Optimization of Biodiesel Production through Enzymatic Transesterification of Jatropha curcas Oil

Fahad Al Basir, Priti Kumar Roy

Abstract—Enzymatic transesterification of Jatropha curcas plant oil with an alcohol is described as a two-step process. In the first step, hydrolysis of Jatropha oil to produce free fatty acid and the second step is the esterification of methanol with fatty acid to form the desired product, biodiesel. In this article, effect of stirring on enzymatic transesterification of Jatropha oil has been studied by formulating a mathematical model. Suitable reaction conditions such as molar ratio, enzyme load, stirring etc. are determined using the mathematical model. In order to find a unique optimum stirrer profile (a function of time), mathematical control theory is applied on stirring and make the process cost effect. The validity of the model is established by simulated result of the model and experimental results available in the literatures.

Keywords—Biodiesel, Jatropha curcas oil, Enzyme catalyst loading, Transesterification, Stirring, Mathematical Modeling, Optimization, Uniqueness.

I. INTRODUCTION

Biodiesel is considered as the most appropriate alternative fuel for diesel engines. It is gaining the most importance due to diminishing petroleum sources and the environmental consequences of exhaust gases from petroleum based engines. To reduce the coat of biodiesel production, less expensive feedstock such as Jatropha oil is used as feed stock [1, 2, 3].

Biodiesel production through enzymatic transesterification of *Jatropha curcas* oil is gaining more importance for its selective and eco-friendly nature. Most of the studies on biodiesel production using enzyme as catalyst (lipase) are purely experimental [5]. Limited number of kinetic modeling studies can be found in the literature [3, 4]. Al-Zuhair et al. established a kinetic model for lipase-catalyzed biodiesel production from waste cooking oil. Mathematical modeling approach for the enzymatic production of biodiesel using different feedstock have been investigated by many researchers [4,6-8]. Liu et al.[4] have investigated the transesterification of waste cooking oil catalyzed by immobilized lipase. They established a mathematical model and determine the kinetic parameters used in the system.

Stirring is the most important which directs the mass transfer between reaction phases. Appropriate mixing is important to reduce mass transfer limitations in transesterification [10]. External mass transfer limitations can be minimized by operation the reaction at an optimum stirrer speed. Effect of mass transfer on the production of biodiesel may be observed through different mixing strategy in a stirred vessel [11]. Optimization of mechanical agitation and evaluation of the mass transfer resistance is essential for maximum biodiesel production [9]. Yadav et al. [12] studied the effect of agitation speed on conversion in the range of 100-700 rpm and shown that the optimum speed for transesterification reaction was found to be 300 rpm. Sharma and Singh have reported that the yield of biodiesel increased from 85 – 89.5% when mechanical stirrer is applied along with the addition of excess amount of biocatalyst. This method produced higher diffusion and low effectiveness factor [13]. Thus, optimal stirring for the enzyme catalysed transesterification should be identified for maximum production and to make the process cost effective.

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In this research article, a mathematical model is formulated and effect of stirring is studied. Using optimal control theory, an optimal stirring profile is obtained for cost effective production of biodiesel. It is shown analytically that the control profile is unique for the optimal system. Simulation results of the model system are in a good agreement with experimental results.

II. THE MATHEMATICAL MODEL

The following assumptions are taken to formulate a simple mathematical model for the enzyme catalytic transesterification reaction of Jatropha Curcas oil:

Jatropha oil contains mainly triglycerides (TG) and free fatty acid (F). Both components can be converted to biodiesel using enzymatic transesterification process. Enzymatic transesterification of Jatropha oil with an alcohol (AL) can be described as two-step process. In the first step, hydrolysis of TG to produce free fatty acid (F) and release of glycerol through a complex C1 (i.e. E.TG) and the second step is the esterification of methanol (AL) with F to form the desired product i.e. biodiesel with the release of free enzyme (E) through a second complex $C2$ (F.AL) [5, 6, 14].

All the mechanistic steps for the biodiesel production can be represented by the following sequence of reactions:

I. Hydrolysis of TG:
$$E + TG \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} [E.TG] \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} F + GL,$$

II. Esterification of methanol:
$$F + AL \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} [F.AL] \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} E + BD, \tag{1}$$
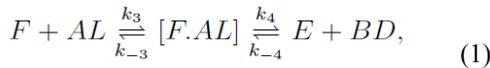
Here, k_1 and k_{-1}, k_2 and k_{-2} are the rate constants for the reversible formation of complex $C1$, acylated enzyme and by product glycerol respectively in the first step of biodiesel formation. k_3 and k_{-3}, k_4 and k_{-4} are the rate constants for the reversible formation of complex $C2$ and biodiesel formation respectively in the final step.

Mixing intensity directs the mass transfer between reaction phases, so mechanical stirring has an effect biodiesel yield. Here, we use k_s as the mass transfer rate constant due to stirring and the term has been defined as below [7, 15]:

$$k_s = \frac{a}{1 + e^{-b(N-c)}}, \tag{2}$$

where N is the speed of stirrer and a, b and c are constants.

The term is used in the fourth equation of the model by the expression $k_s x_B (1 - \frac{x_B}{B_{max}})$. Here B_{max} represents maximum production of biodiesel in a an ideal reaction conditions.

Denoting the concentration of TG, E, F, C1, C2, AL, BD and GL as x_T, x_E, x_F, x_{C1}, x_{C2}, x_A, x_B and x_G respectively and from the above assumptions with the above reaction mechanism followed by law of mass action, the following model system is obtained:

$$\frac{dx_E}{dt} = -k_1 x_T x_E + k_{-1} x_{C1} + k_4 x_{C2} - k_{-4} x_E x_B$$

$$\frac{dx_T}{dt} = -k_1 x_T x_E + k_{-1} x_{C1},$$

$$\frac{dx_F}{dt} = k_2 x_{C1} - k_{-2} x_F x_G - k_3 x_F x_A + k_{-3} x_{C2},$$

$$\frac{dx_B}{dt} = k_4 x_{C2} - k_{-4} x_E x_B + k_s x_B (1 - \frac{x_B}{B_{max}}),$$

$$\frac{dx_A}{dt} = -k_3 x_F x_A + k_{-3} x_{C2},$$

$$\frac{dx_{C1}}{dt} = k_1 x_T x_E - k_{-1} x_{C1} - k_2 x_{C1} + k_{-2} x_F x_G,$$

$$\frac{dx_{C2}}{dt} = k_3 x_F x_A - k_{-3} x_{C2} - k_4 x_{C2} + k_{-4} x_E x_B,$$

$$\frac{dx_G}{dt} = k_2 x_{C1} - k_{-2} x_F x_G. \tag{3}$$

The initial conditions are as follows:

$$x_E(0) = x_{E_0}, x_{C1}(0) = 0, x_F(0) = 0,$$

$$x_A(0) = x_{A_0}, x_T(0) = x_{T_0}, x_{C2}(0) = 0,$$
$$x_B(0) = 0, x_G(0) = 0. \tag{4}$$

2.1 Boundedness of the System

The right hand side of the equation (3) are smooth functions of the variables x_T, x_E, x_A, x_G, x_B, x_{C1}, x_{C2} and so local existence, uniqueness and continuous properties hold. Below, it is shown that every solution of the system is bounded.

Theorem 2.1 *Every solution of the system (3) is uniformly bounded.*

Proof. Define the function $W(t)$: $R_{0,+} \rightarrow R_{0,+}$ by

$$W(t) = x_B + x_T + x_E + x_{C1} + x_A + x_G$$
$$+ x_{C2} + x_F.$$

See that $W(t)$ is well-defined and differentiable on some maximal interval $(0, t_f)$.

Taking the derivative of (3),

$$\frac{dW(t)}{dt} = -k_1 x_T x_E + k_{-1} x_{C1} + k_4 x_{C2} - k_{-4} x_E x_B + k_2 x_{C1}$$
$$- k_{-2} x_F x_G - k_3 x_F x_A + k_{-3} x_{C2} + k_s x_B (1 - \frac{x_B}{B_{max}})$$
$$- [k_{-2}(x_{E_0} + x_{T_0} + x_{A_0})] x_G$$
$$+ (k_{-1} + k_2 + 1) x_{C1} + x_T + k_4 x_{C2} \tag{5}$$

$$\Rightarrow \frac{dW}{dt} + mW \le [k_{-1} + k_2 + k_4][x_{E_0} + x_{T_0} + x_{A_0}] \tag{6}$$

Where,

$$M = [k_{-1} + k_2 + k_4][x_{E_0} + x_{T_0} + x_{A_0}] + k_s a$$

and

$$m = min\{1, k_1 x_{T_0}, k_3 x_{A_0}, k_{-4} x_{E_0}, k_{-3}, x_{E_0}$$
$$+ k_{-2}(x_{E_0} + x_{T_0} + x_{A_0})\}$$

Hence,

$$W \le \frac{M}{m} + W(x_{E_0}, x_{T_0}, x_{F_0}, 0, x_{A_0}, 0, 0, 0) e^{-mt}.$$

Therefore all solution of the system is bounded.

III.   THE OPTIMAL CONTROL PROBLEM

The objective of giving optimal control stirring is to find an optimal profile of stirring to get maximum and cost effective production of biodiesel. We use the control variable $u(t)$, which represents the stirring activator input at time t satisfying $0 \le u(t) \le 1$. Here, $u(t)$ represents control input with values normalized to be between 0 and 1 [7]. Incorporating the control $u(t)$, the system (3) becomes,

$$\frac{dx_E}{dt} = -k_1 x_T x_E + k_{-1} x_{C1} + k_4 x_{C2} - k_{-4} x_E x_B$$

$$\frac{dx_T}{dt} = -k_1 x_T x_E + k_{-1} x_{C1},$$

$$\frac{dx_F}{dt} = k_2 x_{C1} - k_{-2} x_F x_G - k_3 x_F x_A + k_{-3} x_{C2},$$

$$\frac{dx_B}{dt} = k_4 x_{C2} - k_{-4} x_E x_B + u(t) k_s x_B (1 - \frac{x_B}{B_{max}}),$$

$$\frac{dx_A}{dt} = -k_3 x_F x_A + k_{-3} x_{C2},$$

$$\frac{dx_{C1}}{dt} = k_1 x_T x_E - k_{-1} x_{C1} - k_2 x_{C1} + k_{-2} x_F x_G,$$

$$\frac{dx_{C2}}{dt} = k_3 x_F x_A - k_{-3} x_{C2} - k_4 x_{C2} + k_{-4} x_E x_B,$$

$$\frac{dx_G}{dt} = k_2 x_{C1} - k_{-2} x_F x_G, \tag{7}$$

with initial conditions as given by (4).

The above state system can be written in a compact form as:

$$\frac{dx_i}{dt} = f_i(x_1, x_2, ..., x_8, u, t), i = 1, 2, ..., 8. \tag{8}$$

The cost function is thus formulated as

$$J[u(t)] = \int_{t_0}^{t_f} [Pu^2(t) - Qx_B^2(t)] dt \tag{9}$$

Here, we want to maximize biodiesel production and minimize the cost which can be measured by $J(u)$. The parameter $P (> 0)$ is the weight constant on the benefit of the cost of production and $Q > 0$ is the penalty multiplier. Thus, we have to find out the optimal control $u^*(t)$ such that

$$J(u^*) = \min J(u) : u \in U,$$

where U is the admissible control set defined by

$$U = \{u(t) : u(t) \text{ is measurable} , 0 \le u(t) \le 1, \\ t \in [t_i, t_f]\}. \tag{10}$$

Pontryagin Minimum Principle [18, 19] is used to find the optimal stirring in term of $u^*(t)$.

3.1 Existence of an optimal control

The existence of the optimal control can be obtained using a result by Fleming and Rishel in [25] and in [26].

Theorem 3.1 *There exists an optimal control* $(u^*) \in U$ *such that*

$$J(u^*) = \min (J(u) : u \in U). \tag{11}$$

Proof. To use an existence result in [25], we must check the following conditions:

(1) The set of controls and corresponding state variables is nonempty.

(2) The control set U is convex and closed.

(3) The right-hand side of the state system is bounded by a linear function in the state and control variables.

(4) There exists constants $c_1, c_2 > 0$, and $m > 1$ such that the integrand $L(x_B, u)$ of the objective functional satisfies

$$L(x_B, u) \ge c_2 - c_1 (|u|^2)^{\frac{m}{2}}$$

The result from the article by Lukes in [26] is used to verify above four conditions for the existence of solutions of system (7) with bounded coefficients, which gives condition (1). We note that the solutions are bounded. Our control set satisfies condition (2). Since the state system is bilinear in u, the right hand side of system (7) satisfies condition (3), using the boundedness of the solutions (section 2.1). Note that the integrand of our objective functional is convex. Finally, the last condition needs,

$$L(x_B, u) \ge c_2 - c_1 (|u|^2)^{\frac{m}{2}}$$

where c_2 depends on the upper bound on x_B, and $c_1 > 0$ since $P, Q > 0$. Thus, there exists an optimal control for the system (7).

3.2 Dynamics of the Optimality System

The Hamiltonian is formulated as,

$$H = Pu^2(t) - Qx_B^2(t) + \sum_{i=1}^{9} \xi_i f_i, \tag{12}$$

where ξ_1, - ξ_8 are adjoint variables and f_i, i=1, 2, ...,8 are the right side of equation (7), i.e. $f_1 = -k_1 x_T x_E + k_{-1} x_{C1} + k_4 x_{C2} - k_{-4} x_E x_B$, etc.

Theorem 3.2 *If the given optimal control* $u^*(t)$ *and the solution* (x_E^*, x_T^*, x_F^*, x_B^*, x_A^*, x_{C1}^*, x_{C2}^*, x_G *) of the corresponding system (7) minimize* $J(u)$ *over* U *, then there exists adjoint variables* ξ_1 - ξ_8 *which satisfying the following equations,*

$$\frac{d\xi_1}{dt} = k_1 x_T (\xi_1 - \xi_6) + k_{-4} x_B (\xi_4 - \xi_7),$$

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

$$\frac{d\xi_3}{dt} = k_3 x_A (\xi_5 - \xi_7) + k_{-2} x_G (\xi_3 - \xi_6),$$

$$\frac{d\xi_4}{dt} = 2Qx_B + \xi_4 \{k_{-4} x_E + \frac{k_s x_B u(t)}{B_{max}}$$

$$- k_s u(t)(1 - \frac{x_B}{B_{max}})\} - \xi_7 k_{-4} x_E,$$

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

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

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

$$\frac{d\xi_8}{dt} = k_{-2}(\xi_8 - \xi_6), \tag{13}$$

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

$$u^*(t) = max\left(0, min\left(1, \frac{-k_s[\xi_4 x_B(1-\frac{x_B}{B_{max}})]}{2P}\right)\right).$$

(14)

Proof. The Hamiltonian (8) can be written as:

$$H = Pu^2(t) + k_s u[\xi_1 x_B(1 - \frac{x_B}{B_{max}})]$$

$$+terms\ without\ u(t). \qquad (15)$$

According to the Pontryagin Minimum Principle, the unconstrained optimal control variable $u^*(t)$ satisfies

$$\frac{\partial H}{\partial u^*} = 0.$$

Thus from (15),

$$\frac{\partial H}{\partial u^*} = 2Pu^* + k_s x_B(1 - \frac{x_B}{B_{max}})(\xi_4) = 0.$$

Solving one can get,

$$u^*(t) = \frac{-k_s\left[\xi_4 x_B\left(1 - \frac{x_B}{B_{max}}\right)\right]}{2P}.$$

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

$$u^*(t) = max\left(0, min\left(1, \frac{-k_s[\xi_4 x_B(1-\frac{x_B}{B_{max}})]}{2P}\right)\right).$$

According to Pontryagin Minimum Principle, adjoint variables satisfy the following equation,

$$\frac{d\xi_i}{dt} = -\frac{\partial H}{\partial x_i},$$

where $x_i \equiv (x_E, x_T, x_F, x_B, x_A, x_{C1}, x_{C2}, x_{C3}, x_G)$ i.e. $\xi_1 = x_E, \xi_2 = x_T$ etc. and the necessary condition satisfying the optimal control $u(t)$ are

$$H(x_i(t), u^*(t), \xi_i(t), t) = \min_{u \in U}(H(x_i(t), u(t), \xi_i(t), t)).$$

So, adjoint equations (13) can be determined by equation (12) with boundary conditions $\xi_i(t_f) = 0, (i = 1-8)$. Thus equation (7) together with (14) and (13) represents the optimality system.

Now, the optimal profiles for stirring (N^*) can be obtained by the following relations:

$$u^* k_s = \frac{a}{(1 + exp(-b(N^* - c))}. \qquad (15)$$

For further calculation, the adjoint system (13) is written as:

$$\frac{dxi_i}{dt} = F_i(x_1, x_2,..., x_8, \xi_1,..., xi_8, t). \qquad (16)$$

Here, $F_i, i = 1, 2,..., 8$ are right sides of adjoint system (13).

3.3 Uniqueness of the Optimal Control

In this section, we show that the control, u, is unique for the optimal system.

Suppose, x_i, $i = 1, 2,..., 8$ and ξ_j, $j = 1, 2,..., 8$ and $\bar{x}_i$, $i = 1, 2,..., 8$ and $\bar{\xi}_j$ are two solutions of the system (7) and (13).

Let us consider, $x_i = e^{\lambda t} p_i$, and $\xi_j = e^{-\lambda t} q_j$, for i,j=1, 2, ...,8.

(12)

Similarly, $\bar{x}_i = e^{\lambda t} \bar{p}_i$, and $\bar{\xi}_j = e^{-\lambda t} \bar{q}_j$, for i,j=1, 2,..., 8.

Then optimal control takes the following form,

$$u = max(0, min(1, \frac{-k_s[\xi_4 x_4(1-\frac{x_4}{B_{max}})]}{2P})),$$

$$\overline{u} = max(0, min(1, \frac{-k_s[\overline{\xi}_4 \overline{x}_4(1-\frac{\overline{x}_4}{B_{max}})]}{2P}))$$

Thus, we have the following two inequalities,

$$\int_{t_0}^{t_f} (u-\overline{u})^2 dt \leq \widetilde{C}_1 \int_{t_0}^{t_f} [|p_4 - \overline{p}_4|^2 + |q_4 - \overline{q}_4|^2] dt.$$

Substituting $x_i = e^{\lambda t} p_i$, and $\xi_j = e^{-\lambda t} q_j$, (for $i, j = 1,2,...,8$) in (7) and (13),

$$\dot{p}_i + \lambda p_i = e^{-\lambda t} f_i(e^{\lambda t} p_i, t), i = 1,2,...,8,$$

and

$$\dot{q}_j - \lambda q_j = e^{\lambda t} F_j(e^{\lambda t} p_i, e^{-\lambda t} q_j, t).$$

$F_j, (j = 1,2,...,8)$ are given in (15) and as for example, the differential equations for $j = 2$ are,

$$\dot{p}_2 + \lambda p_2 = -e^{\lambda t} k_1 p_2 p_1 + k_{-1} p_6,$$

and

$$\dot{q}_2 - \lambda q_2 = k_1 p_1(q_1 + q_2 - q_6).$$

Another set of sixteen such similar equations can be obtained for the substitution $\overline{x}_i = e^{\lambda t} \overline{p}_i$, $\overline{\xi}_j = e^{-\lambda t} \overline{q}_j$, for $i = 1,2,...,8$. To obtain the equation, we have subtracted the equations for $\overline{x}_i$ from x_j, and $\overline{\xi}_j$ from ξ_j for $i, j = 1,2,...,8$. Next, each subtracted equation is multiplied by an appropriate function and then integrated from initial time (t_0) to final time (t_f).

Thus, the following inequalities are obtained:

$$\frac{1}{2}(p_i - \overline{p}_i)^2(t_f) + \lambda \int_{t_0}^{t_f}(p_i - \overline{p}_i)^2 dt$$

$$\leq \widetilde{C}_2 e^{\lambda t_f} \int_{t_0}^{t_f}[\sum_{i=1}^{8} |p_i - \overline{p}_i|^2] dt$$

$$+ \widetilde{C}_3 \int_{t_0}^{t_f}[\sum_{i=1}^{8} |q_j - \overline{q}_j|^2] dt,$$

and

$$\frac{1}{2}(q_j - \overline{q}_j)^2(t_0) + \lambda \int_{t_0}^{t_f}(q_j - \overline{q}_j)^2 dt \qquad (16)$$

$$\leq \widetilde{C}_4 e^{\lambda t_f} \int_{t_0}^{t_f}[\sum_{i=1}^{8} |q_j - \overline{q}_j|^2] dt.$$

Here, the constants $\widetilde{C}_1$ to $\widetilde{C}_4$ depend on the coefficients and the bounds on states and adjoints.

Adding the inequalities are added and estimated to obtain the following results,

$$\frac{1}{2}[\sum_{i=1}^{8}(p_i - \overline{p}_i)^2(t_f) + \sum_{i=1}^{8}(q_j - \overline{q}_j)^2(t_0)$$

$$+ \lambda \int_{t_0}^{t_f}[\sum_{i=1}^{8}(p_i - \overline{p}_i)^2 + \sum_{i=1}^{8}(q_j - \overline{q}_j)^2] dt$$

$$\leq (\widetilde{C}_5 + \widetilde{C}_6 e^{2\lambda t_f}) \int_{t_0}^{t_f}[\sum_{i=1}^{8}(p_i - \overline{p}_i)^2 + \sum_{i=1}^{8}(q_j - \overline{q}_j)^2] dt.$$

Here, $\widetilde{C}_5$ and $\widetilde{C}_6$ depend on the coefficients and the bounds of p_i, and q_j ($i, j = 1,2,...,8$).

From the above relations we have,

$$(\lambda - \widetilde{C}_5 - \widetilde{C}_6 e^{\lambda t_f}) \int_{t_0}^{t_f}[\sum_{i=1}^{8}(p_i - \overline{p}_i)^2$$

$$+ \sum_{i=1}^{8}(q_j - \overline{q}_j)^2] dt \leq 0.$$

Now, if λ is so chosen such that $\lambda > \widetilde{C}_5 + \widetilde{C}_6$ and

$$t_f < \frac{1}{\lambda} \ln(\frac{\lambda - \widetilde{C}_5}{\widetilde{C}_6}), \quad \text{then} \quad p_i = \overline{p}_i \quad \text{and} \quad q_j = \overline{q}_j,$$

$i, j = 1, 2, ..., 8.$

Hence, the solution set is unique in the time interval $[t_0, t_f]$ and also the control function, $u(t)$, is unique for the optimal system.

IV. RESULTS AND DISCUSSION

In this section, numerical simulation of the model system are shown in the following figures. The effect of enzyme loading and stirring on biodiesel yield has been studied. Simulation result of the optimality system gives the optimal stirring profile $N^*(t)$ for cost effective production of biodiesel.

To prove the possible mass transfer effects on the biodiesel productivity, the simulation of the model has been performed using different agitating speeds (100-500 rpm) keeping all other variables fixed. In Figure 1 (lower panel), raising the stirring rate from 100 to 600 rpm, biodiesel yield is plotted at the fixed molar ratio (4:1). It is clear from this figure that stirring has given a positive effect on biodiesel yield and mass transfer. The conversion could not be enhanced by further intensifying agitation speed of 500 rpm. It appears that the mass transfer limitations are not observed at the stirring rate of 300 rpm while the stirring over 300 rpm decreases the yield, which is possibly due to the shearing of the lipase molecule or

Table 1: Values of rate constants at temperature $40^o C$ and other parameters used for numerical simulation of the model system [4, 7].

Parameters	Value (unit)
k_1	7.5128 $(mol\,/L)^{-1}\ min^{-1}$
k_{-1}	0.1147 $(hour^{-1})$
k_2	0.1032 $(hour^{-1})$
k_{-2}	0.0988 $(mol\,/L)^{-1}\ min^{-1}$
k_3	1.937 $(mol\,/L)^{-1}\ min^{-1}$
k_{-3}	0.0323 $hour^{-1}$
k_4	1.9230 $hour^{-1}$
k_{-4}	0.0011 $(mol\,/L)^{-1}\ min^{-1}$
a	0.320 $-$
b	0.003 (rpm^{-1})

inactivation of the lipase due to the foam formed at this speed. It was also observed that, some immobilized lipases were not in the liquid phase but stuck to the wall of the flask due to the high speed thereby reducing the effective lipase loading in the reaction mixture. Similar observations were found by Halim et al. [22].

Figure 2 shows that optimal stirring produces the highest biodiesel yield within three hours using a lower enzyme loading. Initial mass transfer rate is increased and reaction time is also reduced. Thus, production of biodiesel is more favourable in enzymatic transesterification reaction using optimum stirring profile. It reduces time and cost of production. This figure also shows that stirring in needed for three hours from the beginning and according to Pontryagin principle, the concentration profile of biodiesel is optimal.
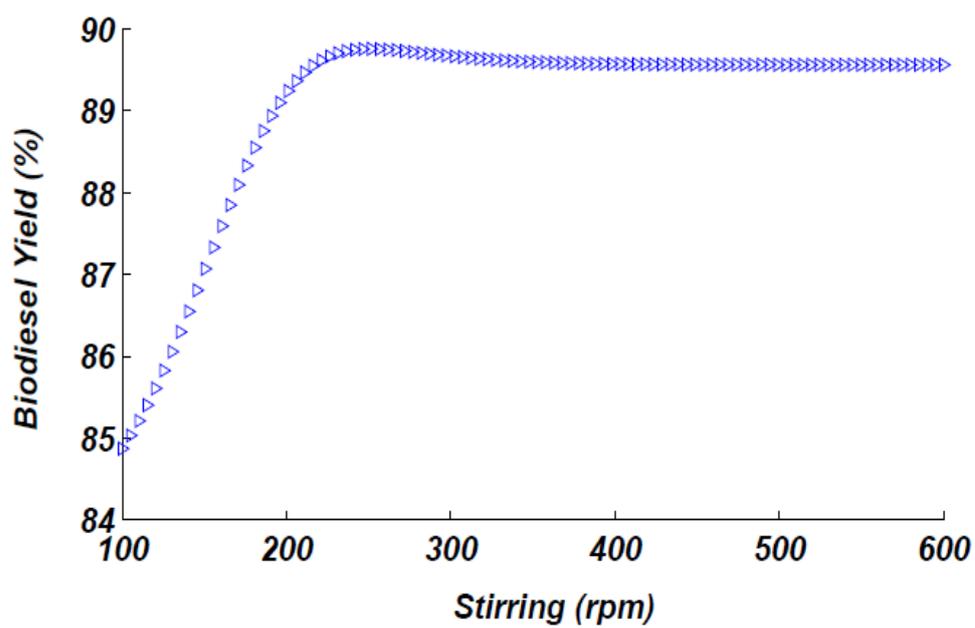
Figure 1: Effect of stirring on biodiesel yield is shown in the figure with parameter as given in **Table 1**. Here, final concentration is plotted as function of stirring taking 4 hours of reaction time.
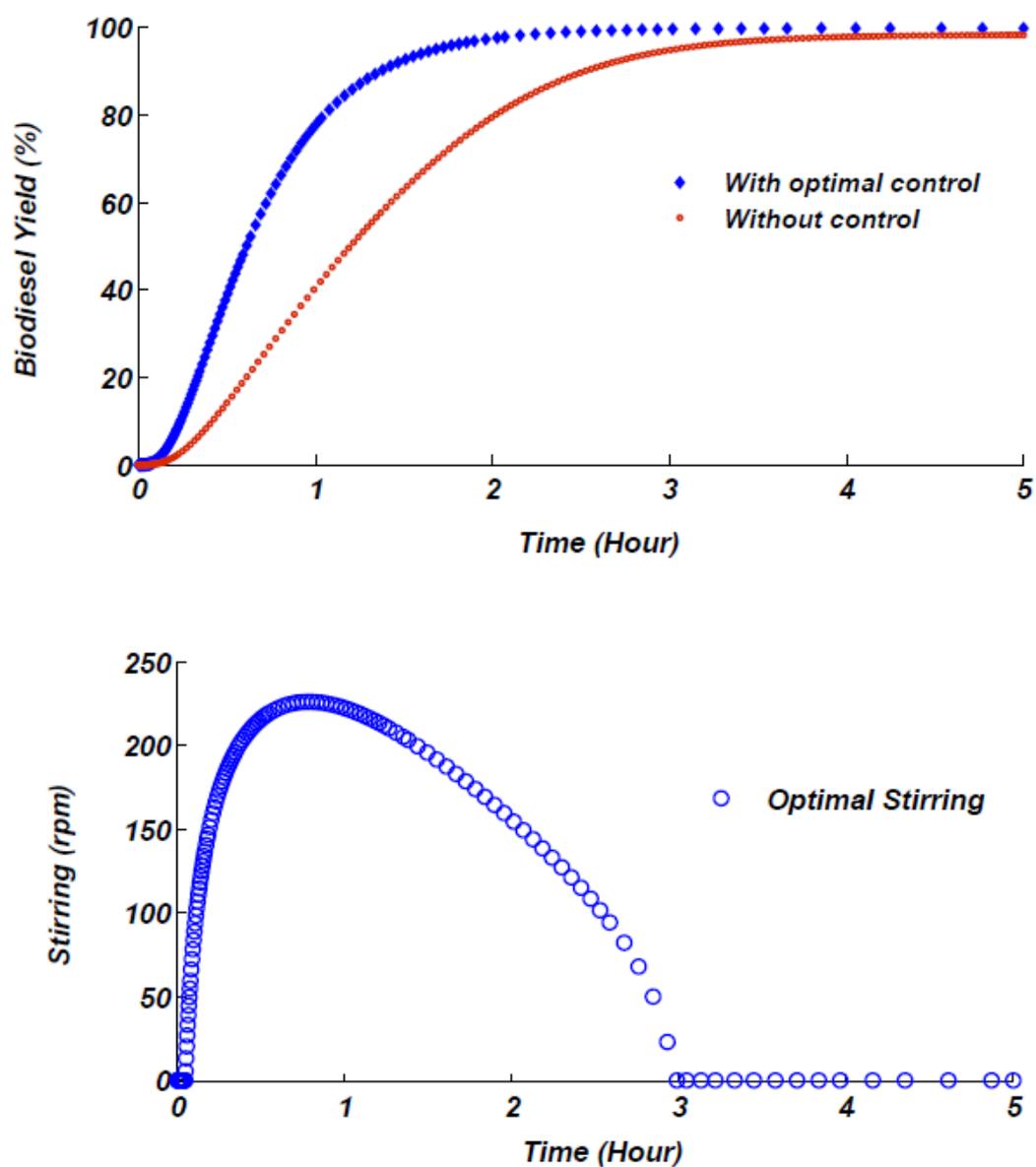
Figure 2: Control profile of stirring ($N^*(t)$) is plotted as a function of time and conversion of biodiesel for two cases, with control and without control with parameter as given in **Table 1.**

V. CONCLUSION

In this article, a mathematical model is formulated to study the effect of stirring on biodiesel production from Jatropha oil using enzymatic transesterification. Influences of agitation speed on biodiesel productivity, in terms of mass transfer are determined numerically. Finally, using optimal control theory, a control profile for stirring is obtained to get maximum biodiesel production and to make the process cost effective and the optimal control profile exists uniquely for the system. Optimization of enzymatic production establish that maximum biodiesel can be produced in 3 hours of reaction time by using optimal stirring profile.

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