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Modeling the Effects of Temperature in Enzymatic Biodiesel Synthesis of Jatropha Oil: An Optimal Control Approach

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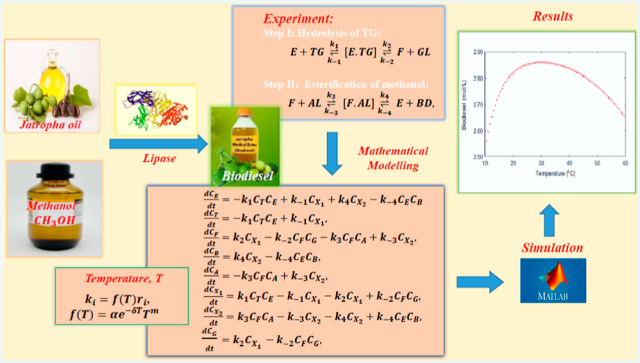
ABSTRACT: Biodiesel, an alternative to diesel, is produced through the enzymatic transesterification of vegetable oil or animal fats. Enzymatic transesterification of oil is gaining more importance, as this method possesses no such disadvantages that are associated with the chemical process. Temperature is the most important factor in enzymatic transesterification for biodiesel synthesis. In this study, a mathematical model is developed to understand the effects of temperature on the enzymatic transesterification of *Jatropha curcas* oil. Reaction rates are expressed as a function of temperature using an appropriate function, and the effects of temperature on the overall enzymatic system are investigated using the mathematical model. A suitable temperature is determined using the mathematical model, keeping the other reaction conditions unchanged that gives maximum yield. Furthermore, an optimal control problem (OCP) is formulated to identify the temperature control strategy that maximizes the biodiesel yield while minimizing production costs. Simulated outcomes obtained from the mathematical model are analogized with the experimental results to make them acceptable. The optimal profile of temperature is determined from the developed OCP, which maximizes the biodiesel yield.



INTRODUCTION

Biodiesel is a type of alternative fuel made from renewable sources such as vegetable oils, animal fats, and recycled cooking oils.[1] It is used in diesel engines in its pure form (B100). It can also be used combined with petroleum diesel.[2] Its importance is increasing as the petroleum sources are decreasing day by day, also, the negative impacts of petroleum-based engines on the environment.[3,4] Biodiesel is produced from less expensive feedstock such as nonedible Jatropha oil to reduce the coat of biodiesel production.[5,6]

Biodiesel is obtained using a process known as transesterification. It includes the reaction of vegetable oils or animal fats with an alcohol and a catalyst. The enzyme may be a chemical or enzymatic compound (generally lipase). The chemical catalytic process gives many side reactions and makes the process complicated. Also, the requirement of high temperature makes this process costly.[7] The use of lipase (as an enzyme catalyst) in biodiesel production offers several advantages over traditional chemical catalysts, such as milder reaction conditions, higher yields, and reduced waste generation.[8] Lipases are enzymes that can break down fats and oils into their parts, making them useful in the production of biodiesel.[9] The alcohol (usually methanol) and lipase are added to the oil or fat in a reactor vessel. The reaction mixture is then stirred and maintained at a specific temperature and pH to allow the lipase to catalyze the conversion of the oil or fat into biodiesel. When the reaction is completed, the produced biodiesel is separated from the byproduct (glycerol). The amount of biodiesel yield depends on the reaction parameters such as reaction time, molar ratio, stirrer rotation, temperature, etc.[10,11] Thus, among the reaction measures, temperature is one of the important factors that is the main focus of this study.

The effects of different reaction parameters on the enzymatic transesterification process have been studied by researchers. Mirosława et al.[11] have prepared biodiesel from soybean oil by enzymatic catalysis using both hydrolysis and esterification reactions and achieved 94% yield of biodiesel. Suhendra et al.[12] have studied the synthesis of biodiesel using transesterification of *Terminalia cattapa* L. kernel oil in the presence of ethanol. They have observed the effect of reaction parameters such as reaction time (3−7 h), temperature (35−60 °C), enzyme loading (0.1−0.3 g), and substrate molar ratio (oil to ethanol as 1:1−1:3). Authors reported an 83.9% yield of biodiesel under optimum. Lee et al.[13] optimized the enzymatic synthesis of

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biodiesel through the transesterification of canola oil and methanol in high-pressure carbon dioxide using response surface methodology, employing a 5-level-5-factor central composite rotatable design that was used to evaluate the effects of temperature, pressure, enzyme loading, substrate molar ratio, and reaction time on the conversion to biodiesel by transesterification.

Among the reaction parameters, temperature plays a critical role in enzymatic transesterification reactions, where lipase enzymes are commonly used as catalysts. Like all enzymes, lipases have an optimal temperature range at which they exhibit maximum catalytic activity.[14] This optimal temperature varies depending on the specific lipase enzyme and its source (e.g., microbial- or plant-derived). Also, increasing the temperature generally increases the reaction rate in enzymatic transesterification up to a point. This is because higher temperatures provide more kinetic energy to the reacting molecules, leading to more frequent collisions and an increased enzymatic activity. Temperature also affects the stability of the enzyme.[15] While increasing the temperature initially enhances activity, excessive heat can denature the enzyme, causing loss of its catalytic function. Therefore, maintaining the temperature within an optimal range is crucial to sustaining the enzyme activity over time. Temperature influences the solubility of the substrates and products in the reaction mixture. In some cases, higher temperatures can improve substrate solubility, which may enhance enzymatic efficiency by facilitating better interactions between the enzyme and substrates. Enzyme kinetics, such as substrate binding, catalytic turnover rate, and affinity, are temperature-dependent. Temperature changes can alter these kinetic parameters, affecting the overall efficiency and specificity of the enzymatic transesterification process.[16]

Mathematical models can be developed to predict and optimize the biodiesel production process. The development of mathematical models for enzymatic biodiesel production can lead to the more efficient and cost-effective production of biodiesel. These models can be used to optimize the reaction parameters and predict the yield and quality of biodiesel produced under different conditions, leading to improved process control and increased production efficiency. The optimization process can be carried out using experimental methods, mathematical modeling, and process simulation and should be based on the specific requirements of the production process.

A few mathematical model-based studies on enzymatic biodiesel synthesis are available in the literature. In refs[17] and[18], kinetic models for lipase-catalyzed biodiesel production from transesterification of waste cooking oil were formulated and analyzed. A mathematical modeling-based study for the enzymatic biodiesel synthesis from different feedstock can be seen in ref 19. Only a few research articles using mathematical models using ordinary differential equations are available in the literature.[20,21]

Optimal conditions for enzyme-catalyzed transesterification are essential for the maximum production of biodiesel. Application of mathematical modeling and optimal control theory in a reacting system is useful for minimizing the cost of production and maximizing the yield.[22−24] Optimization of biodiesel production from vegetable oil through response surface methodology, anaerobic digestion, and artificial neural networking has been studied by researchers.[25,26] Among the reaction parameters, temperature is the most important factor that directs the speed of the reaction.[28] An optimal temperature is important to both speed up the enzyme activity and speed up the transesterification reactions.

Basir et al.[21] have formulated a mathematical model and studied the impact of stirring on mass transfer and biodiesel yield. They also formulated an optimal control problem (OCP) for maximum biodiesel synthesis taking stirring as the controlling agent. In chemical catalytic biodiesel synthesis, the effect of temperature and its optimal control was studied in ref 30. But effects of temperature on biodiesel production using lipase as a catalyst have not been studied yet using any mathematical model. Also, the cost-effectiveness of the transesterification process by finding optimal temperature profiles remains to be explored. Thus, in this article, a mathematical model is established, and an optimal control system is obtained by finding the optimal temperature profile for the enzyme-catalyzed transesterification for both the maximum yield and the cost-effectiveness of the process.

This research aims to establish a mathematical model using ordinary differential equations for enzymatic biodiesel synthesis and to study the effect of temperature on the biodiesel yield and enzyme activity. We considered the fact that reaction rates depend on the reaction temperature and proposed a temperature-dependent function for the reaction rates (with proper justification) to study the role of temperature on biodiesel productivity. Moreover, we have formulated an OCP for maximum biodiesel yield from enzymatic transesterification considering temperature as the controlling parameter. Using optimal control theory, an optimal temperature profile is obtained for the cost-effective and maximum production of biodiesel.

The paper is structured as follows: Section Mathematical Model Derivation introduces the mathematical model and key assumptions and section Optimal Control Problem provides the formulation of the OCP. Simulated results of the proposed model with and without control are provided in section Numerical Simulations. The key findings from the simulations are discussed in section Discussion. The study is concluded with section Conclusions, which highlights the primary findings of the investigation.

MATHEMATICAL MODEL DERIVATION

In this section, a mathematical model for enzymatic biodiesel synthesis has been proposed with proper assumptions. The following hypotheses are used to formulate the mathematical model for the dynamics of transesterification of *Jatropha curcas* oil:

H1: Enzymatic biodiesel synthesis of *Jatropha curcas* oil can be considered as a two-step process,[7] namely, step 1: the hydrolysis of Jatropha oil to produce free fatty acid (FFA), and step 2: esterification of alcohol (methanol) with fatty acid to obtain fatty acid methyl ester, i.e., biodiesel.

H2: Triglycerides (TG) and FFAs (F) are the main components of Jatropha oil. Both components are converted to ester using a two-step transesterification process in the presence of lipase (enzyme). First, hydrolysis of triglycerides (TG) gives FFA (F) and releases the glycerol through the formation of the complex X_1 (i.e., E.TG). In the second step, esterification of methanol (AL) with FFA (F) gives the main product, i.e., biodiesel, and free enzyme (E) is reverted back through the formation of the second complex X_2 (F.AL).[18,21] All the mechanistic steps of transesterification reactions for biodiesel production are given by the diagram stepwise as follows:

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Step 1: hydrolysis of TG

$$\mathrm{E} + \mathrm{TG} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} [\mathrm{E.\ TG}] \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} \mathrm{F} + \mathrm{GL} \tag{1}$$

Step 2: esterification of methanol

$$\mathrm{F} + \mathrm{AL} \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} [\mathrm{F.\ AL}] \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} \mathrm{E} + \mathrm{BD} \tag{2}$$

Here, k_1, k_1, k_2, and k_2 are the rate constants in the first step while complex X_1 is formed. Also, k_3 and k_3 and k_4 and k_4 are the rate constants for the second step while complex X_2 is formed and biodiesel is obtained. Clearly, k_1, k_2, etc. are forward, whereas k_{-1}, k_{-2}, etc. are backward reaction rates as the reactions are reversible.

H3: Considering the impact of temperature on reaction rates, we take the following temperature-dependent form of the reaction rates

$$k_i = f(T) r_i, \qquad i = 1, -1, 2, -2, 3, -3, 4, -4 \tag{3}$$

where

$$f(T) = \alpha\, \mathrm{e}^{-\delta T} T^m \tag{4}$$

Here, α, δ, and m are constants. Also, r_i is the value of the reaction rate constant k_i at ideal reaction conditions. Values of r_i are given in Table 1.

In the following remark 0.2, we have provided the detailed justification of taking the temperature-dependent form of the reaction rates as given in (3).

H4: Denoting the concentration of TG, E, F, X_1, X_2, AL, BD, and GL as C_T, C_E, C_F, C_{X_1}, C_{X_2}, C_A, C_B, and C_G, respectively, and from the above assumptions with the above reaction mechanism followed by the law of mass action, the following model system is obtained

$$\begin{aligned}
\frac{\mathrm{d}C_\mathrm{E}}{\mathrm{d}t} &= -k_1 C_\mathrm{T} C_\mathrm{E} + k_{-1} C_{\mathrm{X}_1} + k_4 C_{\mathrm{X}_2} - k_{-4} C_\mathrm{E} C_\mathrm{B} \\
\frac{\mathrm{d}C_\mathrm{T}}{\mathrm{d}t} &= -k_1 C_\mathrm{T} C_\mathrm{E} + k_{-1} C_{\mathrm{X}_1} \\
\frac{\mathrm{d}C_\mathrm{F}}{\mathrm{d}t} &= k_2 C_{\mathrm{X}_1} - k_{-2} C_\mathrm{F} C_\mathrm{G} - k_3 C_\mathrm{F} C_\mathrm{A} + k_{-3} C_{\mathrm{X}_2} \\
\frac{\mathrm{d}C_\mathrm{B}}{\mathrm{d}t} &= k_4 C_{\mathrm{X}_2} - k_{-4} C_\mathrm{E} C_\mathrm{B} \\
\frac{\mathrm{d}C_\mathrm{A}}{\mathrm{d}t} &= -k_3 C_\mathrm{F} C_\mathrm{A} + k_{-3} C_{\mathrm{X}_2} \\
\frac{\mathrm{d}C_{\mathrm{X}_1}}{\mathrm{d}t} &= k_1 C_\mathrm{T} C_\mathrm{E} - k_{-1} C_{\mathrm{X}_1} - k_2 C_{\mathrm{X}_1} + k_{-2} C_\mathrm{F} C_\mathrm{G} \\
\frac{\mathrm{d}C_{\mathrm{X}_2}}{\mathrm{d}t} &= k_3 C_\mathrm{F} C_\mathrm{A} - k_{-3} C_{\mathrm{X}_2} - k_4 C_{\mathrm{X}_2} + k_{-4} C_\mathrm{E} C_\mathrm{B} \\
\frac{\mathrm{d}C_\mathrm{G}}{\mathrm{d}t} &= k_2 C_{\mathrm{X}_1} - k_{-2} C_\mathrm{F} C_\mathrm{G}
\end{aligned} \tag{5}$$

with initial concentration

$$\begin{aligned}
&C_\mathrm{E}(0) = C_{\mathrm{E}_0}\ \mathrm{mol/L}, \qquad C_\mathrm{T}(0) = C_{\mathrm{T}_0}\ \mathrm{mol/L}, \\
&C_{\mathrm{X}_1}(0) = 0, \qquad C_\mathrm{F}(0) = 0 \\
&C_\mathrm{A}(0) = C_{\mathrm{A}_0}\ \mathrm{mol/L}, \qquad C_\mathrm{T}(0) = C_{\mathrm{T}_0}, \\
&C_{\mathrm{X}_2}(0) = 0 \\
&C_\mathrm{B}(0) = 0, \qquad C_\mathrm{G}(0) = 0
\end{aligned} \tag{6}$$

Remark 1. At the beginning of the reaction, only triglycerides (TG), alcohol (AL), and enzyme (E) lipase are present in the system. Thus, the concentrations of the other reactants are assumed to be zero.

Remark 2. In maximum biochemical reactions, the reaction rate of the process catalyzed by enzyme increases as the temperature is increased and gets its maximum value at a temperature. However, if the temperature is raised further, the rate starts to decrease because the enzyme is denatured and loses its functionality. Each enzyme has its zone of comfort, or optimal temperature range, within which it functions properly. During the formation of biodiesel, the performance of the enzyme is maximum at 30−35 °C because the enzyme can its structure at that particular temperature allowing it to break down the complex molecule efficiently. Above 30−35 °C, the enzyme structure begins to break down (denature) since at higher temperatures intra- and intermolecular bonds are broken as the enzyme molecules acquire even more kinetic energy. At a particular pH, the reaction also has an optimum temperature and at that temperature, the enzyme function is highest.

Table 1. Values of Parameters Used for Numerical Simulation[21]

parameters	value (unit)
r_1	7.5128 mol L^{-1} h^{-1}
r_{-1}	0.1147 h^{-1}
r_2	0.1032 h^{-1}
r_{-2}	0.0988 mol L^{-1} h^{-1}
r_3	1.937 mol L^{-1} h^{-1}
r_{-3}	0.0323 h^{-1}
r_4	1.9230 h^{-1}
r_{-4}	0.0011 mol L^{-1} h^{-1}

According to ref 31, enzymatic synthesis of biodiesel is usually carried out at a temperature between 20 and 60 °C. The

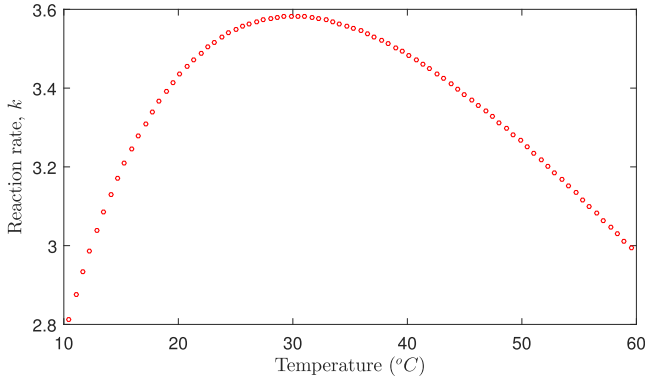

Figure 1. Temperature effect on the reaction rate is shown using the relation (4) and α = 0.3, δ = 0.02, and m = 0.6.

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researchers of the work in ref[32] have shown that the optimal temperature for enzymatic biodiesel synthesis is in the range of 30−35 °C. In ref[33], the calculation of enzyme stability over repeated batch reactors was made by immobilizing the enzymes with *n*-hexane. Around 90% of the enzyme activity was present after seven synthesis cycles, and nearly 100% yield of biodiesel was attained at 30 °C reaction temperature.

In Figure 1, the effects of temperature on the reaction rate are shown using eqs 4 and 3. This figure shows that the reaction rate increases with temperature but decreases when temperature crosses the critical value of 30 °C. Thus, this temperature is favorable for biodiesel synthesis using lipase. Also, at very high temperatures, the enzyme (generally lipase) becomes less active. Thus, the function form of reaction rate as proposed in (4) is appropriate for the present study.

From the above discussion and results, we supposed the temperature-dependent forms of the reaction rates as given in (4) and (3).

OPTIMAL CONTROL PROBLEM

The OCP is proposed here to obtain an optimal profile of temperature in terms of a control parameter that can give maximum biodiesel yield and also minimizes the cost of production.

We have introduced the control variable $u(t)$ in the system which manages the temperature input at any time t. It works on the reaction rates as the rates are a function of temperature. The values of $u(t)$ lie in the range $0 \le u(t) \le 1$. When the control takes the value of $u(t)$ unity, we mean the maximum use of the control corresponding to the temperature for which the value of the reaction rate is maximum. Also, when $u(t)$ is zero implied that temperature is not required, that means, the reaction is completed.[21,22]

Incorporating the control parameter $u(t)$, the state system is obtained as follows

$$\begin{aligned}
\frac{dC_E}{dt} &= -uk_1C_TC_E + uk_{-1}C_{X_1} + uk_4C_{X_2} - uk_{-4}C_EC_B\\
\frac{dC_T}{dt} &= -uk_1C_TC_E + uk_{-1}C_{X_1}\\
\frac{dC_F}{dt} &= uk_2C_{X_1} - uk_{-2}C_FC_G - uk_3C_FC_A + uk_{-3}C_{X_2}\\
\frac{dC_B}{dt} &= uk_4C_{X_2} - uk_{-4}C_EC_B\\
\frac{dC_A}{dt} &= -uk_3C_FC_A + uk_{-3}C_{X_2}\\
\frac{dC_{X_1}}{dt} &= uk_1C_TC_E - uk_{-1}C_{X_1} - uk_2C_{X_1} + uk_{-2}C_FC_G\\
\frac{dC_{X_2}}{dt} &= uk_3C_FC_A - uk_{-3}C_{X_2} - uk_4C_{X_2} + uk_{-4}C_EC_B\\
\frac{dC_G}{dt} &= uk_2C_{X_1} - uk_{-2}C_FC_G
\end{aligned} \tag{7}$$

with the initial reaction conditions as given in (6).

For later use, system (7) is rewritten as below

$$\frac{dC_i}{dt} = f_i(C_1, C_2, ..., C_8, u, t), \qquad i = 1, 2, ..., 8 \tag{8}$$

Now, we formulate the objective cost function. Here, the aim is to maximize the biodiesel yield and also to minimize the cost of production. Thus, we assume the objective cost function $J(u)$ as defined below

$$J[u(t)] = \int_{t_0}^{t_f} [P_1u^2(t) + P_2v^2(t) - QC_B^2(t)]dt \tag{9}$$

In eq 9, the parameter $P(>0)$ is the weight constant due to the benefit of the cost of production and the constant $Q > 0$ is used as the penalty multiplier. We had to calculate the optimal control parameter $u^*(t)$ so that the cost $J(u^{(t)})$ is minimized. Mathematically, this is written as

$$\begin{aligned}
&J(u^*) = \min J(u): u \in U\\
&\quad \text{where } U \text{ is the admissible control set and}\\
&U = \{u(t): u(t) \text{ is measurable, } 0 \le u(t) \le 1\\
&t \in [t_i, t_f]\}
\end{aligned} \tag{10}$$

The optimal value of $u(t)$, i.e., $u^*(t)$, is obtained with the help of Pontryagin's maximum principle.[27,29] According to the maximum principle, we need to define a Hamiltonian as

$$H = P_1u^2(t) + P_2v^2(t) - QC_B^2(t) + \sum_{i=1}^{9} \xi_i f_i \tag{11}$$

where ξ_i, $i = 1, 2, ..., 8$ are adjoint variables and f_j, $j = 1, 2, ..., 8$ are the right side of the state system (7), e.g., $f_1 = -k_1C_TC_E + k_{-1}C_{X_1} + k_4C_{X_2} - k_{-4}C_EC_B$, etc.

Optimal System. We have the following theorem that characterizes the optimality of the system.

Theorem 1. If the given optimal control $u^*(t)$ and the solution (C_E^*, C_T^*, C_F^*, C_B^*, C_A^*, $C_{X_1}^*$, $C_{X_2}^*$, and C_G) of the corresponding system (7) minimize the functional $J(u)$ over the set U, then there exists adjoint variables ξ_i, $i = 1, 2, ..., 8$ which satisfy the following adjoint equations

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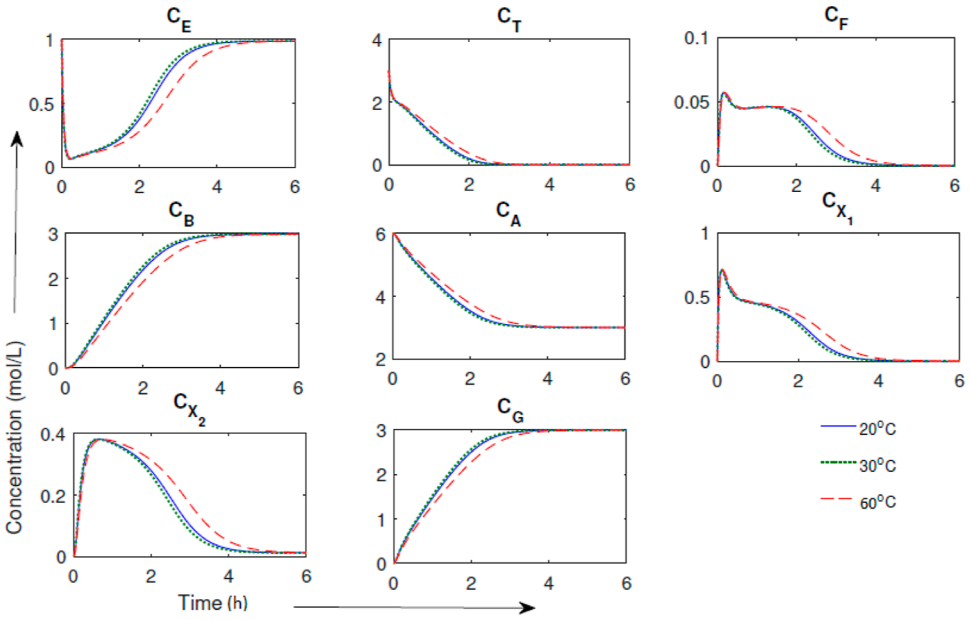

Figure 2. Numerical solutions of the model system (5) are plotted for three temperatures ($T = 20$, 30, and 60). Values of the rate constants r_i, $i = 1, -1, 2, -2, 3, -3, 4, -4$ are taken from Table 1.

$$\frac{d\xi_1}{dt} = k_1 C_T(\xi_1 - \xi_6) + k_{-4} C_B(\xi_4 - \xi_7)$$

$$\frac{d\xi_2}{dt} = k_1 C_E(\xi_1 + \xi_2 - \xi_6)$$

$$\frac{d\xi_3}{dt} = k_3 C_A(\xi_5 - \xi_7) + k_{-2} C_G(\xi_3 - \xi_6)$$

$$\frac{d\xi_4}{dt} = 2QC_B + \xi_4 k_{-4} C_E - \xi_7 k_{-4} C_E$$

$$\frac{d\xi_5}{dt} = k_3 C_F(\xi_5 - \xi_7)$$

$$\frac{d\xi_6}{dt} = k_{-1}(\xi_6 - \xi_2) + k_2(\xi_6 - \xi_3)$$

$$\frac{d\xi_7}{dt} = -k_4\xi_4 - k_{-3} + k_{-3}\xi_7$$

$$\frac{d\xi_8}{dt} = k_{-2}(\xi_8 - \xi_6) \tag{12}$$

with boundary conditions as $\xi_i(t_f) = 0$ *for* $i = 1$ to 8. Furthermore, the optimal control $u^*(t)$ can be written as

$$u^*(t) = \max\left(0, \min\left(1, \frac{\sum \xi_i f_i}{2P_2}\right)\right) \tag{13}$$

Proof. The Hamiltonian (11) can be rewritten as

$$H = Pu^2(t) + r_s u\left[\xi_1 C_B\left(1 - \frac{C_B}{B_{max}}\right)\right] + \text{terms without } u(t) \tag{14}$$

According to the maximum principle,[34] the unconstrained optimal control variable $u(t)$ satisfies

$$\frac{\partial H}{\partial u} = 0 \tag{15}$$

Thus, from (14) and (15), we have

$$\frac{\partial H}{\partial u} = 2Pu + r_s C_B\left(1 - \frac{C_B}{B_{max}}\right)(\xi_4) = 0$$

Simplifying, we obtain

$$u(t) = \frac{-r_s\left[\xi_4 C_B\left(1 - \frac{C_B}{B_{max}}\right)\right]}{2P} \tag{16}$$

Due to the boundedness of the standard control, the compact form of $u^*(t)$ takes the following form

$$u^*(t) = \max\left(0, \min\left(1, \frac{-r_s\left[\xi_4 C_B\left(1 - \frac{C_B}{B_{max}}\right)\right]}{2P}\right)\right) \tag{17}$$

Pontryagin's maximum principle states that the adjoint variables satisfy

$$\frac{d\xi_i}{dt} = -\frac{\partial H}{\partial C_i} \tag{18}$$

where $C_i \equiv (C_E, C_T, C_F, C_B, C_A, C_{X_1}, C_{X_2}, C_{C_3}, C_G)$, i.e., $\xi_1 = C_E$, $\xi_2 = C_T$, etc. The necessary conditions of the optimal control $u(t)$ are

$$H(C_i(t), u^*(t), \xi_i(t), t) = \min_{u \in U}(H(C_i, u, \xi_i, t)) \tag{19}$$

So, the relation (18) gives the adjoint eq 12. The boundary conditions for the adjoint system are $\xi_i(t_f) = 0$, $(i = 1, 2, ..., 8)$.

Remark 3. The state system (7) along with the adjoining system (12) and optimal control given in (17) represents the optimal system. Clearly, the optimal system is a two-point boundary problem. We solve the state system as an initial value

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problem, and the adjoint system as a boundary value problem, in MATLAB using the *bve4c* solver.

NUMERICAL SIMULATIONS

In this section, numerical simulations of the proposed model system without control and with optimal control are plotted and discussed. The effect of temperature on the biodiesel yield was studied using the simulated results. Simulation of the OCP system gives the optimal temperature profile for the cost-effective maximum production of biodiesel.

Numerical simulation of the model system (5) has been performed in Figure 2, and the dynamics of the system (without control) and the effects of temperature on the yield have been studied by taking different values of T (T = 20, 30, and 60 °C). Figure 2 shows the dynamics of the reacting system for three different temperatures taking a fixed molar ratio (C_{A_0}/C_{T_0} = 4:1) and with a fixed reaction time of 3 h. It is observed that complexes X_1 and X_2 direct the synthesis of biodiesel. Complex X_2 gives the desired product (biodiesel). This figure indicates that the enzymatic transesterification of Jatropha oil depends on the stability of the formed intermediate complexes. The stability of complex X_1 is higher than complex X_2 because the transformation from the complex X_1 (E.TG) to glycerol (GL) requires more time while breaking the ester bond in triglyceride (TG) molecules than the ester bond formation between acid and alcohol in X_2 to produce ester. From Figure 2, the yields of biodiesel can also be compared for different temperatures. From this, it is evident that the concentration of biodiesel is the maximum when the temperature is near 30 °C. A temperature higher than 30 °C gives a lower yield.

In Figure 3, when the temperature is increased from 10 to 60 °C, the biodiesel yield is plotted taking a fixed molar ratio, (4:1).

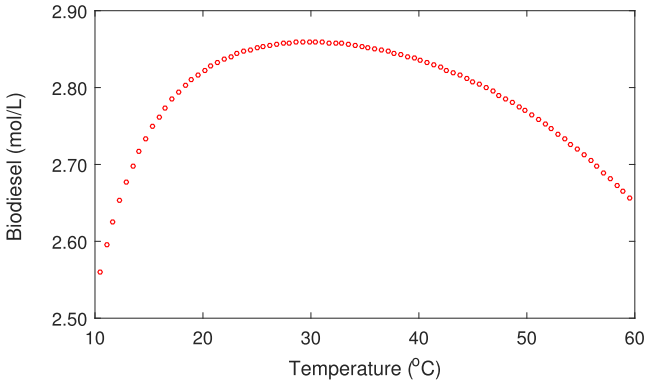

Figure 3. Concentration of biodiesel is shown as a function of temperature (T) using the model system (5). Final reaction time is taken as 3 h.

It is clear from this figure that temperature has given a positive effect on biodiesel yield, but the temperature should not cross the optimal value of 30 °C as the yield is decreased when the temperature is higher than 30 °C. From this figure, the temperature 30 °C can be recommended as optimal for enzymatic biodiesel production from Jatropha oil.

The solution of the optimal system (see remark 0.3) is plotted in Figures 4−6 taking a fixed temperature T = 40 °C. Figure 4 shows that optimal temperature produces the highest biodiesel yield within 3 h.

The optimal control parameter $u^*(t)$ is plotted as a function of time t in Figure 5. The result of this figure is the most

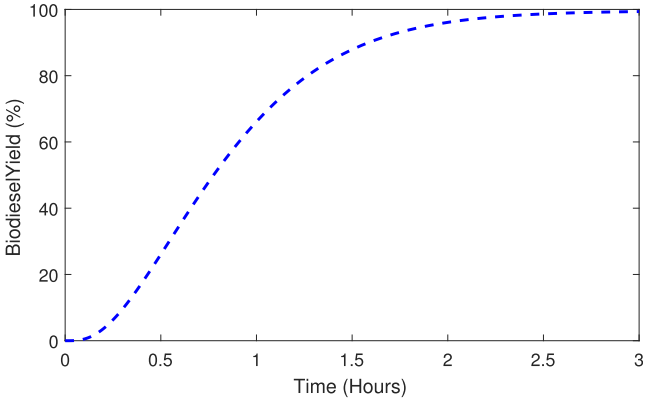

Figure 4. Concentration of optimal biodiesel yield is shown simulating the OCP.

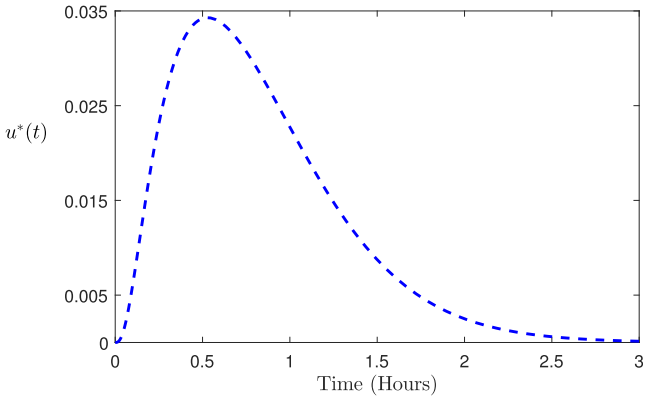

Figure 5. Optimal profile of the optimal control $u^*(t)$ is plotted.

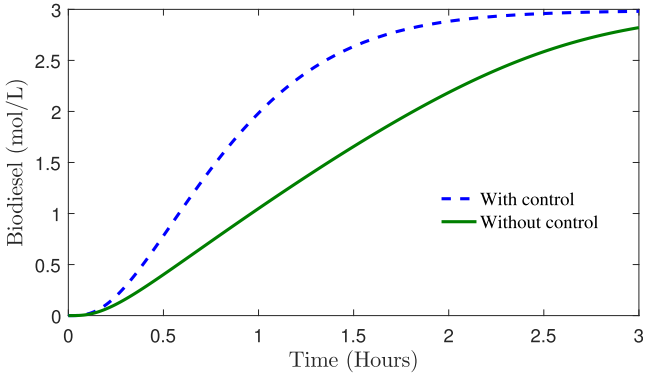

Figure 6. Comparison between the two concentrations of biodiesel: (i) with control and (ii) without control (with fixed temperature, 30 °C).

important for this research. This figure shows that initially, high control is needed, meaning that a high temperature is required but comparatively, temperature should be decreased gradually after 1 h of reaction. After 3 h, no control is required, denoting that the reaction is terminated.

The production of biodiesel is more favorable in enzymatic transesterification reactions using the optimum temperature profile $T^*(t)$. In Figure 6, concentrations of biodiesel are compared for two cases: (i) with an optimal control and (ii) without control. More biodiesel yield can be obtained using optimal temperature than applying a fixed temperature (40 °C). The optimal control approach reduces reaction time and the cost of production is also minimized as the cost functional $J(u)$ is

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minimum for optimal control $u^*(t)$.[27,29] Applying optimal control on the temperature, an almost 100% yield can be achieved from *Jatropha curcas* oil by a lipase-catalyzed transesterification process.

DISCUSSION

In this article, a mathematical model is developed to study the effect of temperature on enzymatic biodiesel synthesis from *Jatropha curcas* oil. The influence of temperature on transesterification, in terms of yield, is determined using the proposed mathematical model, keeping the other reaction conditions such as the molar ratio of substrates (triacylglycerides/alcohol), reaction time, etc. as fixed for this reaction. Optimization theory has been applied to minimize the cost and maximize the yield by finding an optimal profile of temperature.

Results show that the reaction rate increases with the temperature as desired. After a certain temperature, it decreases. Using this fact, we have proposed temperature-dependent profiles for the rate constants. We have seen that biodiesel yield is increased as the temperature is increased from 20 to 30 °C. But with temperature beyond 30 °C, the yield is decreased significantly. At higher temperatures, the enzyme does not revert completely due to the loss of activity at higher temperatures.

From the OCP, an optimal control profile for temperature is obtained in terms of the optimal control parameter $u^*(t)$ to get the optimal biodiesel yield, keeping the production cost at a minimum level. Optimization of the enzymatic output establishes that maximum biodiesel can be obtained within 3 h of reaction time. Almost 100% biodiesel yield can be achieved using optimal temperature with minimum cost.

CONCLUSIONS

Temperature is an important factor in the enzymatic biodiesel synthesis. However, there is no such mathematical model or relation that can help in studying the effects of temperature on biodiesel yield. Thus, we have expressed the reaction rate constant as a function of temperature and consequently developed a mathematical model for studying the effects of temperature on the enzymatic system. Moreover, using optimal control theory, we have determined an optimal temperature profile in the form of the optimal control parameter for maximum yield with a minimum cost of production.

In summary, the proposed model is functional. The impact of temperature on biodiesel yield can be studied using the mathematical model. From this research, it can be recommended that temperature significantly influences the enzymatic transesterification process by affecting enzyme activity, reaction rates, reaction times, and overall process efficiency. This study shows that when temperatures are higher than 30 °C, enzyme catalysts do not work properly and the yield of biodiesel is also lowered. Thus, the temperature should be carefully applied to confirm that the reaction proceeds efficiently while reducing the chance of enzyme deactivation. Optimization of temperature in enzymatic biodiesel synthesis can lead to higher output and diminish the cost of biodiesel production.

ASSOCIATED CONTENT

Data Availability Statement

The experimental result data supporting this article are from previously reported studies and data sets, which have been cited.

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Notes

The authors declare no competing financial interest.

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