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Nonlinear state-dependent impulsive system and its parameter identification in microbial fed-batch culture

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ABSTRACT

In fed-batch culture of glycerol to 1,3-propanediol by *Klebsiella pneumoniae*, glycerol and alkali are fed in batches into the bioreactor to provide sufficient nutrition and maintain a suitable environment for cells growth. In this paper, taking the feeding process as a state-dependent impulses process, a nonlinear state-dependent impulsive system is proposed to formulate the fed-batch process. Some important properties of the solution to the system are discussed, i.e., the existence, uniqueness and regularity of solution to the system and continuous dependence of the solution on initial value and parameters. Regarding the errors between the experimental results and calculated values as the performance index, a parameter identification model is presented. The identifiability of the parameter identification model is also proved. Finally, an improved particle swarm optimization (PSO) algorithm is constructed to seek the optimal parameters. Numerical results show that the nonlinear state-dependent impulsive system can be used to describe the fed-batch culture reasonably .

1. Introduction

1,3-Propanediol (1,3-PD) is a bulk chemical that can be used for synthesizing many polymers with attractive features, such as polyesters, polyethers and polyurethanes [1]. 1,3-PD has traditionally been manufactured by chemical synthesis, which requires a high temperature, a high pressure and expensive catalysts, resulting in very high manufacturing cost. Recently, microbial production has attracted much attention throughout the world. Among various microbial productions of 1,3-PD, glycerol bioconversion to 1,3-PD by *Klebsiella pneumoniae* (*K. pneumoniae*) has been widely investigated due to its high productivity and yield since the 1980s [2].

Cultivation methods for bioconversion of glycerol to 1,3-PD by *K. pneumoniae* can be divided into batch culture, continuous culture and fed-batch culture. The most efficient cultivation method appears to be fed-batch culture which corrects the pH by alkali addition with glycerol supply [3]. The fed-batch culture of glycerol to 1,3-PD by *K. pneumoniae* begins with a batch culture, then glycerol and alkali are added into the bioreactor to provide sufficient nutrition and to maintain a suitable environment for cell growth.

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Determining a valid mathematical model is often a very vital task since the use of a non-accurate model in subsequent optimization and control may lead to undesirable results. Recently, nonlinear dynamical systems have been extensively investigated to formulate fed-batch fermentation. A nonlinear impulsive dynamical system was investigated to formulate fed-batch culture in [4]. For this system, properties, parameter identification and optimal control were studied in [5–7]. In this system, impulses occurred at fixed times which were decided a priori. A nonlinear multistage dynamical system [8] and a switched system with variable switching instants [9] were also proposed to formulate the fed-batch culture, in which the feeding of glycerol and alkali were taken as a time-continuous process. Liu et al. [10–12] discussed modeling, optimal control, sensitivity analysis and parameter identification for time-delayed switched system and nonlinear time-delay system in fed-batch fermentation. However, glycerol fermentation by *K. pneumoniae* is a complex bio-process since the microbial growth is subjected to multiple inhibitions of substrate and products [13]. In order to reduce inhibition of glycerol to the cell growth, glycerol concentration in the bioreactor must be maintained near to a certain value [14], i.e., glycerol and alkali are added instantaneously to the fermentor when the glycerol concentration drop to a certain value. Furthermore, since the feeding process is very short it can be taken as an impulsive form in the actual fermentation process.

Here, a nonlinear state-dependent impulsive system is proposed to formulate the fed-batch culture of glycerol bioconversion to 1,3-PD by *K. pneumoniae*. Some important properties of the system, such as the existence, uniqueness and regularity of the solution are investigated. Regarding the errors between the experimental results and computational values as the performance index, a parameter identification model is presented. The identifiability of the parameter identification model is also proved. An improved particle swarm optimization (PSO) algorithm is constructed to seek the optimal parameters. Numerical results show that the nonlinear impulsive system can describe the fermentation process reasonably.

This paper is organized as follows. In Section 2, a nonlinear state-dependent impulsive system of fed-batch culture is described. In Section 3, some important properties of the system are investigated. In Section 4, a parameter identification model is established and an improved PSO algorithm is constructed to solve the identification model. In Section 5, a numerical example is provided. Conclusions are presented in Section 6.

2. Nonlinear state-dependent impulsive system

The fed-batch culture of glycerol bioconversion to 1,3-PD by *K. pneumoniae* begins with a batch culture, then glycerol and alkali are fed in batches into the fermentor. According to the factual process, we assume that

(H1) The concentrations of reactants are uniform in the bioreactor, time delay and nonuniform space distribution are ignored.
(H2) The feed rate of glycerol can be infinitely large. Moreover, the feeding velocity ratio r of alkali to glycerol is constant.

The whole fed-batch process includes a batch culture in the early stage. Thus, under the assumption (H1), mass balances of biomass, substrate and products in the batch fermentation are written as follows [15]:

$$\begin{cases} \dot{x_1}(t) = \mu x_1(t), \\ \dot{x_2}(t) = -q_2 x_1(t), \\ \dot{x_3}(t) = q_3 x_1(t), \\ \dot{x_4}(t) = q_4 x_1(t), \\ \dot{x_5}(t) = q_5 x_1(t)), \\ x(0) = \xi, \end{cases} \tag{2.1}$$

where $x_1(t), x_2(t), x_3(t), x_4(t)$ and $x_5(t)$ are the concentrations of biomass, glycerol, 1,3-PD, acetic acid and ethanolat time t in the bioreactor, respectively. The vector $x(t) = (x_1(t),\ x_2(t),\ x_3(t),\ x_4(t),\ x_5(t))^T \in \mathbb{R}^5$ is the state variable, $\xi \in \mathbb{R}^5$ is the initial concentrations of the culture. Furthermore, the specific cellular growth rate μ, the specific consumption rate of glycerol q_2 and the specific product formation of 1,3-PD, acetic acid and ethanol q_3, q_4 and q_5 are expressed by the following equations [15].

$$\mu = \mu_m \frac{x_2(t)}{x_2(t) + K_s} \prod_{i=2}^{5} \left(1 - \frac{x_i}{x_i^*}\right)^{n_i}, \tag{2.2}$$

$$q_2 = m_2 + \frac{\mu}{Y_2} + \Delta_2 \frac{x_2(t)}{x_2(t) + k_2}, \tag{2.3}$$

$$q_3 = -m_3 + \mu Y_3 + \Delta_3 \frac{x_2(t)}{x_2(t) + k_3}, \tag{2.4}$$

$$q_4 = -m_4 + \mu Y_4 + \Delta_4 \frac{x_2(t)}{x_2(t) + k_4}, \tag{2.5}$$

$$q_5 = q_2 \left(\frac{b_1}{c_1 + \mu x_2(t)} + \frac{b_2}{c_2 + \mu x_2(t)} \right). \tag{2.6}$$

Under anaerobic conditions at 37° C and pH 7.0, the critical concentrations of biomass, glycerol, 1,3-PD, acetate and ethanol for cells growth are $x_1^* = 10\ \mathrm{g\,L^{-1}},\ x_2^* = 2039\ \mathrm{mmol\ L^{-1}},\ x_3^* = 939.5\ \mathrm{mmol\ L^{-1}},\ x_4^* = 1026\ \mathrm{mmol\ L^{-1}}$ and $x_5^* = 360.9\ \mathrm{mmol\ L^{-1}}$,