\gamma}. \end{aligned} \quad (4.10)$$

Similar to the work [5, 18], we can prove the following theorem.

Theorem 4.2 Let $\mathbf{u}_{\epsilon,\gamma}^*$ be the optimal solution of the approximate problem OCP $_{\epsilon,\gamma}$. Suppose that there exists an optimal solution \mathbf{u}^* of the original problem OCP. Then

$$\lim_{(\epsilon,\gamma) \rightarrow (0,0)} J(\mathbf{u}_{\epsilon,\gamma}^*) = J(\mathbf{u}^*).$$

5 Modified Particle Swarm Algorithm

In our previous work [26], we have proved the existence of the optimal control, and constructed a gradient-based algorithm to solve the optimal control problem. The optimal control model is approximated by a sequence of parametric optimization problems, which can be solved using gradient-based optimization techniques. However, those techniques are only designed to find local optimal solutions. It means that the algorithm may lead that the optimal solution is trapped at the local one rather than the global one. Moreover, at each iteration in the procedure, we need to compute the state and costate differential equations simultaneously.

It is well-known that Particle Swarm Optimization (PSO) algorithm is based on a simple concept. A group of birds are randomly searching food in an area, while they don't know where is the food. But they can estimate the distant between itself current position and the food. In PSO algorithm, each potential solution to a problem is a "bird" in the search space, called by "particle". All the particles have fitness values evaluated by the fitness function, and have velocities which direct the flying of the particles. In every iteration, the particles will be updated by two best values and in this way, particles move towards the best position [7].

PSO algorithm is a kind of random search algorithm and the continuous state inequality constraints are also need to be satisfied by all particles for our problem. In this paper, on the basis of the theory of PSO algorithm, we use the gradient information obtained in Theorem 1 to update the information of the particles when the constraints do not satisfy equation (4.6). Although we still need to solve the costate equations, we only calculate at the time when particles hit the related boundary. Since these kind of time is not too much, the algorithm greatly reduces the computational cost when compared with the pure gradient-based algorithm. That is a kind of combination of the gradient-based algorithms and the random search algorithms. The optimization algorithm is given below.

Algorithm 1

Step 1. Set constants $w_{start}, w_{end} \in (0, 1)$, c_1, c_2 are positive constants and R_1, R_2 are random numbers in $[0, 1]$. Let k be the sequence number and K_{max} be the Maximum number of iterations. Initialize $k = 0, J_{gbest} = 0, J_{best} = 0, p_{gbest} = [p_1^g, p_2^g, p_3^g]^\top$ and $p_{best}(k) = [p_1^b(k), p_2^b(k), p_3^b(k)]^\top$.

Step 2. Randomly generate N initial particles with a uniform distribution on U . Denote position and velocity of the n th particles by $u^n(k) := [u_1^n(k), u_2^n(k), u_3^n(k)]^\top$ and $p^n(k) := [p_1^n(k), p_2^n(k), p_3^n(k)]^\top$, respectively.

Step 3. If $\bar{G}_{\epsilon, \gamma}(u^n(k)) \geq 0$, goto Step 4; else compute

$$h(u^n(k)) := \left. \frac{\partial \bar{G}_\epsilon(u)}{\partial u} \right|_{u=u^n(k)},$$

and update the positions of particles as follows

$$u^n(k) \leftarrow u^n(k) + \rho(u^n(k))h(u^n(k)),$$

where $h(u^n(k))$ is the search direction and $\rho(u^n(k))$ is the step-size selected by Armijo line search.

Step 4. Compute equation (4.10) with $u^n(k)$ and update J_{best} and p_{best} as follows:

$$J_{best}(k) = \max\{J(u^n(k)), n = 1, 2, \dots, N\}, \tag{5.1}$$

$$p_{best}(k) = \arg_{u^n(k)} \max\{J_{best}(u^n(k))\}. \tag{5.2}$$

Step 5. If $J_{best}(k) \geq J_{gbest}$, let $J_{gbest} = J_{best}(k), p_{gbest} = p_{best}(k)$.

Step 6. Set $k = k + 1$, if $k > K_{max}$, then stop. Otherwise, update particles for the next iteration:

$$u^n(k) = u^n(k - 1) + p^n(k - 1), \tag{5.3}$$

where,

$$p_j^n(k) = w * p_j^n(k - 1) + c_1 * R_1 * (p_j^b(k) - u_j^n(k)) + c_2 * R_2 * (p_j^g - u_j^n(k)), \tag{5.4}$$

and

$$w = \frac{(w_{start} - w_{end})(K_{max} - k)}{K_{max}} + w_{end}. \tag{5.5}$$

Then, go to Step 3. Here, we cope with velocities and positions of particles as follows [28]:

$$p_j^n(k) = \begin{cases} p_j^{max}, & \text{if } p_j^n \geq p_j^{max}, \\ p_j^{min}, & \text{if } p_j^n \leq p_j^{min}, \end{cases}$$

$$u_j^n(k) = \begin{cases} u^*, & \text{if } u_j^n \geq u_j^*, \\ u_{*j}, & \text{if } u_j^n \leq u_{*j}. \end{cases}$$

where $p_j^{max} = (u_j^* - u_{*j})/5, p_j^{min} = -(u_j^* - u_{*j})/5$.

Table 1: Parameters values in dynamical system (2.1)

Substrate/products	t_l	t_m	μ_m	m_i	Y_i
$i = 1$ (Biomass)	1.7924	2.4508	0.9192	–	–
$i = 2$ (Glycerol)	–	–	–	1.358	0.01558
$i = 3$ (1,3-PD)	–	–	–	-8.9346	64.69
<i>Acetic acid</i>	–	–	–	2.1098	4.541
<i>Ethanol</i>	–	–	–	-0.183	3.046

Table 2: Performance index with respect to the number of iterations and computation time.

Number of iterations	Value of the performance index	time (seconds)
2	67.9196	10.6
4	70.4733	17.2
6	70.5344	23.9
8	69.1484	30.8
10	71.2427	37.9
15	71.2687	53.0
20	71.1074	71.7
25	71.3358	86.1
35	71.4776	114.8
50	71.3898	164.4

6 Numerical Results

According to the model and algorithm mentioned above, we have programmed the software and applied it to the optimal control problem of microbial fermentation in batch culture. The system parameters are listed in Table 1 (see [26]).

The basic data are listed, respectively, as follows:

boundary value of control vector:

$u_{*1} = 0.01 \text{ mmol/L}$, $u_1^* = 1 \text{ mmol/L}$, $u_{*2} = 200 \text{ mmol/L}$, $u_2^* = 939.5 \text{ mmol/L}$, $u_{*3} = 2 \text{ h}$, $u_3^* = 10 \text{ h}$.

boundary value of state vector:

$x_{*1} = 0.001 \text{ mmol/L}$, $x_1^* = 10 \text{ mmol/L}$, $x_{*2} = 0.001 \text{ mmol/L}$, $x_2^* = 2039 \text{ mmol/L}$, $x_{*3} = 0.01 \text{ mmol/L}$, $x_3^* = 939.5 \text{ mmol/L}$, $x_{*4} = 0.01 \text{ mmol/L}$, $x_4^* = 1026 \text{ mmol/L}$, $x_{*5} = 200 \text{ mmol/L}$, $x_5^* = 360.9 \text{ mmol/L}$.

In Algorithm 1, $w_{start} = 0.9$, $w_{end} = 0.4$, $c_1 = c_2 = 2$, $K_{max} = 20$ and $N = 1000$. The optimal control vector u^* and objective function $J(u^*)$ obtained by Algorithm 1 are 0.985241, 582.004, 5.02762 and 71.5578, respectively. Fig. 1 shows the convergence curve of the algorithm for the performance index. In Fig. 1, the value of the performance index basically lives up to stabilization, so the number of the sample points with $N \times K_{max} = 20000$ are appropriate. Compare with corresponding optimal control vector u^* and objective function $J(u^*)$, 0.973186, 547.04, 5.17509 and 54.5911, respectively, in [26]. Numerical results show that, by employing the optimal control, the concentration of 1,3-PD at the terminal time can be increased, compared with the previous results. The concentration change of biomass, glycerol, 1,3-PD under the optimal control variables are shown in Fig 2.

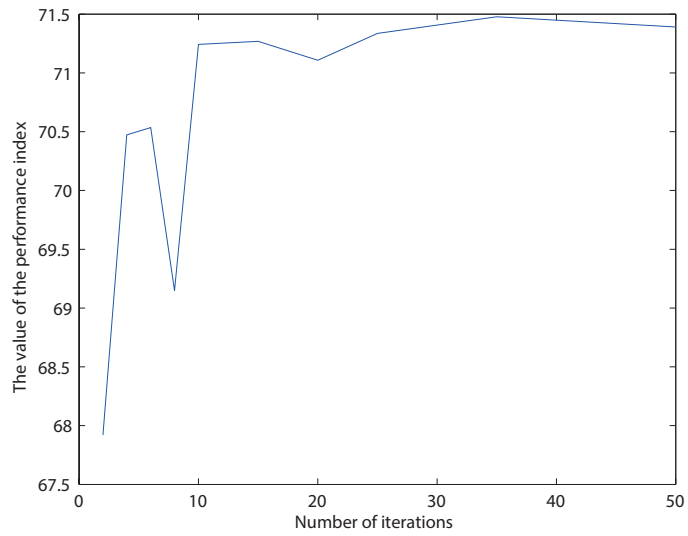


Figure 1: The convergence curve of the algorithm for the performance index.

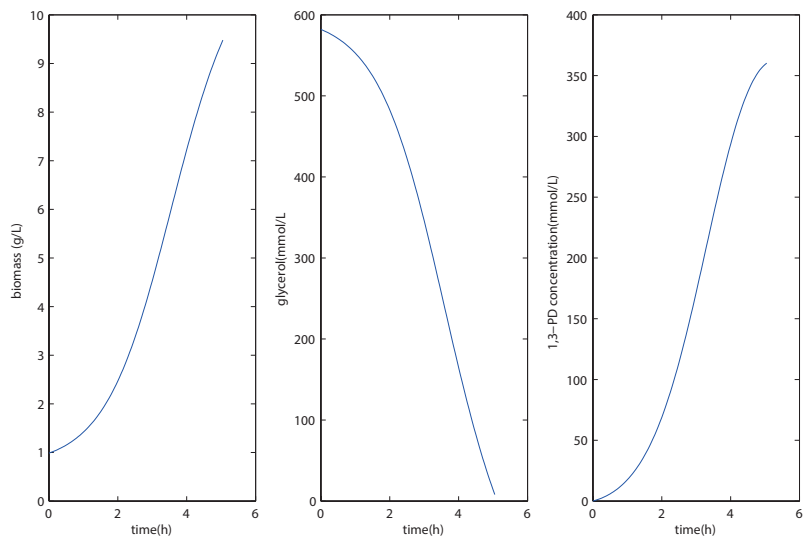


Figure 2: The concentration change of biomass, glycerol, 1,3-PD with respect to the optimal control vector u^* .

7 Conclusions

In this paper, different from the previous approach proposed in [26], based on the theory of swarm intelligence algorithm, we propose a modified particle swarm algorithm to find the global solution of the optimal control problem. Time-scaling technique and smoothing method are adopted to overcome the difficulties of free terminal time and continuous state inequality constraints. Numerical results show that, by employing the optimal control obtained in this paper, the concentration of 1,3-PD at the terminal time can increase when compared with the previous results.

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