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Modelling and properties of a nonlinear autonomous switching system in fed-batch culture of glycerol

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ABSTRACT

A nonlinear autonomous switching system is proposed to describe the coupled fed-batch fermentation with the pH as the feedback parameter. We prove the non-Zeno behaviors of the switching system and some basic properties of its solution, including the existence, uniqueness, boundedness and regularity. Numerical simulation is also carried out, which reveals that the proposed system can describe the factual fermentation process properly.

1. Introduction

The microbial conversion of glycerol by *Klebsiella pneumoniae* (*K. pneumoniae*) to 1,3-propanediol (1,3-PD) in fed-batch culture is of interest to industry because of the increasing glycerol surplus on the market, the potential uses of 1,3-PD and the highest production concentration and productivity [1,2].

In the laboratory, glycerol and alkali are discontinuously added to the reactor in order that the glycerol concentration keeps in a given range and the pH in the bioreactor maintains 7 or so, which can provide nutrition and maintain a suitable environment for the cells' growth [3,4]. Modelling the fermentation process is a premise to carry out optimal control and to increase the productivity of 1,3-PD. Over the past years, a number of models have been established to formulate the fed-batch fermentation process [5–7]. However, the above models are all developed to describe the operation that the addition of alkali coupled with glycerol is determined by a pre-determined fixed schedule, which have difficulties in achieving the requirement of the pH of the solution.

In fact, incorporating the pH feedback control into the feeding system is based on the phenomenon that the pH will gradually reduce to its allowable lower bound because of the accumulation of acid byproducts during batch process and that the pH will increase to reach its allowable upper bound due to the fed alkali [8]. In order to realize pH feedback control, the mathematical relationship among the pH, the concentrations of the fed substances and acid byproduct, and others should be known. According to the literature [9], the pH of the solution can be formulated as a function of the concentrations of acetic acid and alkali in the reactor. Therefore the switches determined by the pH are actually state dependent, or "autonomous", and the whole fed-batch process can be formulated by a nonlinear autonomous switching system [10,11].

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Autonomous switching system describes one of discrete phenomena, where the vector field changes discontinuously, or "switches", when the state hits certain "boundaries" [11]. In fact, the study of nonlinear autonomous switching system is not an easy task due to pathological behaviors that may occur. However, some existing results indicate that when we exclude the occurrence of pathological behaviors such as Zeno phenomenon, some important properties of the solutions could be obtained in the piecewise classical sense [12–14].

In the present work, a nonlinear autonomous switching system is proposed to describe the coupled fed-batch fermentation with the pH as the feedback parameter. Under some assumptions, we prove the non-Zeno behaviors of the switching system. Then, applying the definition of piece classical solution, we discuss the existence, uniqueness and boundedness of the solution to the system in the piecewise classical sense. Furthermore, through verifying the continuity dependence of the switching instants with respect to the initial state and parameters, the regularity of the piecewise classical solution is also proved. Finally, numerical simulation of a factual experiment is carried out, which shows the appropriateness of the proposed system.

This paper is organized as follows. In Section 2, some notations are explained and a nonlinear autonomous switching system is proposed. Section 3 devotes to some important properties of the piecewise classical solution of the switching system, including the existence, uniqueness, boundedness and regularity. In Section 4, numerical simulation is carried out. Conclusions are presented at the end of this paper.

2. Nonlinear autonomous switching system

The fed-batch culture of glycerol bioconversion to 1,3-PD begins with a batch fermentation. After the exponential growth phase, glycerol and alkali (5 mol/L NaOH is used in the laboratory) are continuously fed into the reactor in order that the glycerol concentration keeps in a given range and the pH of the solution in the desirable level. After the feeding ends, another batch culture starts again. Namely, the fed-batch process is switched between fed process and batch process. Regarding batch process as mode 0 and fed process as mode 1, we shall formulate the whole fed-batch process by a switching system including two candidate modes.

In this paper, we consider a fed-batch fermentation process, in which the addition of alkali coupled with glycerol is dependent on the pH of the solution. For details, at the beginning of the fermentation, the pH is adjusted to an expected point; it then gradually decreases as the fermentation time elapsed because of the accumulation of acid byproducts; once it reduces to its allowable lower bound, glycerol coupled with alkali will be added to neutralize the acids in the solution until the pH value reaches its allowable upper bound.

According to the factual experiments, we make the following assumptions.

(H_1) The concentrations of reactants are uniform in reactor, while time delay and nonuniform space distribution are ignored.
(H_2) The feeding media includes fixed concentrations of glycerol and alkali.

Denote $\mathbf{x} := (x_1, x_2, \ldots, x_7)^T \in \mathbb{R}^7_+$ be the continuous state vector, where x_1, x_2, x_3, x_5 are the concentrations of biomass, glycerol, 1,3-PD and ethanol in reactor, respectively; x_4 is the total concentration of acetic acid in reactor, including Ac^- and acetic acid molecules; x_6 denotes the concentration of Na^+ ions coming from the added NaOH and x_7 the volume of the solution. To formulate the fed-batch process with pH feedback, we firstly give an output equation for the pH of the solution. According to the factual experiments, only the fermentation under acidic environment is discussed in this paper. Since the NaOH is the only basic source, we can make the following assumption.

(H_3) During the whole process of fed-batch culture, there exists a constant $M > 0$ such that $x_4 - \gamma x_6 \geqslant M$, where $\gamma > 0$ is the ratio of acetic acid concentration to the total acid byproducts concentrations.

Let $\mathcal{T} := [t_0, t_f]$ be the entire fermentation time. Under the above assumptions (H_1)–(H_3), the pH at time t ($\in \mathcal{T}$) can be formulated by the following output equation [9].

$$y(\mathbf{x}(t)) := \begin{cases} pK_a - \lg\frac{x_4 - \gamma x_6}{\gamma x_6} & \text{if } x_6 \geqslant \epsilon, \\ -\lg\left(\frac{-K_a + \sqrt{K_a^2 + 4K_a x_4/(1000\gamma)}}{2} + \sqrt{K_w^-}\right) & \text{otherwise}. \end{cases} \tag{1}$$

Here K_a is the averaged dissociation constant of acid byproducts, and $pK_a = -\lg(K_a)$; $K_w^- = 1 \times 10^{-14}$ is the dissociation constant of water; $\epsilon > 0$ is a sufficient small constant, below which the concentration of NaOH can be ignored while computing the pH. According to the actual experiments, the pH of the solution cannot deviate from the given allowable range $pH_{\mathrm{ad}} := [\mathrm{pH}_*, \mathrm{pH}^*]$ during the whole fermentation process, so we can assume that

(H_4) During the whole process of fed-batch culture, there exists a constant $\epsilon_0 \geqslant \epsilon > 0$ such that $x_6 > \epsilon_0$.

Under the assumption (H_4), the pH defined in (1) can be reformulated by

$$\tilde{y}(\mathbf{x}(t)) := pK_a - \lg\frac{x_4 - \gamma x_6}{\gamma x_6}. \tag{2}$$