Robust optimal control of a nonlinear impulsive time-delay system for 1,3-PD fed-batch culture

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Abstract. In this paper, taking the feeding process as a form of impulsive and considering the time-delay in fermentation process. A robust model with the time-delay system as the control variable and the time-delay system as the constraint is established. In order to solve this optimal control problem, we have propose a particle swarm optimization method to solve problem. Numerical results show that 1,3-PD yield at the terminal time increases compared with the experimental result.

1. Introduction

The main raw of a new polyester material is 1,3-Propanediol (1,3-PD) is the production, antifreeze and protective agent. Traditional chemical synthesis of 1,3-PD requires expensive catalysts and complex environment. In recent years, microbial fermentation technology has received attention from experts and scholars at home and abroad.

There are three types of microbial fermentation for the production of 1,3-PD. Fed-batch fermentation includes both batch and continuous fermentation modes. Compared to other fermentation methods, fed-batch fermentation has the ability to overcome the inhibition of catabolic metabolites produced during the chemical production process. Therefore, the industrial production of 1,3-PD has been widely used in the replenishment fermentation of wholesale fermentation[1]. During fed-batch fermentation materials are added to the fermerter in batches to maintain a suitable fermentation environment and improve the yield of 1,3-PD. Therefore, the optimal control of glycerol and alkali addition in fed-batch fermentation has received much attention. The literature[2] propose the optimal switching control problem for the fermentation processes of the replenishment batch is studied. However, the above optimal control studies ignore the time-delay phenomenon in the reaction process and the robustness of the intracellular material.

In this article, an impulsive time-delay differential equation with control is proposed to describe the time-delay replenishment batch, using the addition of glycerol and alkali as control vectors. In order to maximize production, we use the end-moment 1,3-PD production as a performance indicator, we propose a optimal control model with time-delay.

2. Nonlinear impulsive time-delay system

In the production of replenishment sub-wholesale fermentation, alkali and glycerol are added to the fermenter in batches to provide sufficient nutrients. Based on the fermentation process, this paper assumes that:
(H1): The concentration of substance in the container is uniform, ignoring the inhomogeneity of spatial distribution.

(H2): In the batch flow process, only alkali and glycerol are added to the fermenter.

(H3): The concentrations of extracellular material at moment $t-\tau$.

Under assumptions (H1)-(H3), biomass, substance and reaction in an intermittent process can expressed by the differential equation

$$
\dot{x}_i(t) = \mu(x(t))x_i(t - \tau),
$$

$$
\dot{x}_2(t) = q_2(x(t))x_1(t - \tau),
$$

$$
\dot{x}_3(t) = q_3(x(t))x_1(t - \tau),
$$

$$
\dot{x}_4(t) = q_4(x(t))x_1(t - \tau),
$$

$$
\dot{x}_5(t) = q_5(x(t))x_1(t - \tau),
$$

$$
\dot{x}_6(t) = \frac{1}{V_s} [J_{\text{max}} x_2(t) x_2(t) + \frac{1}{A_s} \{x_2(t) - x_6(t) - q_2(x(t))\} - \mu(x(t))x_6(t)],
$$

$$
\dot{x}_7(t) = \beta C_{\text{protein}} \left[ \frac{x_7(t)}{k_{\text{GDH}} (1 + x_6(t) x_6(t)) + x_6(t)} - k_{\text{PDOR}} U_{\text{PDOR}}(x(t)) \right],
$$

$$
\dot{x}_8(t) = \beta C_{\text{protein}} k_{\text{PDOR}} U_{\text{PDOR}}(x(t)) \left[ \frac{x_8(t)}{k_{\text{PDOR}} (1 + x_7(t) x_7(t)) + x_7(t)} - K_{\text{PDOR}} (x_8(t) - x_4(t)) \right]
$$

where $\tau$ is the delay arguments; $J_{\text{max}}$ is a maximal of glycerol; $K_m$ represents mMichealis-Menten constant of permease; $k_{\text{GDH}}$ and $k_{\text{PDOR}}$ are the ratios of activities of 1,3-PD oxydoreductase (PDOR) and glycerol dehydratase (GDHt) in vitro, respectively; $C_{\text{protein}}$ is the average in vitro protein concentration; $\beta$ is a the enzyme for activity coefficient; $K_{\text{GDH}}$ and $K_{\text{PDOR}}$ are GDHt and PDOR for respectively Michaelis-Menten constants; $K_{\text{GDH}}$ and $K_{\text{PDOR}}$ represent inhibitor constants of 3-hydroxypropionaldehyde, respectively; and $U_{\text{GDH}}(x(t))$ and $U_{\text{PDOR}}(x(t))$ are the specific activities, respectively. Based on the work[2], functions $\mu(\cdot), U_{\text{GDH}}(\cdot)$ and $U_{\text{PDOR}}(\cdot)$ are expressed as

$$
\mu(x(t)) = u_m \frac{x_2(t)}{x_2(t) + K_s \sum_{j=2}^{5} (1 - \frac{x_j}{x_j})},
$$

$$
U_{\text{PDOR}}(x(t)) = U_{\text{PDOR}}^{0} - \mu(x(t)) U_{\text{PDOR}}^{1} - \Delta U_{\text{PDOR}}^{m} \frac{x_2(t)}{x_2(t) + K_{\text{PDOR}}},
$$

the above parameters values are given in the literature[3].

Now, let $f_i(x(t), x(t-\tau), u(t)), i = 1,2, \ldots, 8$, be the right-hand sides of delay differential equation. Moreover, define

$$
f(x(t), x(t-\tau), u(t)) := (f_1(x(t), x(t-\tau), u(t)), \ldots, f_8(x(t), x(t-\tau), u(t)))^T.
$$

Then, the whole fed-batch process can be written as
\[
\begin{aligned}
\dot{x}(t) &= f(x(t), x(t-\tau), u(t)), \quad t \neq l_k, \\
\Delta x(t) &= I(x(t)), \quad t = l_k, \quad k = 1, 2, \ldots, N-1, \\
u(t) &\in U(t), \\
x(t) = \phi(t), \quad t \leq 0,
\end{aligned}
\]

where \( u(t) = (u_1(t), u_2(t))^T \in R^2 \) is control function; \( N \) is the number of jumps; \( l_k, k = 1, 2, \ldots, N-1 \), are given impulsive moments; \( T = l_N \) is a given terminal time; and \( \phi : R \rightarrow R^8 \) is a given continuous function. Additionally, to meet the actual conditions of cell growth, the substance concentrations in the biological reaction process must be strictly limited in a certain range. Hence, define

\[
W_{ad} := \prod_{i=1}^{8} [x_{q_i}, x_{q_i}^*], \quad \forall t \in [-\tau, T].
\]

3. Optimal control model

3.1. Optimal control model

During batch fermentation process, the producer expects to maximize the yield at end moment. Therefore, with the addition of glycerol and alkali as the control function and the yield of 1,3-PD at the terminal moment as the performance index, the following optimal control model is proposed in this paper:

\[
\begin{aligned}
(OCP) \quad &\max J(u, T) = x_3(T \mid u, T) \\
&\text{s.t. } x^T(t \mid u, T) \in W_{ad}, \\
&\quad u(t) \in U(t), \\
&\quad T \in [T_{\min}, T_{\max}].
\end{aligned}
\]

3.2. Numerical solution method

In this article, in order to overcome the localization of the particle swarm algorithm, a new velocity and position strategy is proposed. In addition, a new strategy of dealing with position outside parameter bounds is also introduced.

(1) (Updating strategy) In the previous iterations, balance development and exploitation by modifying the update speed and location as follows.

\[
\begin{aligned}
\nu(m) &= (-1 + c_1 \times r_1) \times \nu(m-1) + c_2 \times (pbest(m-1) - \sigma(m-1)) + r_2 \times c_2 \times (gbest - \sigma(m-1)), \\
\sigma(m) &= \frac{\sigma(m-1) + w(m) \times \nu(m)}{M_{ler}}, \\
w(k) &= w_2 - \frac{(w_1 - w_2)}{M_{ler}}; \quad w_1 \text{ and } w_2 \text{ are the inertia weights.}
\end{aligned}
\]

(2) (Processing parameter bounds) Assuming that the position component of the particle violates the parameter bound constraint, the particle update position component reflected back by parameters.

\[
\sigma(m) = \begin{cases} 
2\sigma - \sigma(m), & \text{if } \sigma > \sigma^*, \\
2\sigma(m) - \sigma, & \text{if } \sigma < \sigma^*.
\end{cases}
\]

4. Numerical results

In the numerical experiments, we use the same settings initial condition for the experimental to optimize the feeding amount. The initial concentration, initial volume of fermenting material, and end
time are $x_0, V_0 = 5L,$ and $T = 24.16h,$ respectively. Based on experiment, the fermentation process is divided into eight stages. Material are added at 100s in each stage. Table 1 and Table 2 given the upper and lower bounds of the amounts of glycerol and alkali added at each stage. Applying the PSO algorithm to solve OCP, the obtained optimal feeding strategy of material are listed in Table 3. From Figure 1, we can obtain that product is better than experiment data.

Table 1. The bounds of feeding amount of glycerol.

| Stage | I     | II    | III   | IV    | V     | VI    | VII   | VIII  |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Upper | 0.0017000 | 0.0024000 | 0.0025000 | 0.0020000 | 0.0014000 | 0.0012000 | 0.0008000 | 0.0004000 |
| Lower | 0.0004206 | 0.0005888 | 0.0006374 | 0.0005074 | 0.0003542 | 0.0002924 | 0.0002308 | 0.0001019 |

Table 2. The bounds of feeding amount of alkali.

| Stage | I     | II    | III   | IV    | V     | VI    | VII   | VIII  |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Upper | 0.0012750 | 0.0018000 | 0.0018750 | 0.0015000 | 0.0010500 | 0.0009000 | 0.0006000 | 0.0003000 |
| Lower | 0.0003154 | 0.0004416 | 0.0004780 | 0.0003805 | 0.0001593 | 0.0002193 | 0.0001731 | 0.0000764 |

Table 3. Optimal feeding strategy of glycerol and alkali.

| Stage | I     | II    | III   | IV    | V     | VI    | VII   | VIII  |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| glycerol | 0.0016750 | 0.0017140 | 0.0024750 | 0.000650 | 0.0010500 | 0.0009000 | 0.0002160 | 0.0003947 |
| alkali | 0.0003145 | 0.0004416 | 0.0004780 | 0.0003805 | 0.0001593 | 0.0002193 | 0.0001731 | 0.0000764 |

Figure 1. The changes of extracellular 1,3-PD concentration with time.

5. Conclusions
In this article, an impulsive time-delay system with multiple control variables to descr-ible the 1, 3-PD fed-batch process. Taking the 1, 3-PD at terminal time as performance index, the optimal control model of impulsive time-delay is established. The improved PSO is applied to sol-ve the optimal control problem. Numerical shows that the production of 1,3-PD is significantly hi-gher than experimental data at terminal time.
References

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