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Multi-objective optimization of nonlinear switched time-delay systems in fed-batch process

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ABSTRACT

Maximization of productivity and minimization of consumption are two top priorities for biotechnological industry. In this paper, we model a fed-batch process as a nonlinear switched time-delay system. Taking the productivity of target product and the consumption rate of substrate as the objective functions, we present a multi-objective optimization problem involving the nonlinear switched time-delay system and subject to continuous state inequality constraints. To solve the multi-objective optimization problem, we first convert the problem into a sequence of single-objective optimization problems by using convex weighted sum and normal boundary intersection methods. A gradient-based single-objective solver incorporating constraint transcription technique is then developed to solve these single-objective optimization problems. Finally, a numerical example is provided to verify the effectiveness of the numerical solution approach. Numerical results show that the normal boundary intersection method in conjunction with the developed single-objective solver is more favourable than the convex weighted sum method.

1. Introduction

Fed-batch processes are extensively used in the biotechnological industry. To ensure product quality and economic viability of a fed-batch process, it is important to optimally design its operating strategy. Typically, in the literature, a single objective, e.g., maximization of product productivity, is considered [1–4]. However, product productivity alone is not sufficient to provide a full indication of the economic viability of the fermentor, since the substrate consumption must also be taken into consideration. Thus, optimization of the fermentation processes is, in fact, a multi-objective optimization (MOO) problem.

1,3-Propanediol (1,3-PD) is a bulk chemical used as a monomer in the production of polyesters, polyethers and polyurethanes. These polymers possess fine qualities and will continue to be used widely in the future [5]. Production methods for 1,3-PD can be divided into two categories: chemical synthesis and microbial conversion. Compared with chemical synthesis, microbial conversion method has become increasingly attractive in the industry due to easy availability of renewable feedstock, such as glycerol – a byproduct of biodiesel production [6]. Glycerol is converted to 1,3-PD via bacterial fermentation [7]. Glycerol fermentation to produce 1,3-PD is a complex bioprocess, since the microbial growth is subjected

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to multiple inhibitions of substrate and products [5] and there exist time-delays in the process [8,9]. Regarding the various fermentation techniques, which include batch mode, fed-batch mode and continuous mode, the fed-batch fermentation is typically implemented by switching between batch mode (in which the feeding of substrate is closed) and feeding mode (in which the feeding of substrate is open). This switching manner can reduce effectively the substrate inhibition and improve the 1,3-PD productivity, making the fed-batch fermentation being the most efficient cultivation method in 1,3-PD production [10]. The fed-batch process for converting glycerol to 1,3-PD begins with a batch operation. During this initial batch phase, the biomass tends to grow exponentially. Once the exponential growth phase ends, glycerol and alkali are added to the reactor to provide nutrition and regulate the pH level. The process then reverts to batch mode, and so on until the end of the final batch mode.

To achieve economically competitive production of 1,3-PD, optimization of the microbial conversion process is critical. Thus, many studies have been carried out on modelling and optimization of fed-batch process. The process is modelled as a nonlinear impulsive system in [11], where the addition of glycerol and alkali is assumed to be in an impulsive form. For this system, the corresponding parameter identification problem was investigated in [11,12]. Furthermore, by taking the concentration of 1,3-PD at the terminal time as the objective function, a dynamic optimization problem was discussed in [13]. However, in reality, glycerol and alkali are added continuously. Thus, the fed-batch process is modelled as a nonlinear multistage system in [14]. Again, taking the concentration of 1,3-PD at the terminal time as the objective function, dynamic optimization problems involving the nonlinear multistage system were discussed in [14–16]. However, time-delays are ignored in the nonlinear systems mentioned above. In fact, like most real systems, fed-batch process is also influenced by time-delays. For this, a nonlinear multistage time-delay system was proposed in [17], where the corresponding parameter identification problem was also discussed. More recently, many important results obtained from the optimization of 1,3-PD production processes are summarized in [18]. However, only one objective function is involved in these optimization problems, meaning that they are single-objective optimization (SOO) problems.

In this paper, we model the 1,3-PD fed-batch process as a nonlinear switched time-delay system with free terminal time. By taking both maximization of 1,3-PD productivity and minimization of consumption rate of substrate as the objectives, we then present a MOO problem involving this nonlinear switched time-delay system with free terminal time and subject to continuous state inequality constraints, where the feeding rate of glycerol, switching instants between batch and feeding modes, and duration of the fermentation process are regarded as the decision variables. As pointed out in [19–21], it is cumbersome to solve this free time optimization problem numerically, because numerical integration of the dynamic system must be conducted over a variable time interval at each optimization iteration. Thus, we introduce a time-scaling transformation [21] to convert the free time MOO problem into an equivalent one with fixed terminal time. However, unlike the case involving delay-free optimization problem, this time-scaling transformation causes the involving dynamic system to become a new switched system with variable time-delay. For the transformed MOO problem, it is conceptually different from a SOO problem. A key characteristic of a MOO problem is that the optimality is characterized by a set of solutions, called Pareto set, denoting the trade-offs between the competing objectives [22]. A solution is said to be Pareto optimal, if there is no other solution with better values of both objectives. Hence, when moving from one Pareto solution to another, any improvement in one objective can only occur with the worsening of at least one other. To generate the Pareto set of the MOO problem, two different approaches are often used [23]. The first approach, which is known as a scalarization method, transforms a MOO problem into a sequence of parametric SOO problems. By varying the parameters of the method involved, a representation of the Pareto set is obtained. This approach includes the classic convex weighted sum (CWS) [24] and normal boundary intersection (NBI) [25]. The second approach is referred to as a vectorization method. It utilizes heuristic optimization methods, such as genetic algorithm [26] and particle swarm optimization [27], to generate the Pareto set directly from the multi-objective formulation. Note that, for the scalarization approach, gradient-based deterministic optimization routes can be combined with to find (at least locally) optimal solutions for large-scale and highly constrained MOO problems in a fast and efficient way [28]. Consequently, such scalarization approach has been extensively used to solve MOO problems in biochemical processes [29–32].

To solve the MOO problem considered in this paper, we transcribe the equivalent MOO problem into a sequence of SOO problems by using the CWS and the NBI methods. It should be noted that the existing single-objective solvers, including those solvers mentioned in [29–32], only deal with problems involving ordinary differential systems and thus cannot be used to solve the resulting SOO problems, which involve switched time-delay systems. Furthermore, it is well known that variable switching times pose a significant challenge for conventional numerical optimization techniques [33–35]. To overcome this challenge, an extended version of the time-scaling transformation in [21] is typically used to map the variable switching times to fixed time points in a new time horizon. However, this extended time-scaling transformation is not applicable to switched time-delay systems [36]. For these reasons, we develop a new single-objective solver to solve the resulting SOO problems. On the one hand, by employing the constraint transcription technique [37], we approximate the continuous state inequality constraints by constraints in canonical form. On the other hand, we derive the gradients of the objective functions and the constraint functions with respect to the decision variables. On this basis, the CWS and the NBI methods in conjunction with the new gradient-based single-objective solver are used to solve the MOO problem, respectively. A numerical example is used to verify the effectiveness of the solution approach. Numerical results show that the NBI method is more favourable than the CWS method.

The rest of the paper is organized as follows. Section 2 gives the nonlinear switched time-delay system for describing the fed-batch process. Section 3 presents the MOO problem and its equivalent form. The numerical solution methods for the