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Optimal control of a batch fermentation process with nonlinear time-delay and free terminal time and cost sensitivity constraint

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ABSTRACT

In this paper, we consider a nonlinear time-delay dynamic system with uncertain system parameters to characterize the process of batch fermentation. Our goal is to design an optimal control scheme to maximize the productivity of 1,3-propanediol (1,3-PD). Accordingly, we introduce an optimal control problem governed by the nonlinear time-delay dynamic system, in which the control variables are the free terminal time of the batch fermentation process and the initial concentrations of biomass and glycerol. The optimal control problem is subject to a cost sensitivity constraint for ensuring that an acceptable level of the system performance is achieved and continuous state inequality constraints for ensuring that the concentrations of biomass, glycerol, 1,3-PD, acetate, ethanol lie within specified limits. Then, the optimal control problem with free terminal time is transformed, via a hybrid time-scaling strategy, into an equivalent problem with fixed terminal time, which is much preferred for numerical computation. Using the constraint transcription and local smoothing approximation techniques, we approximate these continuous state inequality constraints by conventional inequality constraints to yield an approximate optimal control problem. Because of the highly complex nature of this approximate problem, a parallel algorithm based on the filled function method is constructed to solve this approximate problem. Finally, it is observed that the optimal control obtained is satisfactory through numerical simulations.

1. Introduction

1,3-Propanediol (1,3-PD) is one of the important products with numerous applications, in particular for production of a new type of polyester, which is referred to as polytrimethylene terepthalate [1]. Currently, the process of producing 1,3-PD can be divided into two types: microbial conversion and chemical synthesis [2]. Compared with chemical synthesis approaches, microbial conversion methods have received attention recently because it is a choice for cheaply renewable feedstock, high region specificity and no harm to environment [3]. From both the economical and ecological point of view, it is an effective method to produce 1,3-PD by glycerol bioconversion induced by *Klebsiella pneumoniae* (*K. pneumoniae*) [4]. At present, there are three microbial conversion methods for producing 1,3-PD: batch, continuous and fed-batch fermentations [5]. In batch fermentation, bacteria and substrate are presented at the beginning of the process, and nothing is added or removed from the fermentor during the process [6]. In continuous fermentation, fresh medium is added continuously to replenish consumed substrate while old medium is removed during the reaction [7,8]. In fed-batch fermentation, glycerol and alkali are discontinuously added to the reactor at constant rates, so as to keep the substrate concentration and the pH in the desirable levels, without the removal of medium [9,10]. There are several reasons for the necessity of studying batch fermentation [11]: (1) in batch fermentation, 1,3-PD yield, which is defined as the ratio between the formation of 1,3-PD and the consumption of glycerol, is high. The main reason is that the batch fermentation can be expressed as an excessive metabolism process of glycerol. That is, the high concentration of glycerol

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leads to the high formation of 1,3-PD and the low formation of by-product in batch fermentation of glycerol. In particular, note that the high target product yield in batch fermentation is only applicable to the bioconversion of glycerol. Not all the batch fermentations are of the high target product yield; (2) batch fermentation is a simple and easy operation mode compared with fed-batch and continuous fermentations; (3) batch fermentation is basic for understanding or controlling fed-batch and continuous fermentations.

In the laboratory, it is impractical to carry out lots of batch experiments to obtain high production concentration and molar yield of 1,3-PD. Consequently, it is necessary to describe the process of batch fermentation through the application of mathematical systems. Relevant literature includes Ref. [12], where a substrate-sufficient kinetic system is proposed to characterize substrate (glycerol) consumption and extracellular substances (1,3-PD, acetate and ethanol) formation in batch fermentation; Ref. [13], where robust identification of enzymatic nonlinear dynamical systems for 1,3-PD transport mechanisms in microbial batch fermentation is researched; Ref. [14], where modelling and pathway identification involving the transport mechanism of a complex metabolic system in batch fermentation is investigated; Refs. [15–17], where robustness analysis and identification of nonlinear multi-stage dynamical system in batch fermentation are considered; Ref. [18], where parameter identification for a nonlinear enzyme-catalytic dynamic system with multiple time-delays is studied; Refs. [19,20], where the different identification problems for nonlinear hybrid dynamical system in batch fermentation are investigated; Ref. [21], where a stochastic model for microbial fermentation process under Gaussian white noise environment is considered; Ref. [22], where joint estimation of batch fermentation is carried out by using unscented Kalman filter.

An optimal control problem, in which both process yield and process sensitivity are considered in the objective function, is discussed in [23]. However, there is one limitation: the presence of time-delay, which is always encountered in real-world applications, is ignored in [23]. In [24], a parameter identification governed by a nonlinear time-delay system is carried out in microbial batch fermentation. The optimal control problem governed by this nonlinear time-delay system is studied in [25]. However, a cost sensitivity corresponding to uncertainty system parameters has not yet been considered. Clearly, a nonlinear dynamic system is an idealized description about the actual behavior of a biological or engineering system. During the life span of the system, the values of some system parameters may change [26,27]. For an optimal control problem governed by a nonlinear dynamical system, the optimal cost function obtained is under the assumption that these system parameters of the dynamical system are fixed. Given some of these system parameters are subject to variation, the cost sensitivity corresponding to uncertainty system parameters should be taken into consideration [28]. Nonetheless, in the process of microbial fermentation, there are few papers dedicated to the cost sensitivity.

In this paper, we consider a nonlinear time-delay dynamic system to characterize the process of batch fermentation of glycerol bioconversion to 1,3-PD induced by *K. pneumoniae*. Our aim is to construct an optimal control to maximize the productivity of 1,3-PD. Therefore, we propose an optimal control problem that depends on system parameters which have some uncertainty as to their exact values. The control variables are the terminal time of the batch fermentation process and the initial concentrations of biomass and glycerol. The optimal control problem governed by a nonlinear time-delay dynamic system, is subject to cost sensitivity (the derivative of the cost function with respect to the uncertain system parameters) constraint for ensuring that an acceptable level of the system performance is achieved and continuous state inequality constraints for ensuring that the concentrations of biomass, glycerol, and reaction products lie within specified limits. Then, the optimal control problem with free terminal time is transformed into an equivalent optimal control problem with fixed terminal time via a hybrid time-scaling strategy that only maps the current state into the new time scale and the delayed state remain in the original time scale. The equivalent problem is much preferred for numerical computation. Through the application of the constraint transcription and local smoothing approximation techniques, we approximate these continuous state inequality constraints by conventional inequality constraints to yield an approximate optimal control problem. On account of the highly computing complexity of this approximate problem, the computational cost is very high. Thus, we develop a parallel algorithm, based on the filled function method, to solve the approximate problem. Finally, numerical results show that the obtained optimal control is satisfactory.

The remainder of this paper is organized as follows. In Section 2, a nonlinear time-delay dynamic system is formulated. In Section 3, an optimal control problem subject to a cost sensitivity constraint and continuous state inequality constraints is proposed. In Section 4, computational approaches are constructed to solve the optimal control problem. In Section 5, numerical results are presented. In Section 6, conclusions and trace the direction for future works are presented.

2. Nonlinear time-delay dynamic system

Nomenclature

- I_n denotes the set $\{1, 2, \ldots, n\}$.
- $\mathbb{R}_+$ denotes the set of nonnegative real numbers.
- $\mathbb{R}$ denotes the set of real numbers.
- A^{T} denotes the transposition of matrix or vector A.
- $T \in [a_3, b_3]$ is the free terminal time for the fermentation process, where a_3 and b_3 are the minimal and the maximal time durations, respectively.
- $[0, T] \subset \mathbb{R}_+$, is the interval of reaction time.
- $x_0 := [x_{01}, \ldots, x_{05}]^{\mathrm{T}} \in \mathbb{R}^5$, is the initial state vector.
- a_1 and b_1 are the values of the minimal and the maximal the initial state x_{01}, respectively.
- a_2 and b_2 are the values of the minimal and the maximal the initial state x_{02}, respectively.
- $x(t) := [x_1(t), \ldots, x_5(t)]^{\mathrm{T}} \in \mathbb{R}^5$, denotes the continuous state vector (whose components are the state variables), where $x_1(t), \ldots, x_5(t)$ denote the concentrations of biomass, glycerol, 1,3-PD, acetate, ethanol at time $t \in [0, T]$, respectively.
- μ_m is the maximum specific growth rate.
- k_1 is the Monod saturation constant.
- m_2 is the maintenance term of substrate consumption under substrate-limited conditions.
- Y_2 is the maximum growth yields.
- m_i, $i = 3, 4, 5$, are the maintenance terms of 1,3-PD, acetate and ethanol under substrate-limited conditions.
- Y_i, $i = 3, 4, 5$, are the maximum 1,3-PD, acetate and ethanol yields.