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Optimal 1,3-propanediol production: Exploring the trade-off between process yield and feeding rate variation

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ABSTRACT

This paper proposes a new optimal control model for the production of 1,3-propanediol (1,3-PD) via microbial fed-batch fermentation. The proposed model is governed by a nonlinear multistage dynamic system with two modes: feeding mode, in which glycerol and alkali substrates are added continuously to the fermentor; and batch mode, in which no substrates are added to the fermentor. The non-standard objective function incorporates both the final 1,3-PD yield and the cost of changing the input feeding rate, which is the control variable for the fed-batch fermentation process. Continuous state inequality constraints are imposed to ensure that the concentrations of biomass, glycerol, and reaction products lie within specified limits. Using the constraint transcription method, we approximate the continuous state inequality constraints by a conventional inequality constraint to yield an approximate parameter optimization problem. We then develop a combined particle swarm and gradient-based optimization algorithm to solve this approximate problem. The paper concludes with simulation results.

1. Introduction

1,3-Propanediol (1,3-PD) is an organic compound with a wide range of applications in cosmetics, adhesives, lubricants and medicines [1]. Due to its unique symmetrical structure, 1,3-PD can act as a monomer for the production of various industrial polymers, including polyesters and polyurethanes [2]. Production methods for 1,3-PD can be divided into two categories: chemical synthesis and microbial conversion. This paper focuses on the latter category, which is now becoming increasingly attractive in industry because of the cheap availability of renewable feedstock such as glycerol, a byproduct of biodiesel production [2,3].

Glycerol is converted to 1,3-PD via bacterial fermentation [4,5]. The fermentation process can be one of three types: batch fermentation (all substrate is present at the beginning of the reaction and nothing is added or removed from the fermentor during the reaction); fed-batch fermentation (fresh medium is added during the reaction to prevent nutrient depletion, but nothing is removed); and continuous fermentation (fresh medium is added during the reaction while old medium is removed). This paper focuses on fed-batch fermentation, which is typically implemented by switching between a batch mode (in which the input feed is closed) and feeding mode (in which the input feed is open). Switching between batch and feeding modes in this manner makes it easier to regulate the pH value for optimal reaction conditions [6–8]. In addition, substrate inhibition (whereby secondary reaction products hinder the consumption of substrate) is greatly reduced, allowing for more glycerol and alkali to be consumed and thus more biomass to be produced with higher 1,3-PD concentration [9].

The fed-batch fermentation process for converting glycerol to 1,3-PD begins with batch operation [10,11]. During this initial batch phase, the biomass tends to grow exponentially. Once the exponential growth phase ends, the glycerol and alkali substrates are added continuously to the reactor to regulate the pH level. The process then reverts to batch mode, and so on until the end of the final batch phase.

To achieve commercially viable concentrations of 1,3-PD, optimization of the microbial conversion process is critical. A major challenge is the presence of undesirable secondary products (acetate and ethanol), which inhibit the production of biomass. To address this challenge, precise mathematical models are required for process control and optimization. Recently in [12], a nonlinear impulsive model was proposed to describe the fed-batch fermentation process for converting glycerol to 1,3-PD. The corresponding parameter identification and optimal control problems were investigated in [13–17]. The impulsive model in [12] is based on the assumption that the addition of glycerol and alkali substrates is a

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discrete process. However, in practice, glycerol and alkali are added continuously, not at discrete times. Thus, a new model involving a nonlinear multistage dynamic system with continuous input variables was proposed in [18–20] for describing the fed-batch fermentation process. This model was further investigated in [21].

The optimal control models described in the previous paragraph only consider the maximization of the final 1,3-PD yield. However, in actual operation, it is also important to consider the cost associated with changing the process inputs: large changes to the glycerol and alkali addition rates are difficult (and potentially very costly) to implement in practice. Accordingly, in this paper, we consider a hybrid objective function that takes both 1,3-PD yield and input volatility into account. The optimal control model involves minimizing this hybrid objective function subject to a nonlinear multistage dynamic model for the fed-batch fermentation process, and continuous inequality constraints to reflect operational requirements. Since the governing multistage dynamic system is highly nonlinear, numerical techniques are unavoidable for solving the proposed optimal control model. We develop a novel approach based on the constraint transcription method [22], particle swarm optimization [23–25] and gradient-based nonlinear programming [26,27].

The remainder of this paper is organized as follows. In Section 2, we present a nonlinear multistage dynamic model to describe the microbial fed-batch fermentation process. Next, in Section 3, we introduce a novel optimal control model with hybrid objective function consisting of two terms: the first term encourages high 1,3-PD yield; the second term penalizes variation in the input feeding rate (the control variable for the process). By using the constraint transcription method, we obtain an approximate parameter optimization problem, which can be solved using the combined particle swarm and gradient-based optimization algorithm described in Section 4. Finally, in Section 5, we present the results from our extensive numerical simulations.

2. Process dynamics

We consider the fed-batch fermentation process described in [1] for converting glycerol to 1,3-PD. The process model is derived by ignoring time-delay effects and non-uniform space distribution. For batch mode, the mass balance relationships for biomass, substrate and reaction products can be expressed by the following differential equations:

$$\begin{aligned}\dot{x}_1(t) &= \mu(t)x_1(t),\\ \dot{x}_2(t) &= -q_2(t)x_1(t),\\ \dot{x}_i(t) &= q_i(t)x_1(t), \quad i=3,4,5,\end{aligned}$$

where t denotes process time (in hours); and $x_i(t)$, $i=1, 2, 3, 4, 5$, are, respectively, the concentrations of biomass, glycerol, 1,3-PD, acetic acid and ethanol ($x_1(t)$ is measured in $\mathrm{g\,L^{-1}}$ and the other state variables are measured in $\mathrm{mmol\,L^{-1}}$). Furthermore, $\mu(t)$ is the specific growth rate of cells (in $\mathrm{h^{-1}}$); $q_2(t)$ is the specific consumption rate of substrate (in $\mathrm{h^{-1}}$); and $q_i(t)$, $i=3, 4, 5$, are, respectively, the specific formation rates of the reaction products 1,3-PD, acetic acid and ethanol.

For feeding mode, the mass balance relationships can be expressed by

$$\begin{aligned}\dot{x}_1(t) &= (\mu(t)-D(t))x_1(t),\\ \dot{x}_2(t) &= D(t)\left(\frac{\rho_g}{R+1}-x_2(t)\right)-q_2(t)x_1(t),\\ \dot{x}_i(t) &= q_i(t)x_1(t)-D(t)x_i(t), \quad i=3,4,5,\end{aligned}$$

where $D(t)$ denotes the dilution rate at time t, ρ_g denotes the concentration of glycerol in the input feed, and R is the ratio of alkali to glycerol in the input feed.

Based on the work in [1], the specific growth rate of cells can be expressed as follows:

$$\mu(t) := \frac{\Delta_1 x_2(t)}{x_2(t)+k_1}\prod_{l=2}^{5}\left(1-\frac{x_l(t)}{x_l^*}\right)^{n_l},$$

where Δ_1 is the maximum specific growth rate; x_l^*, $l=2, 3, 4, 5$, are the maximum residual concentrations of substrate and reaction products; k_1 is the Monod saturation constant; and n_l, $l=2, 3, 4, 5$, are given exponents. Moreover the specific consumption rate of substrate can be expressed as follows:

$$q_2(t) := m_2 + \frac{\mu(t)}{Y_2} + \frac{\Delta_2 x_2(t)}{x_2(t)+k_2},$$

where m_2 is the maintenance term of substrate consumption under substrate-limited conditions; Y_2 is the maximum growth yield; Δ_2 is the maximum increment of substrate consumption rate under substrate-sufficient conditions; and k_2 is the saturation constant for substrate.

The specific formation rates of 1,3-PD and acetic acid are defined as

$$q_i(t) := m_i + Y_i\mu(t) + \frac{\Delta_i x_2(t)}{x_2(t)+k_i}, \quad i=3,4,$$

where m_3 and m_4 are the maintenance terms of 1,3-PD and acetic acid formations under substrate-limited conditions; Y_3 and Y_4 are the maximum 1,3-PD and acetic acid yields; Δ_3 and Δ_4 are the maximum increments of 1,3-PD and acetic acid formation rates under substrate-sufficient conditions; and k_3 and k_4 are the saturation constants for 1,3-PD and acetic acid.

The specific formation rate of ethanol can be expressed by

$$q_5(t) := q_2(t)\left(\frac{c_1}{c_2+\mu(t)x_2(t)}+\frac{c_3}{c_4+\mu(t)x_2(t)}\right),$$

where c_1, c_2, c_3 and c_4 are given parameters.

Furthermore, the dilution rate $D(t)$ and volume $V(t)$ are given by

$$\begin{aligned}D(t) &:= \frac{u(t)}{V(t)},\\ V(t) &:= V_0 + \int_0^t u(s)ds,\end{aligned}$$

where V_0 denotes the initial volume of solution in the fermentor and $u(t)$ denotes the input feeding rate.

Let

$$f^b(t,x(t)) := \begin{pmatrix}\mu(t)x_1(t)\\ -q_2(t)x_1(t)\\ q_3(t)x_1(t)\\ q_4(t)x_1(t)\\ q_5(t)x_1(t)\end{pmatrix}$$

and

$$f^c(t,x(t),D(t)) := \begin{pmatrix}(\mu(t)-D(t))x_1(t)\\ D(t)(\frac{\rho_g}{R+1}-x_2(t))-q_2(t)x_1(t)\\ q_3(t)x_1(t)-D(t)x_3(t)\\ q_4(t)x_1(t)-D(t)x_4(t)\\ q_5(t)x_1(t)-D(t)x_5(t)\end{pmatrix},$$