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Studying various optimal control problems in biodiesel production in a batch reactor under uncertainty

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HIGHLIGHTS

- ▶ Various optimal control problem encountered in biodiesel production reactor.
- ▶ Used novel approach to solve the stochastic optimal control problem.
- ▶ Uncertainties in feed composition is considered.
- ▶ Significant improvement in profitability with the stochastic optimal control problem as compared to base cases.

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ABSTRACT

The optimal control problem encountered in biodiesel production can be formulated using various performance indices, namely, maximum concentration, minimum time, and maximum profit. The problems involve determining optimal temperature profile so as to maximize these performance indices. This paper presents the formulations of these optimal control problems and analyzes the solutions. Optimal control problems involve the solution of partial or second order differential equation depending on the method used, resulting in difficult tasks to solve due to their mathematical representation. This difficulty becomes more challenging when uncertainty in any parameter is considered. It has been shown that the application of maximum principle in optimal control problems provides the same results but its formulation avoids the solution of second order or partial differential equations. In this work, we use the maximum principle to solve the problems in the deterministic case. Further, we consider uncertainty in the feed composition and their effects on the optimal control solution.

1. Introduction

Biodiesel is generally manufactured using batch reactors [1,2]. Some advantages are their flexibility and they are often preferred when feedstock availability is limited (e.g. seasonal demand). Biodiesel (methyl ester) is one of the most well-known examples for alternative energy and it is also renewable and domestic resource with an environmentally friendly emission profile [3]. This biofuel is derived from vegetables oils (e.g. soybean oil) and it is produced by transesterification reaction with an alcohol (e.g. methanol). Several factors that can affect the process in terms of yield have been investigated. Among of these factors, the most relevant are: the alcohol ratio, catalyst concentration, reaction temperature, and reaction time. Ref. [4] has an excellent summary of important aspects of biodiesel production. The economic performance of batch processes is determined by the supply of raw material, design of the heating/cooling system (meaning energy requirements), productivity, and the time required to achieve the productivity of the reaction. When analyzing the economic estimation of biodiesel production, it has been found that the most relevant factor of the total manufacturing cost is the raw material, specifically, the feedstock, since corresponds to around 80 to 90% of the total estimate production cost [5–7]; another important factor is the energy cost which compromises 5% of the total cost. The percentage of energy distribution in each unit operation of the biodiesel process was also studied by [7]. They found that, although most energy was consumed by methanol recovery with 66% of the total energy consumption, the reactor consumed 17% of the energy. On the other hand, [2] compared the performance of batch with continues reactors for biodiesel production from different feedstock. In their study, they found that a single CSTR was not capable of achieving the same productivity of batch reactor and demands an absurdly large residence time to

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maintain the productivity. To compensate the loss in productivity caused by the implementation of continuous reactors, they proposed some alternatives, such as, the use of CSTRs in series, the increase the catalyst concentration or the use of two reactors with half size of a single CSTR but this arrangement required enormous sizes. However, these alternatives did not favor the total manufacturing costs. For these reasons batch reactors are commonly used to produce biodiesel. Therefore, it is important to optimize the performance of this unit operation and is the focus of current endeavor.

Optimal control problems are defined in the time domain and their solutions require establishing an optimal operation policy that maximizes or minimizes a performance index. This optimal operation policy is obtained using dynamic optimization techniques. Due to the dynamic nature of the decision variables, optimal control problems are much more difficult to solve compared to normal optimization where the decision variables are scalars. Optimization in batch processes can lead to different types of problems depending on the objective of the process. For instance, in batch distillation there are maximum concentration problems [8,9], minimum time problems [10] and maximum profit problems [11,8]. On the other hand, papers [12–16] present optimal control problems for batch reactors. In general, these examples address the optimization problems to achieve the theoretical optimal temperature profile since it provides useful information for designing and controlling the reaction process.

In this paper, we study three optimal control problems in a batch reactor for biodiesel production: maximum concentration of methyl ester (MCP), the minimum reaction time (MTP), and the maximum profit problem (MPP). The purpose is to find a temperature control policy that can change with time using the dynamic optimization. To solve optimal control problems, direct and indirect methods can be used [17]. When direct methods are used, the problem can be discretized into partial or full discretization depending on the level of discretization. In this case, dynamic and NLP methods can be employed; however, since these types of problem are large, they require large-scale NLP solvers and most of the time they need good initial values to converge. Besides, discretization methods cannot be used in stochastic systems. We propose an alternative approach that avoids the use of these large-scales NLP solvers. As a result, the MCP and MTP illustrated in this paper are founded on the maximum principle theory, and the approach is based on the Steepest Ascent of Hamiltonian, also shown in [18]. Furthermore, the MPP is solved using an algorithm that combines the maximum principle and NLP techniques [19]. This algorithm is an efficient approach which avoids the solution of the two-point boundary value problem that results in the pure maximum principle or in the solution of the partial differential equations for the pure dynamic programming formulation.

Optimal control problems become more challenging when variability or uncertainty is considered. In biodiesel production, there are inherent uncertainties that have a significant impact on the product quantity, quality and process economic. For example, uncertainties with respect to the model parameters (e.g. kinetic parameters), uncertainties in the input variables, and uncertainties in the initial conditions such as feed composition variability. Later is considered as uncertainty factor since the percentage and type of triglycerides in soybean oil varies considerably. Thus, the triglyceride composition existing in soybean contains five types of hydrocarbon chains which are: tripalmitin, tristearin, triolein, trilinolein, trilinolein, and trilinolenin and their percentage in triglycerides are 6–10%, 20–30%, 2–5%, 50–60%, and 5–11%, respectively [20]. This uncertainty can be modeled using probabilistic techniques, and it can be propagated using stochastic modeling iterative procedures [21]. Therefore, optimization under uncertainty in the feed composition is also considered in this paper.

The outline of this paper is as follows. Section 2 shows the formulation and mathematical model of the optimal control problems, MCP, MTP, MPP (deterministic and stochastic case) followed by Section 3, which presents the numerical results and discussion section. Finally, Section 4 shows conclusions of this work.

2. Optimal control problem

The commonly used methods for solving optimal control problems include maximum principle, dynamic programming, and NLP algorithm with ODE discretization by collocation. However, maximum [8,11] principle is preferable because avoids the solution of partial differential equations and second order differential equations [19]. Maximum principle was proposed first by Pontryagin and coworkers [22–24] and it has been widely used to solve a variety of optimal control problems. In the following subsections, three different problems are shown for the case study of biodiesel production. All of them are solved using the maximum principle. Table 1 summarizes the optimization problems presented in this paper.

2.1. Maximum concentration problem (MCP)

The formulation of the optimal control problem for maximum concentration of biodiesel production in a batch reactor is presented in this subsection. In this problem, the objective is to maximize the concentration of methyl ester (biodiesel) by finding the best temperature profile in a given reaction time (t_f = 100 min). The numerical model for biodiesel production presented here is based on kinetic model studied by [25].

Objective function:

$$\max J = \int_{to}^{tf} k_1 C_{TG} C_A = k_2 C_{DG} C_E + k_3 C_{DG} C_A - k_4 C_{MG} C_E + k_5 C_{MG} C_A - k_6 C_{GL} C_E = C_E(t_f) \quad (1)$$

Subject to:

$$F_1 = \frac{dC_{TG}}{dt} = -k_1 C_{TG} C_A + k_2 C_{DG} C_E \quad (2)$$

$$F_2 = \frac{dC_{DG}}{dt} = k_1 C_{TG} C_A - k_2 C_{DG} C_E - k_3 C_{DG} C_A + k_4 C_{MG} C_E \quad (3)$$

$$F_3 = \frac{dC_{MG}}{dt} = k_3 C_{DG} C_A - k_4 C_{MG} C_E - k_5 C_{MG} C_A + k_6 C_{GL} C_E \quad (4)$$

$$F_4 = \frac{dC_E}{dt} = k_1 C_{TG} C_A - k_2 C_{DG} C_E + k_3 C_{DG} C_A - k_4 C_{MG} C_E + k_5 C_{MG} C_A - k_6 C_{GL} C_E \quad (5)$$

$$F_5 = \frac{dC_A}{dt} = -\frac{dC_E}{dt} \quad (6)$$

$$F_6 = \frac{dC_{GL}}{dt} = k_5 C_{MG} C_A - k_6 C_{GL} C_E \quad (7)$$

Table 1
Optimal Control problems in Biodiesel production.

Problem	Concentration	Batch time	Objective
Maximum concentration (MCP)	Free	Fixed	Maximize C_E
Minimum time (MTP)	Fixed	Free	Minimize t_f
Maximum profit (MPP)	Free	Free	Maximize profit