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Optimal control for nonlinear dynamical system of microbial fed-batch culture

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ABSTRACT

In fed-batch culture of glycerol bio-dissimilation to 1, 3-propanediol (1, 3-PD), the aim of adding glycerol is to obtain as much 1, 3-PD as possible. So a proper feeding rate is required during the process. Taking the concentration of 1, 3-PD at the terminal time as the performance index and the feeding rate of glycerol as the control function, we propose an optimal control model subject to a nonlinear dynamical system and constraints of continuous state and non-stationary control. A computational approach is constructed to seek the solution of the above model in two aspects. On the one hand we transcribe the optimal control model into an unconstrained one based on the penalty functions and an extension of the state space; on the other hand, by approximating the control function with simple functions, we transform the unconstrained optimal control problem into a sequence of nonlinear programming problems, which can be solved using gradient-based optimization techniques. The convergence analysis of this approximation is also investigated. Numerical results show that, by employing the optimal control policy, the concentration of 1, 3-PD at the terminal time can be increased considerably.

1. Introduction

The microbial conversion of glycerol to 1, 3-propanediol (1, 3-PD) is particularly attractive in that the process is relatively easy and does not generate toxic byproducts. 1, 3-PD has numerous applications in polymers, cosmetics, food, lubricants, and medicines. Industrial 1, 3-PD production has attracted much attention as an important monomer to synthesize a new type of polyester, polytrimethylene terephthalate (PTT) [1]. However, compared with chemical production, it is difficult to obtain a high 1, 3-PD concentration in the fermentor using the microbial culture. Hence, it is an area of interest to develop an improved technique to improve the productivity of 1, 3-PD.

Glycerol can be converted to 1, 3-PD by several microorganisms [2,3]. Among these, *Klebsiella pneumoniae* (*K. pneumoniae*) ferments glycerol to 1, 3-PD in a high yield and productivity [4–6]. With regard to fermentation, almost all of existing culture techniques, including batch culture, fed-batch culture and continuous culture, have been practiced. During the bioconversion of glycerol to 1, 3-PD, the most efficient cultivation method appears to be a fed-batch culture which corrects pH by alkali addition for glycerol supply [7]. In the actual fermentation process, the fed-batch culture begins with batch culture. After the exponential growth phase (a period in which the number of new bacteria appearing per unit time is proportional to the present population) ends, glycerol and alkali are added continuously to the fermentor. This helps to maintain a suitable environment for cells growth. At the end of the feeding, a batch phase starts again. The above processes are repeated until the end of the final batch phase.

The fermentation of glycerol by *K. pneumoniae* under anaerobic conditions is a complex bioprocess, since microbial growth is subjected to multiple inhibitions of substrate and products [8]. Modeling the fermentation process is a premise to carry out optimal control and to improve the productivity of product. Therefore, it is a key step to formulate the fermentation

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process by a precise mathematical model. In recent years, nonlinear dynamical systems have been extensively investigated to formulate the fermentation process [9–13]. Although the achieved results are interesting, these dynamical systems are based on an assumption that the feeding of glycerol only occurs at impulsive time. In fact, the feeding rate of glycerol is finite, so the feeding is not an impulsive form but a time-continuous process. Therefore, the impulsive dynamical system cannot rationally describe the actual fed-batch fermentation process.

Compared with the previous systems, a controlled dynamical system which does not take the feeding process as an impulsive form, but a time-continuous process, is proposed in this work. To maximize the concentration of 1, 3-PD at the terminal time, we develop an optimal control model subject to our proposed dynamical system and constraints of continuous state and non-stationary control. There exist many methods to solve the problem of optimal feeding rate, such as Luus–Jaakola search method [14], multiple shooting technique [15], genetic algorithm [16] and so on. However, these methods are all applied to the fed-batch process in which the substrates are fed to the fermentor continuously. In the actual fermentation, glycerol and alkali are intermittently fed in fermentor. As a result, the computation is more complex. Hence, it is necessary to present a new method to solve this class of problem.

Optimal control problems involving continuous state and/or control inequality constraints have been extensively studied in the literature. Many interesting theoretical results can be found in books such as [17]. For numerical computation, several successful families of algorithms have already been developed, see, for example [18–23]. In particular, the parametrization method (PM) in [20] is based on sequential development of a simple idea to account that solutions of real optimal control problem have a rather simple structure and control functions can be well approximated in some parametric function classes. Consequently, control functions can be finitely parametrized, and the optimal control problem will become a finite-dimensional nonlinear programming problem. In addition, optimal control problems can be solved by the PM with the help of the information about the derivatives of performance indices.

In view of the characteristic of the proposed optimal control model, we construct a computational approach to find the optimal control in two aspects. Firstly, we transcribe the optimal control model into an unconstrained one based on the penalty functions and an extension of the state space. Secondly, the PM is applied to approximating the above unconstrained optimal control problem. The convergence analysis of this approximation is investigated. The first and second derivatives of the performance index with respect to control parameters are also presented. Numerical results show that, by employing the optimal control policy, the concentration of 1, 3-PD at the terminal time can be increased by 28.32% compared with the experimental result.

The remainder of this paper is organized as follows. In Section 2, a description is carried out about the controlled nonlinear dynamical system of microbial fed-batch culture. Section 3 proposes an optimal control model. A computational approach is developed to solve the optimal control model in Section 4, while Section 5 illustrates the numerical results. Finally, conclusions are provided in Section 6.

2. Controlled nonlinear dynamical systems

In fed-batch culture, the composition of culture medium, cultivation conditions and analytical methods of fermentative products were similar to those previously reported in [24]. According to experiment process, we assume that

(H_1): The concentrations of reactants are uniform in reactor. Time delay and nonuniform space distribution are ignored.
(H_2): During the process of fed-batch culture, only glycerol and alkali are fed into the reactor. Moreover, the feeding velocity ratio r of alkali to glycerol is a constant.

Let $x(t) := (x_1(t), x_2(t), x_3(t), x_4(t), x_5(t), x_6(t))^{\mathrm{T}} \in R^6_+$ be the continuous state, where $x_1(t), x_2(t), x_3(t), x_4(t), x_5(t), x_6(t)$ are the concentrations of biomass, glycerol, 1, 3-PD, acetate, ethanol and the volume of culture fluid at t in fermentor, respectively. $u(t) \in R^1$ is the control function, which is the rate of adding glycerol in the fed-batch culture. Let T be the terminal time of fermentation. Denote t_{2i+1}, the moment of adding glycerol, at which the fermentation process switches to continuous culture from batch culture, and t_{2i+2}, the moment of ending the flow of glycerol, $i \in \Lambda_1 := \{0, 1, 2, \dots, n-1\}$, at which the fermentation process jumps into batch culture from continuous culture. Note that $0 = t_0 < t_1 < t_2 < \cdots < t_{2n} < t_{2n+1} = T$ and these moments are decided a priori in the experiment. Let $\Lambda_2 := \{0, 1, 2, \dots, n\}$. Mass balances of biomass, substrate and products in fed-batch culture can be formulated as the following controlled nonlinear dynamical system:

$$\begin{cases} \dot{x}(t) = f(x(t), u(t)), \\ x(0) = x_0, & t \in [0, T], \\ u(t) \in U(t), \end{cases} \tag{1}$$

where

$$f(x(t), u(t)) = \begin{pmatrix} (\mu - D(x(t), u(t)))x_1(t) \\ D(x(t), u(t)) \left(\dfrac{c_{s0}}{1+r} - x_2(t) \right) - q_2 x_1(t) \\ q_3 x_1(t) - D(x(t), u(t)) x_3(t) \\ q_4 x_1(t) - D(x(t), u(t)) x_4(t) \\ q_5 x_1(t) - D(x(t), u(t)) x_5(t) \\ (1+r)u(t) \end{pmatrix}. \tag{2}$$