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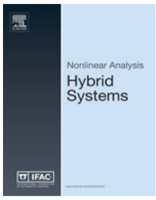

Robust multi-objective optimal switching control arising in 1,3-propanediol microbial fed-batch process

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ABSTRACT

This paper considers optimal control of glycerol producing 1,3-propanediol (1,3-PD) via microbial fed-batch fermentation. The fed-batch process is formulated as a nonlinear switched time-delay system. In general, the time-delay in the fed-batch process cannot be exactly estimated. Our goal is to design an optimal switching control scheme to simultaneously maximize 1,3-PD productivity and 1,3-PD yield under time-delay uncertainty. Accordingly, we propose a robust multi-objective optimal switching control model, in which two objectives, i.e., 1,3-PD productivity and 1,3-PD yield, and their sensitivities with respect to uncertain time-delay are considered in the objective vector. The control variables in this problem are the feeding rate of glycerol, the switching instants and the terminal time of the process. By introducing an auxiliary dynamic system to calculate the objective sensitivities and performing a time-scaling transformation, we obtain an equivalent multi-objective optimal switching control problem in standard form. We then convert the equivalent multi-objective optimal control problem into a sequence of single-objective optimal switching control problems by using a modified normal boundary intersection method. A novel gradient-based single-objective solver combining control parameterization with constraint transcription technique is developed to solve these resulting single-objective optimal control problems. Finally, numerical results are provided to verify the effectiveness of the proposed solution approach.

1. Introduction

1,3-Propanediol (1,3-PD) is a promising bulk chemical which has attracted worldwide attention due to its enormous application in polymers, cosmetics, foods, lubricants and medicines [1]. Currently, the market for 1,3-PD amounts to over 100 million pounds per year and is growing rapidly [2]. In general, production routes for 1,3-PD can be divided into two categories: chemical synthesis and microbial conversion. Compared with chemical synthesis, bioconversion of 1,3-PD via fermentation is particularly attractive in that the process is relatively easy and does not generate toxic byproducts. This conversion could also help to reduce glycerol surplus in the market [3]. Hence, improvement in the microbial production of 1,3-PD is of considerable importance to industries. To maximize the profit of 1,3-PD production, multi-objective optimization should be applied to the production process.

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Glycerol can be converted to 1,3-PD by several microorganisms [4]. Among these, *Klebsiella pneumoniae* (*K. pneumoniae*) ferments glycerol to 1,3-PD in a good yield [5]. Glycerol fermentation to produce 1,3-PD by *K. pneumoniae* is a complex bioprocess [6]. Regarding the various fermentation techniques, fed-batch fermentation appears to be the most efficient cultivation method. The fed-batch fermentation is typically implemented by switching between batch mode and feeding mode. This switching manner can reduce effectively the substrate inhibition and improve the 1,3-PD productivity. Moreover, the concentration of substrate in a fed-batch process can be externally manipulated by using appropriate feeding rate profiles. As a result, optimal control of fed-batch processes has been a topic of research for many years [7–9].

The performance of optimal control depends on the accuracy of the process model. Recently, it is found that the fed-batch process can be accurately modelled as nonlinear dynamical systems. Under the assumption that the feed of glycerol only occurs at impulsive instants, the process is modelled as nonlinear impulsive system [10]. Taking the 1,3-PD concentration at the terminal time as the objective, optimal control of nonlinear impulsive systems is discussed in [11]. However, since the feeding rate of glycerol is finite, it is not reasonable to describe the actual fed-batch process as an impulsive dynamical system. In reality, the feed of glycerol is a continuous process. Thus, the fed-batch process is modelled as nonlinear switched systems [12,13]. Optimal control of nonlinear switched systems is investigated in [14]. However, time-delays are ignored in the above nonlinear systems. In fact, like most real systems, fed-batch bioreactors are influenced by time-delays [15,16]. Several reasons may be responsible for the occurrence of the delays in the fed-batch process: a cell has to undergo some change or growth process for which it needs some time before it reacts with others; the substrate and the products have to be transported across the cell membrane requiring a certain amount of time for the transport; sometimes, either because of lack of knowledge or in order to reduce complexity it is appropriate to omit a number of intermediate steps in the reaction system for which the processing time is not negligible and has to be implemented as a delay [17,18]. As a result, a nonlinear switched time-delay system is proposed in [19]. More recently, a published book [20] summarizes some optimal control results arising in 1,3-PD production processes. Although the results obtained are interesting, only one objective is considered in these optimal control problems and thus they all belong to single-objective optimal control (SOC) problems. Moreover, it is difficult to determine the exact value of time-delay in the dynamic equation describing the fed-batch process and only nominal time-delay can be obtained using experimental data [19].

In this paper, we consider robust multi-objective optimal control (RMOC) of 1,3-PD fed-batch production in the presence of time-delay uncertainty. This fed-batch process is formulated as a nonlinear switched time-delay system. The optimal control problem is to design an optimal switching control scheme that maximizes 1,3-PD productivity and 1,3-PD yield, and also minimizes their sensitivities with respect to uncertain time-delay. Accordingly, we propose a robust multi-objective optimal switching control model that regards the feeding rate of glycerol, switching instants between batch and feeding modes, and the terminal time of the fermentation process as control variables and is subjected to continuous state inequality constraints. By the way, optimal control of switched systems is an important and challenging research topic for applied mathematicians [21–24]. Nevertheless, optimal control for switched systems with time-delays is scarce in the literature. Necessary conditions for determining optimal switching times and/or optimal impulse magnitudes for such systems are derived in [25]. Switching time and parameter optimization for nonlinear switched systems with multiple time-delays is considered in [26]. However, no time-delay uncertainty is considered in these optimal switching control results. On the other hand, multi-objective optimal control (MOC) problems often arise in bioprocesses and have been extensively investigated; see, for example [27–29]. Multiple objective approaches are often employed to tackle these MOC problems: (i) scalarization methods, e.g., convex weighted sum (CWS) method [30], and normal boundary intersection method (NBI) [31], which transform MOC problem into a sequence of parametric SOC problems, and (ii) vectorization methods, e.g., genetic algorithm [32], and particle swarm optimization [33], which generate the Pareto set directly from the multi-objective formulation. It should be noted that scalarization approaches, compared with vectorization methods, can be combined with gradient-based deterministic optimization methods for finding optimal solutions to large-scale and highly constrained MOC problems in a fast and efficient way. As a result, scalarization approaches have been extensively used to solve MOC problems in biochemical processes [34,35].

In this paper, by introducing an auxiliary time-delay system to calculate the objective sensitivities and performing a time-scaling transformation [36], we first transform the RMOC problem into an equivalent one in standard form. The equivalent problem is then converted into a sequence of parametric SOC problems by using a modified NBI method. The advantages of this method are that it can generate evenly distributed points in Pareto set and that it is weakly efficient for MOC problem. Incidentally, the existing single-objective solvers, including those developed in [28,34,35], only deal with SOC problems involving ordinary differential systems and thus cannot be used to solve the resulting SOC problems involving switched time-delay systems. For this reason, we approximate the resulting SOC by a sequence of parameter optimization problems through the application of the control parameterization method [37]. The continuous state inequality constraints are approximated as constraints in canonical form by employing the constraint transcription technique [38]. The gradient formulas of the objectives and constraints with respect to the decision variables are also provided. On this basis, a novel gradient-based solver is developed to solve the resulting SOC problem. Finally, numerical results verify the effectiveness of the proposed solution approach.

The paper is organized as follows. Section 2 gives the process model describing the fed-batch process. Section 3 presents the RMOC problem. Section 4 gives the equivalent form of the RMOC problem. The numerical solution method for the equivalent problem is developed in Section 5. Numerical results are discussed in Section 6. Finally, Section 7 provides the main conclusions.