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Modelling and parameter identification for a nonlinear time-delay system in microbial batch fermentation

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ABSTRACT

Mathematical modelling and parameter identification of a microbial batch fermentation process is considered in this paper. In view of the existence of time delays, a nonlinear time-delay system is firstly proposed to formulate the fermentation process. Some important properties are also discussed. Taking the errors between the computational values and the experimental data as the cost function, a parameter identification model subject to continuous state constraints and parameter constraints is then presented. To seek the optimal time delay and the optimal kinetic parameters, an improved differential evolution algorithm in conjunction with the constraint transcription technique is developed. Finally, numerical results show that the model can describe the batch fermentation process reasonably.

1. Introduction

Time-delay systems are increasingly used in numerous application areas that include physiological kinetics, population dynamics, infectious diseases and so on [1]. Parameter identification problem is usually done by comparing the system output observed in practice with the system output predicted by the model, and then adjusting the parameters accordingly. Works on identification of time-delay systems have shown the complexity of the question [2]. Hence, the problem of identifying unknown parameters and time delays in time-delay systems has been extensively studied, see, for example, [3,4].

1,3-Propanediol (1,3-PD) is a valuable chemical intermediate that is suitable as a monomer for polycondensations to produce polyesters, polyethers and polyurethanes [5]. The fermentation of glycerol to 1,3-PD is particularly attractive in that the process is relatively easy and does not generate toxic byproducts. Glycerol can be converted to 1,3-PD by several microorganisms [6–8]. Among these, *Klebsiella pneumoniae* (*K. pneumoniae*) ferments glycerol to 1,3-PD in a high yield and productivity. The methods of glycerol bioconversion to 1,3-PD consist of batch, continuous and fed-batch cultures. Compared with continuous and fed-batch cultures, glycerol fermentation in batch culture can obtain the highest production concentration and molar yield 1,3-PD to glycerol [9]. As a results, there has been widely used in industrial fermentation process.

The widespread use of batch culture in 1,3-PD fermentation process has aroused an obvious interest in its modelling with a view to facilitating its design, control and optimization. The fermentation of glycerol by *K. pneumoniae* under anaerobic conditions is a complex bioprocess since the microbial growth is subjected to multiple inhibitions of substrate as well as products [10] and time delays exist in the process [11,12]. An excess kinetic model for substrate consumption and product formation was established in [13,14]. Later the model was improved so that it could describe substrate consumption and products formation in a large range of feed glycerol concentrations into medium [15]. The parameter identification problem based on this model and its optimization algorithm were investigated in [16,17]. A two-stage dynamical system to formulate

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the batch culture process was proposed in [18]. A nonlinear dynamical system describing the multistage cell growth in batch culture was presented by a modification at the specific rate of cell growth [19]. More recently, a nonlinear hybrid dynamical system including the transport modes of glycerol and 1,3-PD through the cell membrane was established [20]. Although the achieved results are interesting, time delays are ignored in the above researches.

In this paper, a novel mathematical model including time delay, i.e., nonlinear time-delay system, is proposed to describe the batch fermentations of glycerol by *K. pneumoniae*. Some important properties are also investigated. Taking the errors between the computational values and the experimental data, a parameter identification model subject to continuous state constraints and parameter constraints is then presented to identify the delay argument and the kinetic parameters in the nonlinear time-delay system. The constraint transcription and smoothing techniques [21] are applied to dealing with the continuous state constraints in the parameter identification model. On this basis, an improved differential evolution algorithm is developed to solve the identification problem. Finally, comparisons between simulated and experimental results indicate that the model can be used to describe the batch fermentation process reasonably.

This paper is organized as follows. In the next section, Section 2, the nonlinear time-delay system in the batch fermentation process is presented. Section 3 gives the parameter identification problem. Section 4 illustrates the numerical results, while conclusions are provided in Section 5.

2. Nonlinear time-delay systems

In batch culture, a quantity of biomass and glycerol are added to the reactor only once and stirred uniformly under given conditions. During the process of the culture, the concentration of the glycerol decreases gradually and tends to zero finally. According to the fermentation process, we assume that.

(H_1) Do not input or output the biomass, substrate and products in reactor during the batch fermentation process.
(H_2) The concentrations of reactants are uniform in reactor.

Although the uptake of nutrient by cells is an essential instantaneous process, cells have to undergo growth process before they produce products [22]. Thus, a time delay should be taken into account in modelling the fermentation process. Under the assumptions (H_1) and (H_2), mass balances of biomass, substrate and products in batch culture can be formulated as the following nonlinear time-delay system:

$$\begin{cases} \dot{x}_1(t) = \mu x_1(t-\tau), \\ \dot{x}_2(t) = -q_2 x_2(t), \\ \dot{x}_3(t) = q_3 x_1(t-\tau), \quad t \in (0, T], \\ \dot{x}_4(t) = q_4 x_1(t-\tau), \\ \dot{x}_5(t) = q_5 x_1(t-\tau), \\ x(0) = x_0, \end{cases} \tag{1}$$

where $x(t) := (x_1(t), x_2(t), x_3(t), x_4(t), x_5(t))^T$ is the state vector whose components are, respectively, the concentrations of biomass, glycerol, 1,3-PD, acetate and ethanol in the reactor at time t; x_0 is a given initial state; T is the terminal moment of the batch culture and τ is the delay argument. On the basis of previous work [15], the specific growth rate μ of cells can be expressed as

$$\mu = \begin{cases} \frac{\mu_m x_2(t)}{k_1 + x_2(t)} \prod_{\ell=2}^{5} \left(1 - \frac{x_\ell(t)}{x_\ell^*}\right), & \text{if } x_\ell < x_\ell^*, \\ 0, & \text{otherwise}, \end{cases} \tag{2}$$

where μ_m is the maximum specific growth rate; k_1 is the Monod saturation constant; x_ℓ^* are the critical concentration for cells growth. The specific consumption rate of substrate q_2 is

$$q_2 = m_2 + \frac{\mu}{Y_2}. \tag{3}$$

In (3), m_2 is the maintenance term of substrate consumption under substrate-limited conditions. Y_2 is the maximum growth yield. The specific formation rates $q_\ell, \ell = 3, 4$, of 1,3-PD and acetate are defined as

$$q_\ell = -m_\ell + \mu Y_\ell, \tag{4}$$

in which m_ℓ are the maintenance terms of product formations under substrate-limited conditions; Y_ℓ are the maximum product yields. The specific formation rates q_5 of ethanol is defined as

$$q_5 = m_5 + \mu Y_5, \tag{5}$$

where m_5 is the maintenance terms of ethanol formations under substrate-limited conditions; Y_5 is the maximum ethanol yields.