

OPTIMAL CONTROL ON SAPONIFICATION TO MAXIMIZE BIODIESEL PRODUCTION FROM JATROPHA CURCAS OIL

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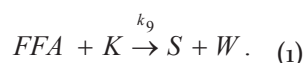
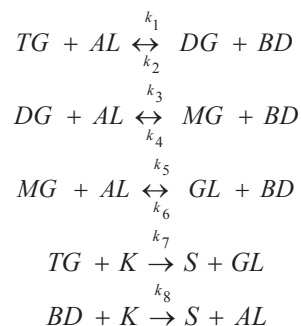
Abstract: Biodiesel is supposed to be the most demanding alternative energy sources in the future world. Maximum production of biodiesel from vegetable oils in the presence of alkaline catalyst is severely hampered by some side reactions amongst which saponification or soap formation is the most important one. Free fatty acids, produced in the oils by hydrolysis during storage, are responsible for this saponification which has a negative impact on biodiesel production. It reduces the yield of biodiesel, complicates the separation and purification procedure through emulsification. Thus, control of saponification is important to enhance smooth biodiesel production. In this research article, a mathematical model of transesterification of Jatropha Curcas oil with alcohol using alkaline catalyst is formulated. We analyze the effect of temperature, catalyst concentration, and mixing intensity on saponification during biodiesel production. Optimal control theoretic approach is applied on saponification reactions to maximize biodiesel production by alkali-catalyzed transesterification.

Keywords: Biodiesel, Jatropha Curcas Oil, Transesterification, Saponification, Control Theoretic Approach.

Introduction: Biodiesel (BD) is long chain fatty acid esters derived from vegetable oils or animal fats that can be recognised as an alternative energy sources in diesel engines[1]. There are several methods for production of BD such as esterification [2], transesterification [3] and two-step methods [4] using different vegetable oils and alcohols (AL) in presence of catalyst. Most widely used method today for BD production is transesterification of non edible vegetable oils or triglycerides (TG) with AL such as methanol, ethanol and butanol in presence of catalyst [5]. Among the non edible vegetable oils, Jatropha Curcas oil (JCO) is considered as a prominent feed stock to produce BD due to its availability and higher oil content as well as it can be cultivated in barren and waste land in simple conditions. Free fatty acids (FFA) in JCO react with the alkaline catalyst (K) to produce soap (S) through saponification reactions [6]. This reaction causes lower yield, incomplete reaction, washing difficulties and purity of BD [7]. So controlling the formation of S can minimize the difficulty in smooth production of BD. Mathematical modeling for the formation of BD from vegetable oils are available but modeling based on control approach on saponification reactions with a view to maximize biodiesel production is very few. Based on this scenario, in this research article, we formulate and analyze a mathematical model of transesterification reaction kinetics with a view to optimize BD production from high FFA JCO by reducing saponification reactions through control theoretic approach in the system kinetics.

Formulation of Control Induced Mathematical Model: Formation of BD through transesterification reaction with AL in the presence of K consists of three reversible reactions. In the first reversible step, TG reacts with AL to produce diglycerides (DG)

which further reacts with AL to produce monoglycerides (MG) in the second reversible step. Finally MG reacts with AL to produce glycerol (GL) as a byproduct. At each reaction step, one molecule of BD is produced. Side saponification reactions of TG, BD and FFA with K produces soap alongwith GL, AL and water (W) respectively which are schematically described below.



We denote the concentrations of TG, DG, MG, BD, AL, GL, K, FFA, S and W by $x_T, x_D, x_M, x_B, x_A, x_G, x_K, x_F, x_S$ and x_W respectively. B_{max} represents maximum concentration of BD. Here, k_1 to k_9 are reaction rate constants. The reaction constant, k_i , is expressed by the equation $k_i = a_i e^{\frac{-b_i}{T}}$. Here, T is the reaction temperature, a_i is the frequency factor, and $b_i = \frac{Ea_i}{R}$ in which Ea_i is the activation energy for each component and R is the universal gas constant.

The values of a_i and b_i are given in Table 1. As mixing intensity has a significant impact on the reaction optimization, we use k_s as the stirring rate and define the term as [8]: $k_s = \frac{a}{1 + \exp\{-b(N - c)\}}$ where N is the speed of stirrer and a, b and c are parameters. It is given to our model in logistic fashion by the term $k_s x_B (1 - \frac{x_B}{B_{max}})$. We apply control inputs $u_1(t)$,

reactions so that we can get more BD in each step of transesterification reaction where u_i satisfy $0 \leq u_i(t) \leq 1$. Here $u_i(t)$ represents control input with values normalized between 0 and 1 [9]. Also $u_i(t) = 1$ represents the maximal use of control and $u_i(t) = 0$ signifies no control. From the law of mass action with three control parameters taking into consideration, we have the following optimal control problem corresponding to equation (1):

$u_2(t)$ and $u_3(t)$ to minimize saponification

$$\frac{dx_B}{dt} = k_1 x_T x_A - k_2 x_D x_B + k_3 x_D x_A - k_4 x_M x_B + k_5 x_M x_A - k_6 x_G x_B - k_8 u_2 x_B x_K + k_s x_B (1 - \frac{x_B}{B_{max}}),$$

$$\frac{dx_T}{dt} = -k_1 x_T x_A + k_2 x_D x_B - k_7 u_1 x_T x_K,$$

$$\frac{dx_D}{dt} = k_1 x_T x_A - k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B,$$

$$\frac{dx_M}{dt} = k_3 x_D x_A + k_4 x_M x_B - k_5 x_M x_A + k_6 x_G x_B,$$

$$\frac{dx_A}{dt} = -k_1 x_T x_A + k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_B - k_5 x_M x_A + k_6 x_G x_B,$$

$$\frac{dx_G}{dt} = k_5 x_M x_A + k_6 x_G x_B + k_7 u_1 x_T x_K,$$

$$\frac{dx_K}{dt} = -(k_7 u_1 x_T x_K + k_8 u_2 x_B x_K + k_9 u_3 x_K x_F),$$

$$\frac{dx_F}{dt} = -k_9 u_3 x_F x_K,$$

$$\frac{dx_S}{dt} = k_7 u_1 x_T x_K + k_8 u_2 x_B x_K + k_9 u_3 x_K x_F,$$

$$\frac{dx_W}{dt} = k_9 u_3 x_F x_K. \tag{2}$$

With initial conditions: $x_B(0) = 0, x_T(0) = x_{T_0}, x_D(0) = 0, x_M(0) = 0, x_A(0) = x_{A_0}, x_G(0) = 0$.

Theoretical study of the system: Here we want to maximize bio-diesel x_B and minimize soap x_S , so that we define the objective cost function for the minimization problem as,

$$J(u_1, u_2, u_3) = \int_{t_0}^T [P u_1^2(t) + Q u_2^2(t) + R u_3^2(t) - A x_B^2(t) + T x_S^2(t)] dt \tag{3}$$

subject to the system (2). The parameters P, Q, R, A and T are the positive weight constants on the benefit of the cost of production. The benefit

is based on the minimization of cost together with maximization of biodiesel concentration. Our aim is to find out the optimal control $u^*(t) = (u_1^*(t), u_2^*(t), u_3^*(t))$ such that

$$u^*(t) = \min (J(u_1, u_2, u_3) : (u_1, u_2, u_3) \in U).$$

Here, $U = U_1 \times U_2 \times U_3$,

$$U_1 = \{u_1(t) : u_1 \text{ is measurable and } 0 \leq u_1 \leq 1, t \in [t_i, t_f]\}$$

$$U_2 = \{u_2(t) : u_2 \text{ is measurable and } 0 \leq u_2 \leq 1, t \in [t_i, t_f]\}$$

$$U_3 = \{u_3(t) : u_3 \text{ is measurable and } 0 \leq u_3 \leq 1, t \in [t_i, t_f]\}.$$

We use ‘‘Pontryagin Minimum Principle’’ [10] to find $u^*(t)$.

$$\frac{\partial H}{\partial u_i^*} = 0, i = 1, 2, 3.$$

Basically this $u^*(t)$ indicates the control on reaction parameters which reveal the temperature, mixing intensity and catalyst concentration to produce maximum production of biodiesel with suppression of saponification.

Dynamics of the optimal system: For optimal control of the system, we define the Hamiltonian as follows:

$$H = [Pu_1^2(t) + Qu_2^2(t) + Ru_3^2(t) - x_B^2(t) + Tx_S^2] + \sum_{i=1}^{10} \xi_i f_i \tag{4}$$

where f_i 's are the right hand side of the control induced system and ξ_i are adjoint variables. The corresponding adjoint equations are given by,

$$\frac{d\xi_i}{dt} = -\frac{\partial H}{\partial x_i}, i = 1, 2, \dots, 10,$$

where $x_1 = x_B, x_2 = x_T, \dots, x_{10} = x_W$.

(5)

According to Pontryagin Minimum Principle [10], the unconstrained optimal control variables u_1^*, u_2^* and u_3^* satisfy,

Thus from (4) and (6), we have

$$u_1^*(t) = \frac{k_7 x_T x_K (\xi_2 - \xi_6 + \xi_7 - \xi_9)}{2P}, \tag{7}$$

$$u_2^*(t) = \frac{k_8 x_B x_K (\xi_1 - \xi_5 + \xi_7 - \xi_9)}{2Q}, \tag{8}$$

$$u_3^*(t) = \frac{k_9 x_F x_K (\xi_7 - \xi_8 - \xi_9 + \xi_{10})}{2R}. \tag{9}$$

Due to the boundedness of the standard control we

$$u_1^*(t) = \max(0, \min(1, \frac{k_7 x_T x_K (\xi_2 - \xi_6 + \xi_7 - \xi_9)}{2P})). \tag{10}$$

$$u_2^*(t) = \max(0, \min(1, \frac{k_8 x_B x_K (\xi_1 - \xi_5 + \xi_7 - \xi_9)}{2Q})). \tag{11}$$

$$u_3^*(t) = \max(0, \min(1, \frac{k_9 x_F x_K (\xi_7 - \xi_8 - \xi_9 + \xi_{10})}{2R})). \tag{12}$$

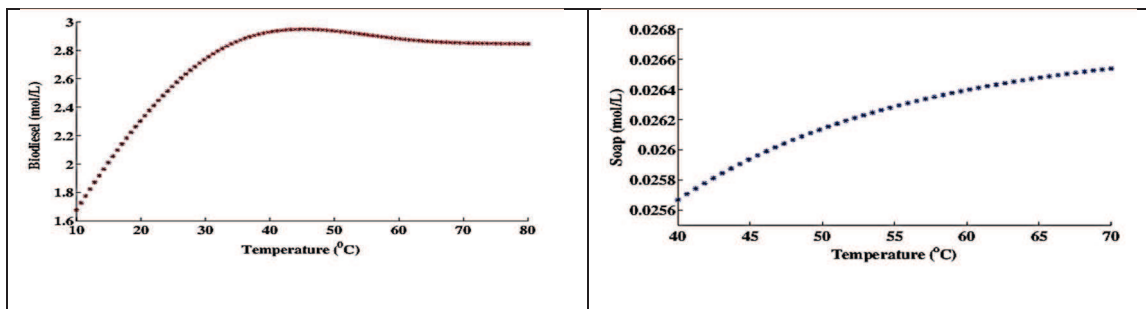


Figure 1: Effect of the temperature on biodiesel production and saponification at 600 rpm stirrer at 60 minutes of reaction.

Table 1: Values of parameters used in numerical calculation.					
Parameters	Value (Sec ⁻¹)	Parameters	Value (K ² /Sec)	Parameters	Value
a_1	3.92e7	b_1	6614.83	B_{max}	3 moles/litre
a_2	5.77e5	b_2	4997.98	a	0.12
a_3	5.88e12	b_3	9993.96	b	0.003 rpm ⁻¹
a_4	0.098e10	b_4	7366.64	c	300 rpm
a_5	5.35e3	b_5	3231.18		
a_6	2.15e4	b_6	4824.87		
a_7	3.92e7	b_7	6614.83		
a_8	5.77e5	b_8	4997.98		
a_9	5.88e11	b_9	9993.96		

Numerical Simulation: Numerical simulation has been done on the basis of analytical results. We have analysed the effect of temperature, catalyst concentration and mixing intensity at 60 minutes of reaction time. Figure 1 shows the effect of the temperature on BD production and saponification at 600 rpm stirrer speed, 6:1 methanol to oil molar ratio. It is evident from figure that the initial reaction rate increases as the reaction temperature and increase upto 50°C. After that rate of BD decreases due to excessive saponification. Thus we can take 50°C as the optimum temperature for biodiesel production.

Figure 2 reveals that more amount of catalyst produces excess soap over time which yields a lower amount of BD. So minimum amount of catalyst is required for smooth production of BD. Figure 3 shows that the maximum BD can be achieved by using a stirrer speed of 600 rpm. The higher stirring speed more than 600 rpm causes saponification which reduces the production of BD. Thus 600 rpm is the optimum stirrer speed to get maximum BD.

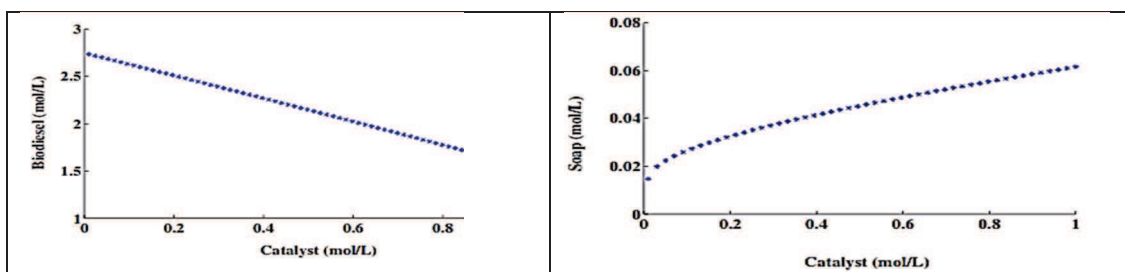


Figure 2: Effect of catalyst on biodiesel production and soap formation at 50°C and 600 rpm stirrer speed with 60 minutes of reaction.

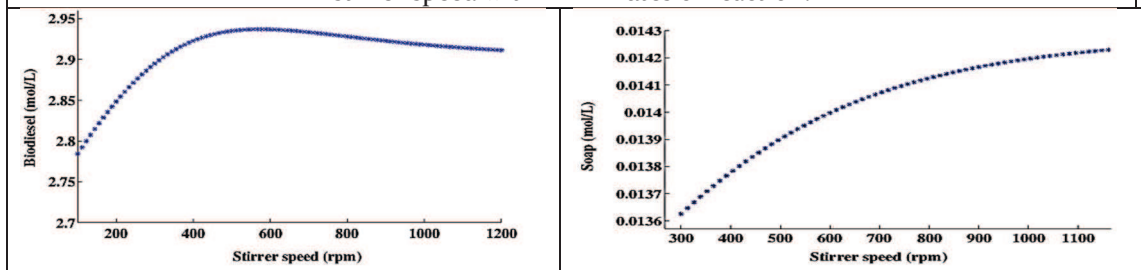


Figure 3: Effect of mixing speed on biodiesel production and soap formation at 50°C using 6:1 methanol to oil molar ratio with catalyst concentration 1.5% (w/w) of oil at 60 minutes of reaction.

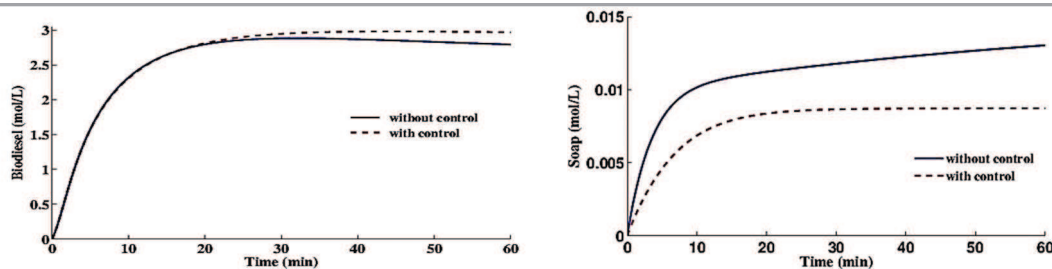


Figure 4: Concentration of biodiesel and soap with control and without control.

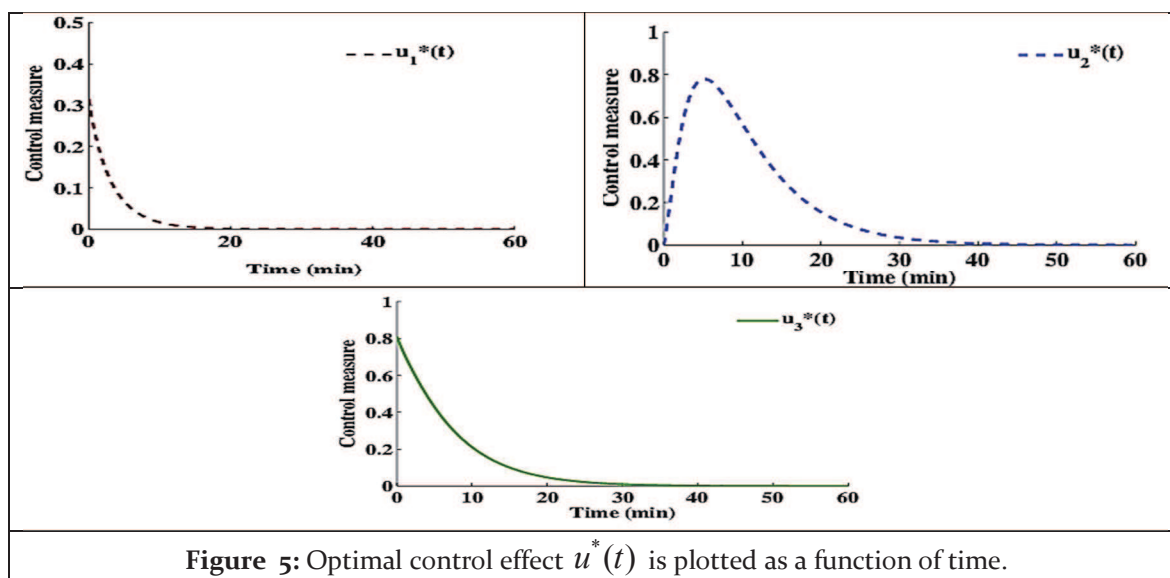


Figure 5: Optimal control effect $u^*(t)$ is plotted as a function of time.

Figure 4 represents the concentration profile of BD and S without control and with control on the system kinetics. From this figure, it is observed that the control induced system gives more production of BD alongwith reduction of saponification. Our numerical result shows that the concentration of BD at optimal level reaches its maximum value, 2.98 mole/L, while the maximum concentration is 2.795mole/L if there is no control on the system. We can achieve 6% more BD by applying control on transesterification reaction.

Figure 5 illustrates how the control parameters act on the system with respect to time. From this figure, we see that control approach is required for the initial thirty minutes of reaction by which saponification reaction is minimized and we can get the desired amount of BD.

Discussion: We have formulated and analysed a mathematical model of transesterification reaction for BD production considering saponification

reactions. Numerically we have shown that the reaction depends significantly on mixing intensity, catalyst concentration and temperature. As saponification reaction significantly reduces BD production so, applying mathematical control approach on each step saponification reaction gives smooth and optimum BD production alongwith GL as by product.

Conclusion: We suggest that our mathematical model of biodiesel production can be applied to experimental researchers for maximum production in industrial scale. Numerical analysis gives a better understanding of optimal control theory. We successfully optimize biodiesel production as well as minimize soap formation by applying control approach in the system kinetics. Thus our mathematical model of transesterification is more functional and provides an idea to reduce saponification and maximize biodiesel production.

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