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.

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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 vegetable 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...
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 quality, quantity 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, 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:

\[
\max J = \int_0^{t_f} \left( C_{TG} - C_A \right) \, dt
\]

Subject to:

\[
F_1 = -k_1 C_{TG} C_A + k_2 C_{DG} C_E
\]

\[
F_2 = k_1 C_{TG} C_A - k_2 C_{DG} C_E - k_3 C_{DC} C_A + k_4 C_{MC} C_E
\]

\[
F_3 = k_3 C_{DC} C_A - k_4 C_{MC} C_E - k_5 C_{MC} C_A + k_6 C_{GL} C_E
\]

\[
F_4 = \frac{dC_{DG}}{dt} = k_1 C_{TG} C_A - k_2 C_{DG} C_E + k_3 C_{DC} C_A - k_4 C_{MC} C_E + k_5 C_{MC} C_A - k_6 C_{GL} C_E
\]

\[
F_5 = \frac{dC_{DC}}{dt} = -\frac{dC_{DG}}{dt}
\]

\[
F_6 = \frac{dC_{GL}}{dt} = k_5 C_{MC} C_A - k_6 C_{GL} C_E
\]

<table>
<thead>
<tr>
<th>Problem</th>
<th>Concentration</th>
<th>Batch time</th>
<th>Objective</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum concentration (MCP)</td>
<td>Free</td>
<td>Fixed</td>
<td>Maximize (C_{G})</td>
</tr>
<tr>
<td>Minimum time (MTP)</td>
<td>Free</td>
<td>Fixed</td>
<td>Minimize (t_f)</td>
</tr>
<tr>
<td>Maximum profit (MPP)</td>
<td>Free</td>
<td>Fixed</td>
<td>Maximize profit</td>
</tr>
</tbody>
</table>
where \( \text{C}_{\text{TG}}, \text{C}_{\text{DG}}, \text{C}_{\text{MG}}, \text{C}_{\text{E}}, \text{C}_{\text{A}}, \) and \( \text{C}_{\text{GL}} \) are the state variables and represent concentrations of triglycerides, diglycerides, monoglycerides, methyl ester, methanol, and glycerol, respectively. The initial conditions are: \( \text{C}_i(0) = [\text{C}_{\text{TG}}; 0; 0; 0; \text{C}_{\text{E}}; 0] \) [\text{mol/L}]. The reaction constant, \( k_r \), is expressed by

\[
k_r = a_e e^{- \frac{T}{T_0}}
\]

where \( T \) is the reaction temperature (control variable), \( a_e \) is the frequency factor and \( b_e = E_a/k_z \) for which \( E_a \) is the activation energy for each component \( i \) and \( k_z \) is the gas constant. The maximum concentration problem is solved in our previous paper [26] and detailed information about these constants can be obtained from this paper. This problem formulation is briefly described below.

In the maximum principle, the objective function is reformulated as a linear function in terms of final values of state variables and values of \( A_i \), where \( A_i \) represents a vector of constants, \( A_i = [0; 0; 1; 0; 0] \).

\[
\max f = \sum_{i=1}^{n} A_i C_i(t_f) = A_i^T C_i(t_f) = C_i(t_f)
\]

Moreover, the application of the maximum principle involves the addition of \( n \) adjoint variables \( z_i \), \( n \) adjoint equations and a Hamiltonian, which satisfies the following relations:

\[
\frac{dz_i}{dt} = \sum_{j=1}^{n} z_j \left( \frac{\partial F_i}{\partial C_j} \right)
\]

H \( (z_i, C_i, T, t_f) = z_i^T F_i C_i, T) \)

where \( n \) is the number of components (6 components) and \( F_i \) is the right hand side of differential equation for each component \( i \) (Eqs. (2)–(7)). Eq. (11) shows the general form to obtain the Hamiltonian. The optimal decision vector \( T(t) \) can be obtained by finding the extremum of the Hamiltonian at each time step, in other words, applying the optimality condition \( dH/dt = 0 \) The maximum principle formulation results in two point boundary value problem, where the initial conditions for the state variables \( C_i \) are known, but the conditions for the adjoint variables are only known at the final boundary. In order to obtain a solution, some iterative techniques including the shooting method and steepest ascent of the Hamiltonian method can be used [11]. To reduce the computational intensity, the optimal temperature trajectory for the system is achieved by using the approach proposed by [19,27], which uses the maximum principle and the steepest ascent of the Hamiltonian method. This algorithm starts with the initial guess of temperature, \( T(t) \). Subsequently, Eqs. (2)–(7) and the differential equations resulted from Eq. (10) are solved by employing the Runge Kutta Fehlberg method [28]. Next, the values of \( dH/dt \) at each time are computed and then the convergence criterion \( (dH/dt < \text{tolerance}) \) is verified. If the convergence criterion is not satisfied, the temperature \( T(t) \) is updated using this gradient, in such that the updated temperature profile improves the objective function, shown in Eq. (12). The value of \( M \) is a suitable constant that can be small enough so that no instability will result, or large enough for rapid convergence. Fig. 1 shows the flowchart for this algorithm.

\[
T(t)_{\text{new}} = T(t)_{\text{old}} + M \left( \frac{dH}{dt} (t) \right)
\]

2.2. Minimum time problem (MTP)

For the minimum time problem, the objective is to minimize the batch time given a final concentration. In earlier work [26], we have shown that fixing concentration of methyl ester, the reaction time needed would be 69.5% less than it was at the maximum concentration problem. The maximum concentration and minimum time problem result in similar equations for maximum principle, however, one more equation is introduced due to the new state variable \( t \) (time). The formulation for the minimum time problem is explained next.

The objective function:

\[
\min f = \int_{\text{C}(t_i)}^{\text{C}(t_f)} \frac{dt}{\text{dC}} = \frac{\text{dC}}{\text{dt}} = t(\text{C}(t_f))
\]

Subject to:

\[
\frac{dC_1}{dT} = \frac{dC_2}{dT} = \frac{dC_3}{dT} = \frac{dC_4}{dT} = F_i G_i
\]

where \( F_i \) are the differential Eqs. (2)–(7) and \( G_i \) can be written as:

\[
G_i = \frac{dt}{dC} = \frac{1}{k_1 \text{C}_{\text{TG}} \text{C}_{\text{A}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{E}} + k_3 \text{C}_{\text{DG}} \text{C}_{\text{A}} - k_4 \text{C}_{\text{MG}} \text{C}_{\text{E}} + k_5 \text{C}_{\text{MG}} \text{C}_{\text{A}} - k_6 \text{C}_{\text{GL}} \text{C}_{\text{E}}}
\]

Therefore, this problem is subject to:

\[
F_1 = \frac{dC_1}{dT} = \frac{k_1 \text{C}_{\text{TG}} \text{C}_{\text{A}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{E}}}{k_1 \text{C}_{\text{TG}} \text{C}_{\text{C}} - k_3 \text{C}_{\text{DG}} \text{C}_{\text{C}} + k_2 \text{C}_{\text{DG}} \text{C}_{\text{A}} - k_4 \text{C}_{\text{MG}} \text{C}_{\text{C}} + k_5 \text{C}_{\text{MG}} \text{C}_{\text{A}} - k_6 \text{C}_{\text{GL}} \text{C}_{\text{C}}}
\]

\[
F_2 = \frac{dC_2}{dT} = \frac{k_1 \text{C}_{\text{TG}} \text{C}_{\text{A}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{E}}}{k_3 \text{C}_{\text{TG}} \text{C}_{\text{C}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{C}} + k_3 \text{C}_{\text{DG}} \text{C}_{\text{A}} - k_4 \text{C}_{\text{MG}} \text{C}_{\text{C}} + k_5 \text{C}_{\text{MG}} \text{C}_{\text{A}} - k_6 \text{C}_{\text{GL}} \text{C}_{\text{C}}}
\]

\[
F_3 = \frac{dC_3}{dT} = \frac{k_1 \text{C}_{\text{TG}} \text{C}_{\text{A}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{E}}}{k_1 \text{C}_{\text{TG}} \text{C}_{\text{C}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{C}} + k_3 \text{C}_{\text{DG}} \text{C}_{\text{A}} - k_4 \text{C}_{\text{MG}} \text{C}_{\text{C}} + k_5 \text{C}_{\text{MG}} \text{C}_{\text{A}} - k_6 \text{C}_{\text{GL}} \text{C}_{\text{C}}}
\]

\[
F_4 = \frac{dC_4}{dT} = \frac{k_1 \text{C}_{\text{TG}} \text{C}_{\text{A}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{E}}}{k_1 \text{C}_{\text{TG}} \text{C}_{\text{C}} - k_2 \text{C}_{\text{DG}} \text{C}_{\text{C}} + k_3 \text{C}_{\text{DG}} \text{C}_{\text{A}} - k_4 \text{C}_{\text{MG}} \text{C}_{\text{C}} + k_5 \text{C}_{\text{MG}} \text{C}_{\text{A}} - k_6 \text{C}_{\text{GL}} \text{C}_{\text{C}}}
\]
In the previous section, it is shown the formulation of maximum concentration and minimum time problem using the maximum principle and the application of the steepest ascent of the Hamiltonian as the solution technique. In this section, the maximum profit problem is formulated. This problem determines the optimum batch time and concentration of biodiesel while maximizing the overall profit. Moreover, it is presented here that the maximum profit problem involves the solution of the maximum concentration problem and both the maximum concentration and minimum time problems turn out to be special cases of the maximum profit problem. The objective function for the maximum profit problem in the reaction section is represented by Eq. (26) [11].

The objective function:

$$\max J^* = M_p P_t - B_k C_t$$  \hspace{1cm} (26)

where $M_p$ is the amount of product (kg), $P_t$ is the sales value of the product ($/kg), $B_k$ is the amount of feed $F$ (kg), $C_t$ is the cost of feed ($/kg), $t$ is batch time (minutes) and $t_s$ is the setup time for each batch (minutes). It can be seen that the energy term is not considered in this equation because it does not affect in the same proportion as the raw material. As mentioned before, previous literature agreed that raw material is the largest contributor to the production cost. One possible reason is that the transesterification reactions are exothermic, which increase the temperature of the reactor by itself, so the energy required to heat the reactor is not significant.

In order to solve the complete optimization problem Eq. (26) can be reformulated as:

$$\max J^* = \frac{(\max M_p) P_t - B_k C_t}{t + t_s}$$  \hspace{1cm} (27)

where the problem is solved using two layered optimization.

Table 2 shows the information needed for profit function calculation. The amount of feed involves the quantity of methanol and triglycerides at the beginning of the reaction while the amount of product is the final concentration of methyl ester which is maximized by finding a temperature profile.

### 2.3.1. Solution method

As stated earlier, the maximum profit problem is solved as two level optimization problem. This algorithm combines maximum profit and Non-Linear Programming (NLP) techniques. The solution procedure is shown in Fig. 2. As shown in this figure, there are two levels of optimization which are: NLP optimization at the outer loop with the initial value of temperatures and the inner loop involving calculation of the maximum concentration of biodiesel. This algorithm uses the same MCP to solve the MPP. In brief, it initializes giving the initial guess of temperature and solving the MCP which consists on the system of differential equations for the states and adjoint variables so the derivative of the Hamiltonian is calculated and a new temperature profile is obtained (Level 2). The integration and calculation of the control variable $T$ continues until the specific stopping criterion is met. This Level 2 is the same as summarized in Section 2.1. Once, this criterion is reached, the optimal temperature profile and maximum value of concentration calculated at the given time go to level 1 to compute the objective function (Eq. (27)), then NLP optimization technique is used to find optimum time corresponding to the criterion that the Kuhn Tucker error is less than an allowable tolerance (allowable Kuhn Tucker error), at this stage the algorithm stops, otherwise, a new value of time is updated and the level 2 takes part in the algorithm again. This code uses SQP (Sequential Quadratic Programming) to minimize ($-J^*$). This approach was derived from the solution of optimal control problems in batch distillation presented in [19].

### 2.3.2. Stochastic maximum profit problem (SMPP)

In the previous optimal control problems, it is assumed that all the parameters and variables are known and used the deterministic model. However, this is not a realistic assumption given that there are inherent uncertainties in biodiesel feed composition. Therefore, in this section, we formulate the stochastic maximum profit problem (SMPP) for the biodiesel production. The objective function in this problem is subject to fluctuations due to the

### Table 2

<table>
<thead>
<tr>
<th>Item</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Raw materials</strong></td>
<td></td>
</tr>
<tr>
<td>Soy bean oil (triglycerides)</td>
<td>$0.62/kg</td>
</tr>
<tr>
<td>Methanol</td>
<td>$0.320/kg</td>
</tr>
<tr>
<td><strong>Product</strong></td>
<td></td>
</tr>
<tr>
<td>Biodiesel (methyl ester)</td>
<td>$1/gallon = $0.9/kg</td>
</tr>
<tr>
<td><strong>Additional parameters</strong></td>
<td></td>
</tr>
<tr>
<td>Biodiesel density</td>
<td>0.88 kg/l</td>
</tr>
<tr>
<td>Triglyceride density</td>
<td>885.446 kg/l</td>
</tr>
<tr>
<td>Methanol density</td>
<td>32.04 kg/l</td>
</tr>
<tr>
<td>Setup time ($t_s$)</td>
<td>10 min</td>
</tr>
<tr>
<td>Volume</td>
<td>10000 l</td>
</tr>
</tbody>
</table>

* Ref. [3,29].
variability in the feedstock composition. This uncertainty is represented in the variation of the soybean composition which has five triglyceride components. In a previous work of our group [30], we showed the uncertainty characterization and the stochastic simulation for the feedstock composition of soybean oil. Now the problem is to determine the expected value of the maximum profit. Then, the SMPP can be formulated as it is shown in Eq. (28).

\[ \max J_0 = \frac{\max ME}{C_0^{BoCo} + t_S/C_2} \]  

where the values of \( P_r, B_w, C_n \) and \( t_c \) are the same values shown in Table 2.

The strategy presented in Section 2.3.1 is also used for the solution of SMPP, but in this case the static uncertainties in feed

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**Fig. 2.** Combining maximum principle and NLP optimization techniques.

**Fig. 3.** Concentration profile of methyl Ester (MCP).

**Fig. 4.** Concentration profiles for all components of transesterification reaction.

**Fig. 5.** Time profile for methyl ester (MTP).
composition are propagated through the model to obtain characteristics of dynamic uncertainties in concentrations. These uncertainties are then modeled as Ito processes and the stochastic maximum principle is employed to solve the problem. For details of this method, please refer to [30].

3. Result and discussion

Results of the three optimal control problems in a batch reactor for biodiesel production are shown in this section. To start with, Fig. 3 illustrates the concentration profile of methyl ester for the MCP. Here, we are comparing the concentration values at constant temperature (base case 1: 315 K and base case 2: 323 K) with the values calculated at optimal temperature profile. It can be seen that when the optimal control temperature profile is used at 100 min of reaction time, the concentration of methyl ester reaches its maximum value (0.7927 mol/L); while employing the base cases 1 and 2, the maximum concentration is 0.7324 mol/L and 0.7829 mol/L, respectively. This change represents an increase on the concentration of methyl ester of 8.24% with respect to base case 1% and 1.25% with respect to base case 2. The increment for the second case 2 is not significant compared to the first case since the constant profile at 323 K belongs to the constant optimal profiles reported in the literature [31].

Moreover, if we fix the concentration at 0.7324 mol/L (concentration reached in base case 1) and use the optimal control approach to solve the minimum time problem, the reaction time...

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Maximum concentration</th>
<th>Minimum time</th>
<th>Maximum profit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration of methyl ester (mol/L)</td>
<td>0.7944</td>
<td>0.7324</td>
<td>0.7802</td>
</tr>
<tr>
<td>Time (min)</td>
<td>100</td>
<td>30.5</td>
<td>50</td>
</tr>
<tr>
<td>Profit ($/h)</td>
<td>103,1005</td>
<td>32.8868</td>
<td>149.8260</td>
</tr>
</tbody>
</table>

Fig. 6. Temperature profile for methyl ester. (a) Maximum concentration problem. (b) Minimum time problem.

Fig. 7. Concentration profiles for maximum profit.

Fig. 8. Temperature profile for maximum profit.

Fig. 9. Temperature profile comparison between deterministic and stochastic case.
obtained is 30.5 min which is 69.5% less than the original case (100 min). Compare with base case 2, the reduction in time represents 46%. This improvement does not affect the behavior of the other components because after 50 min of reaction time, their concentration values remain constants. This behavior can be seen in Fig. 4 where the concentration profile for all components is presented after applying the optimal control approach.

Fig. 5 shows the objective function for the three cases in the MTP. As it can be observed, after fixed the concentration of methyl ester to 0.7324 mol/L, the minimum reaction time reached is around 30.6 min when optimal control approach is applied, while in base cases 1 and 2 their minimum time is reached at 100 and 54 min, respectively. This confirms the results obtained from the MCP, concluding that this problem gives the same results as the MTP.

Temperature profile with respect to time for the case of MCP is shown in Fig. 6a while Fig. 6b shows the same profile with respect to concentration of methyl ester for the MTP. The first figure presents how temperature increases up to 336 K at minute 16th and then starting to decrease until 330 K at minute 30.5th. This behavior is also reflected in the concentration profile (Fig. 2) where most part of the reaction occurs in the beginning since this reaction is favored by the increase of temperature [32]. On the other hand, Fig. 6b shows a different temperature profile. In this case, the temperature decreases until 326 K and then it reached a value of 342 K at final concentration of methyl ester (0.7324 mol/L). Although, the optimal control profiles shown in this figure for the two optimal control problems are significantly different, their results are similar showing that this problem has multiple solutions.

Fig. 7 compares the concentration profile of methyl ester using optimal control problem with maximum profit as the objective function with the base cases. It can be seen that at 50 min of time, there is an increase of methyl ester concentration of 25.56% (base case 1) and 8.50% (base case 2). Moreover, if we compute the profit values in the MCP and MTP using Eq. (26) and compare these values with the profit value found in the MPP, there is an increment of 45.32% and 355.58%, respectively; this information is summarized in Table 3. The results show that the MPP, which combines the maximum concentration and minimum time problem, gives better results than employing the problems individually. The optimal temperature profile for MPP is presented in Fig. 8. As it is observed, this optimal profile has higher values of temperature compare to the MCP profile (Fig. 6a). This situation evidences what it is shown in Fig. 7, where the production of methyl ester is favored since it can produce more of methyl ester at the same time if constant profiles are used.

Another objective of this paper was to show how the uncertainty in the feed composition affects to MPP. Fig. 9 presents the optimal temperature profile comparison between deterministic and stochastic case. Although three curves are shown in this figure, the dashed curve is the smoothed version of the stochastic temperature profile. It is observed two noticeable differences, one is that the temperature profile from the stochastic cases (both) maintains higher values after minute 16th, and second, the stochastic case finishes earlier than deterministic case, i.e. around 5 min earlier. These two characteristics are reflected in the optimal profit value. As shown in Table 4, when the variability in the feed composition is considered and stochastic modeling is carried out under uncertainties, it has been found that there is an improvement of 6.68% in the stochastic case as compared to the deterministic case and a very significant improvement compare with the two base cases. Therefore, applying optimal control under uncertainty in the feed composition in biodiesel production (batch reaction section) can provide a better reaction time to produce the same amount of biodiesel. In other words, the SMPP gives 9.992 $/h more than MPP (deterministic case) and 148.163 $/h and 76.951 $/h more than base case 1 and 2, respectively. It can be also seen that the profit value using both the original temperature profile and the smoothed curve are presented in this table, and their values do not have significant difference. However, the smoothed temperature profile is preferred since the ease to implement the control into the process.

### 4. Conclusions

The article presented three optimal control problems encountered in biodiesel production. These problems involved determining optimal temperature profile so as to maximize or minimize performance indices, namely, concentration, time and profit. For the maximum concentration and minimum time problem, the maximum principle along with the steepest ascent of the Hamiltonian method was used as the solution technique. It was shown that the solution of these two problems results in similar equations for maximum principle. While in the maximum profit, the solution technique used was based on combining the maximum principle and NLP techniques. It was shown that the solution of maximum profit involves the solution of maximum concentration in the inner loop and minimum time problem in the outer loop. The maximum profit found was 149.826 $/h. The Simulation results indicated that the maximum profit problem gives better results than using the maximum concentration and minimum time problem individually. We also considered variability and uncertainty in feed composition inherent in biodiesel production. The maximum profit problem became expected profit problem. Again stochastic maximum principle and NLP optimization techniques are used to solve this problem. It has been found that the stochastic maximum profit problem provides 6.7% improvement over the deterministic problem and significantly greater improvement over the base cases.

### References


