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**Optimal Control on Temperature to Maximize Biodiesel
Production from Jatropha Curcas Oil:
A Mathematical Approach**

Fahad Al Basir¹ and Priti Kumar Roy²

^{1,2}Centre for Mathematical Biology and Ecology,
Department of Mathematics, Jadavpur University, Kolkata- 700032, India

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Abstract. *Biodiesel is considered as one of the most possible renewable energy and alternative of petrol based diesel fuel. It is produced through transesterification of vegetable oils. Jatropha Curcas oil is considered as the feedstock for biodiesel production. Production of biodiesel through transesterification of Jatropha oil significantly depends on four parameters such as reaction time, temperature, oil to alcohol molar ratio and stirrer speed. In this research article, We consider a system of biodiesel production with no initial mass transfer resistance i.e. optimal stirring is given to the system. Then, we show the effect of molar ratio and temperature on the system in a fixed stipulated time. Finally, we find an optimal control profile for smooth production of biodiesel using maximum principle. Numerical simulation is also done to fulfill the analytical results.*

Key words: Biodiesel, Jatropha Curcas Oil, Transesterification, Reaction Parameter, Optimal Control, Maximum Principle.

² Corresponding Author: Priti Kumar Roy, E-mail: pritiju@gmail.com, +913324146584, Ph. No. +919432095603.
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1 Introduction

In today's world, petroleum is clearly the most important energy source. It providing more than half of the world's power, as well as being a basic material used in the manufacture of fertilizer, synthetic fibers, plastics and synthetic rubber. Demand is ever increasing worldwide, yet petroleum resources are finite and non-renewable. Concerns about dwindling supplies, its unstable and rising cost and environmental problems have motivated researchers more extensively to seek alternative, renewable energy sources.

Fatty acid methyl esters (FAME) collectively known as biodiesel. Biodiesel is obtained from renewable vegetable oils such as *Jatropha curcas* oil and can be used as an alternative fuel for diesel [1]. Biodiesel is a non-polluting, locally available, accessible, sustainable and reliable fuel obtained from renewable sources such as vegetable oils or animal fats by transesterification [2]. One of the alternative ways of biodiesel productions is produce from *Jatropha Curcas* plant. *Jatropha* is one of such non-edible oils, which has an estimated annual production potential of 200 thousand metric tons in India and it can be grown in waste land [3].

Transesterification or alcoholysis is commonly employed to convert vegetable oil to biodiesel in the presence of catalyst. A number of processes have been developed for biodiesel production involving either chemical catalyst like acids, bases, both liquid and heterogeneous or biological catalyst like immobilized or free enzyme [4]-[10]. There are many research articles where alkaline transesterification for biodiesel production is investigated [10]-[12], where raw material with a high water or free fatty acid (FFA) content needs pretreatment with an acidic catalyst in order to esterify FFA [13], [14].

Transesterification is influenced by different parameters such as molar ratio between alcohol and triglycerides, reaction time, catalyst concentration, and reaction temperature [15]. For instance, an excess of alcohol can guarantee the complete conversion of fats or oils to esters in a short time. Usually, the molar ratio employed is 6:1 in a presence of alkali catalyst. On the other hand, the conversion rate of fatty acids esters increases with time and it has been found that the yield reaches a maximum at the reaction time of less than 90 min. Effects of molar ratio of alcohol and catalyst concentration play a vital role in biodiesel yield [16], [17]. An excess of reaction time will decrease the yield due to the backward reactions and it will cause more fatty acids to form soap. The catalyst also plays an important role since its concentration increases the conversion of triglyceride, which increases the yield of biodiesel [17], [18].

Effects of temperature and the reaction time are investigated in case of biodiesel production from *Jatropha Curcas* oil. With increase in reaction temperature, conversion to biodiesel is also increased. But after a certain level of temperature (above 50°C), biodiesel yield is decreased [19], [20]. Thus, temperature is one of the most important control variables in biodiesel production. So, an optimal temperature profile is required for optimum production of biodiesel.

Transesterification of *Jatropha* oil suffers mass transfer limitation problem initially. This problem can be avoided by applying stirring on the system. Roy et al. [21], successfully shows the effect of stirring on transesterification by formulating a mathematical model. It is shown that 600 rpm stirring is optimal to avoid mass transfer problem. In this research article, we have considered the model [21] and wish to show the effect of temperature on biodiesel yield. Also, we have determined a molar ratio which is suitable for biodiesel production. Then using optimal control theory, an optimal temperature profile is determined so that maximum amount of biodiesel can be obtained from transesterification of *Jatropha Curcas* oil in a fixed reaction time.

2 The Mathematical Model

In a laboratory, biodiesel can be produce by reacting triglycerides with methanol. The reactions happen in three reversible steps. During the course of reaction of triglycerides and methanol, some intermediates (diglyceride and monoglyceride) are considered. Therefore, we consider here that three consecutive reversible reactions occurred during the production of biodiesel. The schematic explanation of the reaction is



Overall reaction : $TG + 3AL \rightleftharpoons 3BD + GL$. For the formulation of mathematical model of transesterification reaction system, the following assumptions are adopted [21]

i) since there is little water (0.2% w/w) in the reaction mixture and negligible free fatty acids are detected in the system, so it is assumed that only three consecutive reactions occurred [22],

ii) The catalyst used in this study has no positional specificity, so it acts concurrently on any acyl-group,

iii) As mixing intensity in the reaction system directs the mass transfer limitations between phases, so mechanical stirring is one of the most effective factors in transesterification reaction. Here, we use k_s as the mass transfer rate constant and its unit is min^{-1} and the term has been defined as below [21]:

$$k_s = \frac{a}{(1 + \exp(-b(N - c)))} \quad (2.2)$$

where N is the speed of stirrer and a, b and c are constants. The term is used in our model by the expression $k_s x_B (1 - \frac{x_B}{B_{max}})$. Here x_B denotes the concentration of biodiesel and B_{max} represents maximum biodiesel production in an ideal situation which is defined as system having no mass transfer resistance. The unit of x_B, B_{max} is represented by moles/L. The term has been used logistically because with the increase of stirrer speed, the mass transfer resistance decreases and beyond a certain stirrer speed the mass transfer resistance is negligible. This is also evident from experimental observations of other workers [23].

We denote the concentration of triglycerides, diglycerides, monoglycerides, methanol (alcohol) and glycerol by x_T, x_D, x_M, x_A, x_G respectively and by applying the laws of mass action and above assumptions, we obtain the following six differential equations.

$$\begin{aligned} \frac{dx_B}{dt} &= k_1 x_T x_A - k_2 x_D x_B + k_3 x_D x_A - k_4 x_M x_B + k_5 x_M x_A - k_6 x_G x_B \\ &\quad + k_s x_B (1 - \frac{x_B}{B_{max}}), \\ \frac{dx_T}{dt} &= -k_1 x_T x_A + k_2 x_D x_B, \\ \frac{dx_D}{dt} &= k_1 x_T x_A - k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B, \\ \frac{dx_M}{dt} &= k_3 x_D x_A + k_4 x_M x_B - k_5 x_M x_A + k_6 x_G x_B, \\ \frac{dx_A}{dt} &= -k_1 x_T x_A + k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B - k_5 x_M x_A + k_6 x_G x_B, \\ \frac{dx_G}{dt} &= k_5 x_M x_A + k_6 x_G x_B. \end{aligned} \quad (2.3)$$

Here $k_1, k_2, k_3, k_4, k_5, k_6, B_{max}$ and k_s are positive constants.

Here k_1, k_3, k_5 are forward reaction rates and k_2, k_4, k_6 are backward reaction rates. The dependency of reaction rate constants on the temperature $k_i, (i = 1$ to 6), is expressed by the Arrhenius equation [20]:

$$k_i = \alpha_i e^{-\frac{\beta_i}{T}}. \quad (2.4)$$

T is the reaction temperature, α_i is the frequency factor, and

$$\beta_i = \frac{E\alpha_i}{R}.$$

in which $E\alpha_i$ is the activation energy for each component and R is the universal gas constant. The values of α_i and β_i are given in Table 1.

3 The Optimal Control Problem

Optimal control is useful for controlling a system. Generally, we solve these type of problems by finding the time dependent profiles of the control variable to optimize a particular performance. Calculus of variations, dynamic programming, Pontryagin Minimum Principle and Maximum Principle are used to solved these problems. Using optimal control theoretic approach, we try to find a temperature profile for biodiesel production. To solve this problem, the maximum principle is used [24].

The objective function for this problem is taken in the following manner,

$$\text{maximize } J = x_B(t_f),$$

subject to the following system

$$\begin{aligned} \frac{dx_B}{dt} &= k_1 x_T x_A - k_2 x_D x_B + k_3 x_D x_A - k_4 x_M x_B + k_5 x_M x_A - k_6 x_G x_B \\ &\quad + k_5 x_B \left(1 - \frac{x_B}{B_{max}}\right), \\ \frac{dx_T}{dt} &= -k_1 x_T x_A + k_2 x_D x_B, \\ \frac{dx_D}{dt} &= k_1 x_T x_A - k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B, \\ \frac{dx_M}{dt} &= k_3 x_D x_A + k_4 x_M x_B - k_5 x_M x_A + k_6 x_G x_B, \\ \frac{dx_A}{dt} &= -k_1 x_T x_A + k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B - k_5 x_M x_A + k_6 x_G x_B, \\ \frac{dx_G}{dt} &= k_5 x_M x_A + k_6 x_G x_B. \end{aligned} \quad (3.1)$$

The initial conditions for this system are,

$$x_T(0) = x_{T_0}, \quad x_B(0) = 0, \quad x_D(0) = 0, \quad x_M(0) = 0, \quad x_A(0) = x_{A_0}, \quad x_G(0) = 0.$$

The system (3.1) can be written in compact form as

$$\frac{dx_i}{dt} = f_i(t, x, T), \quad (3.2)$$

where f_i ($i=1, \dots, 6$) are the right sides of system (3.1) and x_i ($i=1, \dots, 6$) are the state variables representing the concentration of each components x_B , x_T , x_D , x_M , x_A , and x_G and temperature (T) is the control parameter.

We are using the maximum principle and in this method Hamiltonian is taken as

$$H(\xi_i(t), x_i(t), T) = \sum_{i=1}^6 \xi_i f_i(x, T), \quad i = 1, 2, \dots, 6, \quad (3.3)$$

where ξ_i ($i = 1, \dots, 6$) are the adjoint variables. The adjoint equations are given by the following relation

$$\frac{d\xi_i}{dt} = - \sum_{j=1}^6 \xi_j \left(\frac{\partial f_j}{\partial x_i} \right), \quad i = 1, \dots, 6. \quad (3.4)$$

From equation (3.3) we get the Hamiltonian as

$$\begin{aligned} H &= \xi_1 \left\{ k_1 x_T x_A - k_2 x_D x_B + k_3 x_D x_A - k_4 x_M x_B + k_5 x_M x_A - k_6 x_G x_B \right. \\ &\quad \left. + k_5 x_B \left(1 - \frac{x_B}{B_{max}}\right) \right\} + \xi_2 (-k_1 x_T x_A + k_2 x_D x_B) \\ &\quad + \xi_3 (k_1 x_T x_A - k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B) \\ &\quad + \xi_4 (k_3 x_D x_A + k_4 x_M x_B - k_5 x_M x_A + k_6 x_G x_B) \\ &\quad + \xi_5 \{-k_1 x_T x_A + k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B \\ &\quad - k_5 x_M x_A + k_6 x_G x_B\} + \xi_6 (k_5 x_M x_A + k_6 x_G x_B) \end{aligned} \quad (3.5)$$

From equation (3.4) and (3.5) we obtain the adjoint system as

$$\begin{aligned}
 \frac{d\xi_1}{dt} &= -\xi_1 \left\{ -k_2x_D - k_4x_M + k_6x_G - k_5 \left(1 - \frac{2x_B}{B_{max}} \right) \right\} + \xi_2 k_2x_D \\
 &\quad + \xi_3 (-k_2x_D - k_3x_A + k_4x_M) - \xi_4 (-k_4x_M + k_6x_G) + \xi_5 k_2x_D + \xi_6 k_6x_G \\
 \frac{d\xi_2}{dt} &= -\xi_1 k_1x_A + \xi_2 k_1x_A - \xi_3 k_1x_A + \xi_5 k_1x_A \\
 \frac{d\xi_3}{dt} &= \xi_1 (k_2x_B - k_3x_A) - \xi_2 k_2x_B + \xi_3 (k_2x_B + k_3x_A) - \xi_4 k_3x_A - \xi_5 (k_2x_B - k_3x_A) \\
 \frac{d\xi_4}{dt} &= -\xi_1 (-k_4x_B + k_5x_A) - \xi_3 k_4x_B - \xi_4 (-k_4x_B - k_5x_A) - \xi_5 k_4x_B - \xi_6 k_5x_A \\
 \frac{d\xi_5}{dt} &= -\xi_1 (k_1x_T + k_3x_D + k_5x_M) + \xi_2 k_1x_T - \xi_3 (k_1x_T - k_3x_D) \\
 &\quad - \xi_4 (k_3x_D - k_5x_M) - \xi_5 (-k_1x_T - k_3x_D - k_5x_M) + \xi_6 k_6x_B \\
 \frac{d\xi_6}{dt} &= \xi_1 k_6x_B - \xi_4 k_6x_B + \xi_6 k_6x_B.
 \end{aligned}
 \tag{3.6}$$

The boundary conditions for the adjoint variable are $\xi_1(t_f) = 1$, and $\xi_i(t_f) = 0$ for $i=2, 3, 4, 5, 6$. We solve The system of equation (8) by backward integration along with RKF method using RKF45 solver. Since, temperature (T) is given in implicit form, the optimal temperature $T^*(t)$ can be obtained by maximizing the Hamiltonian (H) numerically. Using the optimality condition we have,

$$\frac{dH}{dT^*} = 0
 \tag{3.7}$$

Here, T is in implicit form. Rate constants are taken in Arrhenius form as $k_i = \alpha_i e^{-\frac{\beta_i}{T}}$. Thus, the derivative of Hamiltonian is calculated in the following manner. We apply the total derivative concept to the equation (3.5) and then the derivative of the Hamiltonian is calculated by the following equation

$$\begin{aligned}
 \frac{dH}{dT} &= \sum_{i=1}^6 \frac{\partial H}{\partial x_i} \frac{dx_i}{dT} + \sum_{i=1}^6 \frac{\partial H}{\partial \xi_i} \frac{d\xi_i}{dT} \\
 &= \sum_{i=1}^6 \frac{\partial H}{\partial x_i} \theta_i + \sum_{i=1}^6 \frac{\partial H}{\partial \xi_i} \phi_i.
 \end{aligned}$$

Here $\theta_i = \frac{dx_i}{dT}$ and $\phi_i = \frac{d\xi_i}{dT}$ and the values of θ_i and ϕ_i can be calculated by the following properties

$$\frac{d}{dT} \left(\frac{dx_i}{dt} \right) = \frac{d}{dt} \left(\frac{dx_i}{dT} \right) = \frac{d\theta_i}{dt}
 \tag{3.8}$$

and

$$\frac{d}{dT} \left(\frac{d\xi_i}{dt} \right) = \frac{d}{dt} \left(\frac{d\xi_i}{dT} \right) = \frac{d\phi_i}{dt}
 \tag{3.9}$$

The differential equations for θ_i and ϕ_i are given below in compact form as

$$\frac{d\theta_i}{dt} = F(x_i, \theta_i, T),
 \tag{3.10}$$

$$\frac{d\phi_i}{dt} = G(x_i, \phi_i, T).
 \tag{3.11}$$

For example, the differential equation for θ_1 is given respectively by the following equations

$$\begin{aligned}
 \frac{d\theta_1}{dt} &= \frac{dk_1}{dT} x_T x_A + k_1 \theta_2 x_A + k_1 x_T \theta_5 - \left(\frac{dk_2}{dT} x_D x_B + k_2 \theta_3 x_B + k_2 x_D \theta_1 \right) + \\
 &\quad \frac{dk_3}{dT} x_D x_A + k_3 \theta_3 x_A + k_3 x_D \theta_5 - \left(\frac{dk_4}{dT} x_M x_B + k_4 \theta_4 x_B + k_4 x_M \theta_1 \right) + \\
 &\quad \frac{dk_5}{dT} x_M x_A + k_5 \theta_4 x_A + k_5 x_M \theta_5 - \left(\frac{dk_6}{dT} x_G x_B + k_6 \theta_6 x_B + k_6 x_G \theta_1 \right) + \\
 &\quad k_5 \left(\theta_1 - \frac{2x_B}{B_{max}} \right),
 \end{aligned}$$

and

$$\begin{aligned}
\frac{d\phi_1}{dt} = & \phi_1 k_2 x_D + \xi_1 \frac{dk_2}{dT} x_D + \xi_1 k_2 \theta_3 + \phi_1 k_4 x_M + \xi_1 \frac{dk_4}{dT} x_M + \xi_1 k_4 \theta_4 + \\
& \phi_1 k_6 x_G + \xi_1 \frac{dk_6}{dT} x_G + \xi_1 k_6 \theta_6 + \xi_1 k_5 \left(\theta_1 - \frac{2x_B \theta_1}{B_{max}} \right) + \phi_1 k_5 x_B \left(1 - \frac{x_B}{B_{max}} \right) \\
& + \phi_2 k_2 x_D + \xi_2 \frac{dk_2}{dT} x_D + \xi_2 k_2 \theta_3 + \phi_3 k_2 x_D + \xi_3 \frac{dk_2}{dT} x_D + \xi_3 k_2 \theta_3 + \\
& \phi_3 k_2 x_A + \xi_3 \frac{dk_2}{dT} x_A + \xi_3 k_2 \theta_5 - (\phi_3 k_4 x_M + \xi_3 \frac{dk_4}{dT} x_M + \xi_3 k_4 \theta_4) + \\
& \phi_4 k_4 x_M + \xi_4 \frac{dk_4}{dT} x_M + \xi_4 k_4 \theta_4 - (\phi_4 k_6 x_G + \xi_4 \frac{dk_6}{dT} x_G + \xi_4 k_6 \theta_6) + \\
& \phi_5 k_2 x_D + \xi_5 \frac{dk_2}{dT} x_D + \xi_5 k_2 \theta_3 + \phi_6 k_6 x_G + \xi_6 \frac{dk_6}{dT} x_G + \xi_6 k_6 \theta_6.
\end{aligned}$$

Finally, we solve the system of equations (3.10) numerically for θ_i with initial conditions, $\theta_i(0) = 0, i=1, \dots, 6$. On the other hand, to compute ϕ_i , we solve the system of equation (3.11) by backward integration along with RKF method with the is boundary conditions are, $\phi_i(t_f) = 0, i=1, \dots, 6$.

Table 1 Values of parameters used in numerical calculation [20], [25].

Parameters	Value	Parameters	Value
α_1	3.92e7	β_1	6614.83
α_2	5.77e5	β_2	4997.98
α_3	5.88e12	β_3	9993.96
α_4	0.098e10	β_4	7366.64
α_5	5.35e3	β_5	3231.18
α_6	2.15e4	β_6	4824.87

4 Numerical simulation of the model equations:

We solved the model equations numerically in Matlab to understand the dynamical behavior of the transesterification process. Maximum Principle is used for observing the effect of control parameters in the system dynamics with the help of Hamiltonian.

In Figure 1, the system behaviour is shown at constant temperature 318 K. Initially rate of reaction for the formation of biodiesel is quite high since there is no mass transfer limitation initially as stirring (600 rpm) is applies to the system. Subsequently, concentration of triglycerides is decreasing along with declining nature for the concentration of DG and MG. After 45 minutes of reaction time, the reaction rate becomes slower and the system goes towards stability. However, after 60 min there is no significant change in concentration of biodiesel. This situation also happens with the other components (TG, MG, DG, AL and GL). It is also clear from the figure that steady state production of biodiesel is obtained within 1 hr from the start of the reaction.

Figure 2 (right panel) represents the optimum ratio of alcohol and triglycerides and it is seen from the figure that 6:1 is the ideal ratio for reaction optimization. Increase of methanol in molar ratio with respect to oil would result the increase in biodiesel yield. However, too high molar ratio of alcohol to oil (9:1) could give adverse effect on the yield of biodiesel. Because addition of large amount of methanol could slow down the separation process of esters and glycerol phases that affects the final yield of biodiesel. Mass transfer resistance may also occur which eventually could reduce the yield of esters.

Temperature dependency of biodiesel yield is presented in Figure 2 (left panel). As reaction temperature increases, yield of biodiesel is also increased. But after a certain level of temperature (above 318K), biodiesel yield is decreased and it can be identified that 318 K temperature for transesterification reaction gives maximum biodiesel. Too high temperature (such as 333 K) should be avoided because at the high temperature, alcohol vaporizes which ultimately changes optimum molar ratio of alcohol and triglycerides.

Figure 3 represents the trajectories for temperature profile, Hamiltonian derivative ($\frac{dH}{dT}$) and the biodiesel concentrations. It is observed that initially higher temperature is required for smooth biodiesel production that is also evident for experimental works. Hamiltonian

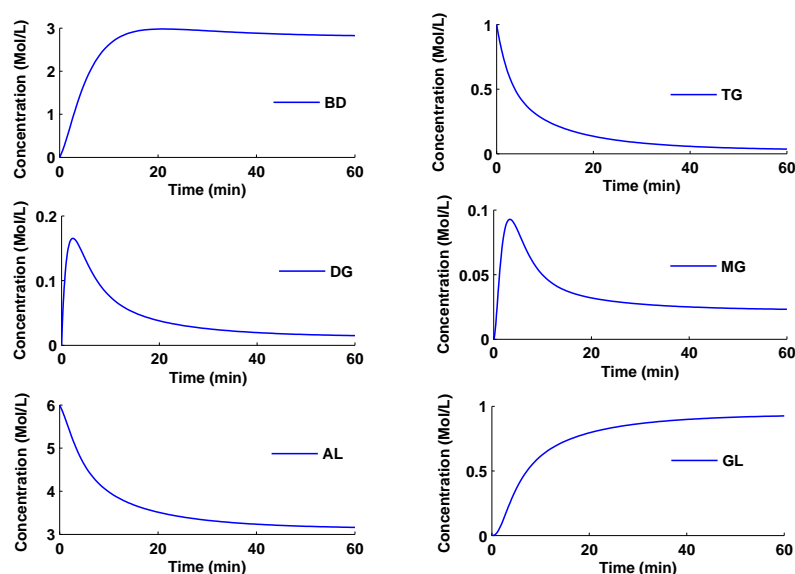


Fig. 1 Concentration trajectories at constant temperature ($318K$) for using parameters as in Table 1 taking stirrer speed $N=600$, $x_T(0) = 1$, $x_A(0) = 6$ and other parameters as in Table 1 .

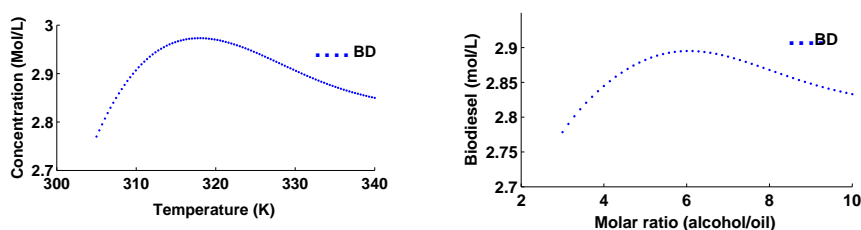


Fig. 2 Concentration of biodiesel is plotted as a function of temperature (left panel) and molar ratio (right panel) at stirrer speed $N=600$ rpm and other parameters as in Table 1.

derivative decreases with time that means temperature goes to its optimum value for maximum production of biodiesel that is indicated clearly by the Hamiltonian derivative. Figure 3 also illustrates the concentration profiles of biodiesel for two cases, case 1: with optimal temperature, and case 2: without control i.e. with fixed temperature. Here we are comparing the concentration profiles at constant temperature at 60 min of reaction time. In this figure, the effect of optimal temperature is reflected on the concentration of biodiesel. In case 1, the concentration of biodiesel at optimal control reaches its maximum value, 2.98 mol/L i.e. 99%; while in case 2, the maximum concentration is 2.75 mol/L i.e. 91% yield is obtained.

5 Discussion

In this article, we have considered a system of biodiesel production that has no mass transfer resistance. Our analysis has showed that maximum concentration of biodiesel can be obtained by introducing control on temperature. Concentration profiles of biodiesel are compared with two cases: (1) at constant temperature $318K$ and (2) at optimal temperature $T^*(t)$ K. Concentration of biodiesel is increased by 8% approximately, when the optimal control on temperature is employed. On the other hand, it is also seen that the biodiesel obtained the maximum concentration in 1 hour.

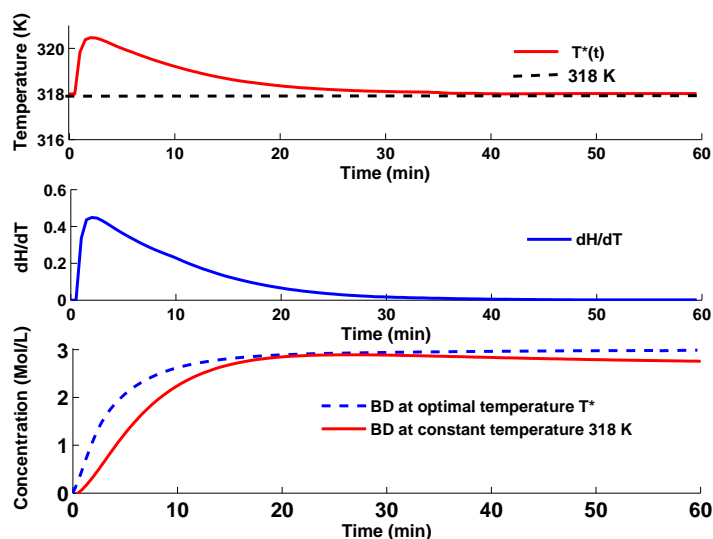


Fig. 3 Optimal concentration of biodiesel, Optimal temperature profile and derivative of Hamiltonian are plotted as a function of time at stirrer speed $N=600$ rpm, $x_T(0) = 1$, $x_A(0) = 6$ and other parameters as in Table 1.

6 Conclusion

Temperature is optimized for which maximum production of biodiesel is obtained which is suitably indicated by Hamiltonian principle. Optimal control provides improvement to the effectiveness of biodiesel production process. The article provides an idea of describing the effect of temperature for faster rate of biodiesel production. So our outcomes will help the experimental researchers for production of future fuel, which may be a possible way for the alternative energy sources for the future generations.

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