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EXTREME SOLUTIONS OF OPTIMAL CONTROL STRATEGY FOR THE PRODUCTION OF BIODIESEL

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Abstract In this paper, without an initial mass transfer resistance, we consider a system of production of biodiesel. We find extreme solutions of temperature profile optimal control strategy for smooth production of biodiesel. We have studied properties and importance of solutions, which is maximal or minimal for a defined differential system.

Keywords. Optimal control, Biodiesel, Jatropha Curcasoil, Transesterification, Reaction parameter, Maximum principal, peano's existence theorem.

1. Introduction

A fuel which is extracted using natural vegetable fats and oils that is clean and renewable is called Biodiesel. This utility of liquid fuels like biodiesel extracted from Jatropha oil by the transesterification process implies as for the use of conventional fossil fuels as an option promisingly. Biodiesel production by the transesterification of Jatropha oil relies on parameters such as temperature, reaction time, speed of the stirrer, molar ratio of oil to alcohol.

The collection of Fatty acid methyl esters (FAME) is Biodiesel. The oil obtained in vegetable oils like Jatropha Curcas oil which is renewable and also an alternate fuel use for diesel is called as Biodiesel [1], which is a pollution free, easily accessible, sustainable, locally available and reliable fuel extracted from sources that are renewable oils from vegetables or animals fats by the process of transesterification [2]. One such alternate way of extracting biodiesel is by production from Jatropha Curcas plant. The oil which is non-edible like Jatropha, in India it acquaints 200 thousand metric tons, an estimated annual production potential and which is grown in any type of waste land [3].

For the convertible process of vegetable oil to biodiesel in the catalyst reaction, the process of Transesterification or alcoholises is employed commonly. More amount of processes such as involving either biological catalyst like free enzyme or immobilized enzyme or chemical catalysts like bases, acids, both heterogeneous and liquid are developed in the production of biodiesel [4]-[10]. The investigation of alkaline transesterification for production of biodiesel are carried out in many research articles [10]-[12], and also where a raw material any with a free fatty acid (FFA) or a high water or content needs a definite pre-treatment for the esterification of FFA with an acidic catalyst[13], [14].

The different parameters like ratio of molar between triglycerides and alcohol, reaction time, catalyst concentration and temperature reaction influences the process of Transesterification [15]. For instance, more quantity of alcohol guarantees the conversion process of oils or fats to the esters completely in a short period of time. In the presence of alkali catalyst, the molar ratio usually carried out is 6:1. The biodiesel yielding attains a maximum quantity only when the time of reaction is less than 90 min, since the conversion rate of fatty acids esters increases when duration prolongs more on the other hand had been determined. Effects of concentration of catalyst and the molar ratio of alcohol play a vital role in yielding biodiesel [16], [17]. But also the yield of biodiesel decreases due to excess reaction time as some backward reactions takes place and it will further cause the formation of soap form fatty acids. Since the concentration raises in the triglyceride conversion, and so the biodiesel yield increases, wherein the reaction of catalyst also plays a very significant role [17], [18].

The various effects of temperature and the reaction time are examined in case of biodiesel extraction from Jatropha Curcas oil. When the temperature increases due to reaction, there is an increase in the conversion of biodiesel. There are some certain temperature readings B (above 50^oC), where the yield of biodiesel decreases [19], [20]. This shows that control variables in production of biodiesel is temperature which is very significant. Thus, for optimum biodiesel production, an optimal profile of temperature is required.

The mass transfer limitation problem is faced initially during the Transesterification of Jatropha oil. While applying stirring on the system, this problem can be avoided. The effect of system on stirring on transesterification is done clearly by formulating a mathematical model which is shown in Roy et al. [21]. To avoid the problem in the mass transfer, it shows that 600 rpm stirring is optimal. Considering the model [21], the temperature effects on the yield of biodiesel is discussed. And also, a molar ratio has been determined which is essential for the production of biodiesel. An optimal temperature profile is determined by using theory of optimal control theory, where from transesterification of Jatropha Curcas, the extreme amount of biodiesel can be obtained oil in a fixed reaction time.

The study of an optimal control of problem [26] in biodiesel production is studied in this paper. For this problem, the maximal and minimal solutions of temperature control policy that changes with time using peano's existence theorem are required.

2 Translating Chemical Knowledge to Ordinary Differential Equations (ODE)

In formulating this model, we shall bring to fore, relating ideas of ordinary differential equation in mathematical modelling, structured as problem statement of optimization control, which are solvable using well known method from numerical methods.

To make ODE's from chemical knowledge, we Consider a model from [26] consisting of a six ordinary differential equations.

By reacting triglycerides with methanol in a laboratory, biodiesel can be produced. Three reversible steps occur in the reaction. Some of the intermediates like diglyceride and monoglyceride are taken into consideration during the reaction of triglycerides and methanol. Hence, here we consider that during the production of biodiesel, there occurs three consecutive reversible reactions. The reaction can be explained schematically as below

$$TG+AL \leftrightarrow DG+BD$$

$$DG+AL \leftrightarrow MG+BD$$

$$MG+AL \leftrightarrow GL+BD$$

Overall reaction: $TG+3AL \leftrightarrow 3BD+GL$.

The following assumptions are carried out for the mathematical model formulation of system of transesterification reaction [21]

i) A little water (0.2% w/w) in the reaction mixture and also free fatty acids which are negligible are detected in the system, so that it assumes to be the occurrence of only three consecutive reactions [22],

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

iii) Since the intensity of mixing in this reaction system insists the limitations of mass transfer in between the phases, and so the foremost effective factors in transesterification reaction is mechanical stirring. Hence, here *ks* is used as the constant of mass transfer rate and its unit is denoted by min^{-1}, wherein that term is defined in [21]:

$$k_s = \frac{a}{1+e^{-bN+c}}$$

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

The term is expressed by $k_s x_B \left[1 - \frac{x_B}{\boldsymbol{B_{max}}}\right]$ in our model.

Here x_B denotes the biodiesel concentration and $\boldsymbol{B_{max}}$ represents maximum production of biodiesel in an ideal situation where it is defined as a system having no resistance of mass transfer. The unit of $x_B, \boldsymbol{B_{max}}$ is represented by moles/L.

Logistically, the term has been handled since when the stirrer speed increases, there is a decrease in resistance of mass transfer and moreover the resistance of mass transfer is negligible beyond a certain stirrer speed. This fact is experimentally evident from the observations done by other workers [23].

The concentration of triglycerides, diglycerides, monoglycerides, methanol (alcohol) and glycerol are denoted as $x_{T,}\ x_D, x_{M,}\ x_A, x_G$ respectively and also by introducing the mass action laws and assumptions made above; the following six differential equations are obtained.

$$\frac{dx_B}{dt} = k_1 x_T x_A - k_2 x_D x_B + k_3 x_D x_A - k_4 x_M x_A + k_5 x_G x_B + k_s x_B \left[1 - \frac{x_B}{\boldsymbol{B_{max}}}\right]$$

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

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

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

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

$$\frac{dx_G}{dt} = k_3 x_D x_A + k_6 x_G x_B$$

Here k_1, k_2, k_3, k_4, k_5, k_6, *Bmax* 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 reaction rate constants dependency on the temperature k_i, (i = 1 to 6), can be expressed by the Arrhenius equation [20]:

$$k_i = \alpha_i e^{-\frac{\beta_i}{T}}$$

T is the reaction temperature, α*i* is the frequency factor, and

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

where $E\alpha_i$ denotes 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. Extreme Solutions to optimal control problem

We aim on studying properties and importance of a solution (or integrals), which is maximal (superior integral) or minimal (inferior integral) for a differential system

$\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$ with initial values of state variables given:

$x_T(0) = x_{T_0}\ x_B(0) = x_D(0) = x_m(0) = x_G(0) = 0, x_A(0) = x_{A_0}$ (3.1)

$D \subset R \times R$, $(0, x_j) \in D$ with maximum interval of existence $\lfloor 0, x_j \rfloor$

Definition 3.1 Let $r_{\max}(t)$ be any solution of differential system

$$\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$$

on the interval $I \cap (0, x_j)$. Then $r_{\max}(t)$ is said to the maximal solution of the differential system

$$\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$$

if, for every solution $x_i(t)$ of $\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$

Existing on the interval $I \cap (0, x_j)$, the inequality $x_i(t) \le r_{\max}(t)$ holds for $t \in I$ (3.2)

$r_{\max}(t) \to Maximal\ Solution$, i.e. all other solutions of the differential system exists and are smaller than $r_{\max}(t)$ over interval $I \cap (0, x_j)$.

Definition 3.2 Let $r_{\min}(t)$ be any solution of differential system

$$\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$$

on the interval $I \cap (0, x_j)$. Then $r_{\min}(t)$ is said to the minimal solution of the differential system

$\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$ if , for every solution $x_i(t)$ of $\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$

Existing on the interval $I \cap (0, x_j)$, the inequality $x_i(t), \le r_{\min}(t)$, $i = 1,2,3,4,5,6$ holds for $t \in I$, $r_{\min}(t) \to Minimal\ Solution$,

i.e., all other solutions of the differential system exists and are larger than $r_{\min}(t)$ over interval $I \cap (0, x_j)$

Definition 3.3 A solution $\frac{r_{\max}(t)}{r_{\min}(t)}$ of the Initial value problem

$$\frac{dx_i}{dt} = f_i(t,x,T), \quad i = 1,2,3,4,5,6$$

with initial values of state variables given:

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

which exist in a interval $I \cap (0, x_j)$ is said to be $\frac{Maximal}{Minimal}$ if for every other solution $x_i(t)$, $i = 1,2,3,4,5,6$ for all $t \in I$, $\frac{\overset{Maximal}{x_i(t) \le r_{\max}(t)}}{\underset{x_i(t) \le r_{\min}(t)}{Minimal}}$ for all $t \in I$.

The Maximal solution $r_{\max}(t)$ and the minimal solution $r_{\min}(t)$ exists, they are unique . This happens only when $f_i(t,x,T)$, $i=1,2,3,4,5,6$ are continuous real valued function on an open set $D \subset R \times R$, $(0,x_j) \in D$.

Note: Interval $I \cap (0,x_j)$ is the common interval of existence for $x_i(t), i=1,2,3,4,5,6$ and $r_{\max}(t)$. Similarly, $I \cap (0,x_j)$ is again the common interval of existence for $r_{\max}(t)$ and $r_{\min}(t)$.

Let $f_i(t,x,T)$, $i=1,2,3,4,5,6$ be a continuous function on a plane (t,x,T) set E by a maximal solution $x_i(t)=r_{\max}(t)$ of Initial value problem.

$$\frac{dx_i}{dt} = f_i(t,x,T), \quad i=1,2,3,4,5,6 \text{ with initial values}$$

$x_T(0) = x_{T_0}\ x_B(0) = x_D(0) = x_m(0) = x_G(0) = 0, x_A(0) = x_{A_0}$ is meant a solution of (3.1) on maximum interval of existence such that if $x_i(t)$ is any solution of (3.1)

Then n a maximal interval $x_i(t) \le r_{\max}(t)$ holds on the common interval of existence of $x_i(t), r_{\max}(t)$. A minimal solution can also be defined similarly.

Lemma 3.4 Let $f_i(t,x,T)$, $i=1,2,3,4,5,6$ be a continuous on a rectangle $\bar{s}_+ : t_0 \le t \le t_0 + a$, $|x_i(t) - r_{\max}(t)| \le b$; Let $|f_i(t,x,T)| \le M$, $i=1,2,3,4,5,6$ $\alpha = \min\left(a, \frac{b}{M}\right)$

Then relation (3.1) has a solution $x(t) = r_{\max}(t)$ on $t_0 \le t \le t_0 + \alpha$ with the property that every solution $x(t) = x_i(t)$ of (3.1) , $x_i(t_0) \le r_{\max}(t_0)$ satisfies $x_i(t) \le r_{\max}(t)$ on $t_0 \le t \le t_0 + \alpha$.

Proof. Let $0 < \alpha < \alpha'$ .Then by Peano's Existence theorem

$$\frac{dx_i}{dt} = f_i(t,x,T) + \frac{1}{n} \quad , \quad i=1,2,3,4,5,6 \quad \text{with initial values} \qquad (3.3)$$

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

has a solution $x(t) = x_n(t)$ on $t_0 \le t \le t_0 + \alpha'$ if n is sufficiently large .

There is sequence $n(1), n(2), n(3), \ldots\ldots\ldots$ such that $r_{\max}(t) = \lim_{k\to\infty} x_{n(k)}(t)$ exists uniformly on $t_0 \le t \le t_0 + \alpha'$ and is a solution of (3.1)

It is to be proved that (3.2) holds on $t_0 \le t \le t_0 + \alpha'$. To this end, it is sufficient to verify $x(t) \le x_n(t)$ on $t_0 \le t \le t_0 + \alpha'$ for all large fixed n .

If $x(t) \le x_n(t)$ on $t_0 \le t \le t_0 + \alpha'$ does not hold, $t = t_1$, $t_0 \le t \le t_0 + \alpha'$ such that $x(t_1) > x_n(t_1)$ hence there is a largest t_2 on $t_0 \le t < t_1$ where $x(t_2) = x_n(t_2)$, so that $x(t) > x_n(t)$ on $t_2 < t \le t_1$.

But (3.3) implies that $x_n'(t_2) = x'(t_2) + \frac{1}{n}$ so that $x(t) < x_n(t)$ for t (> t$_2$) near t$_2$.

This contradiction proves $x(t) \le x_n(t)$ on $t_0 \le t \le t_0 + \alpha'$

Since $\alpha' < \alpha$ id arbitrary, the lemma follows. The uniqueness of the solution $x(t) = x_n(t)$ shows that $x_n(t) \to x_0(t)$ uniformly on $t_0 \le t \le t_0 + \alpha'$ as $n \to \infty$

This lemma indicates an existence theorems for maximal and minimal solution (which are only to be preferred for an open set E). We have the following theorem.

Theorem 3.5 Let $f_i(t,x,T)$, $i=1,2,3,4,5,6$ be a continuous on an open set E and $t_0 < t < r_{\max}(t_0)$. Then initial value problem $x_i(t) = r_{\max}(t)$ has a maximal solution and minimal solution.

4. Conclusions

We have studied properties and importance of a solution (or integrals), which is maximal (superior integral) or minimal (inferior integral) for a defined differential system. We have establishment of the existence of maximal $r_{\max}(t)$ solution and minimal solution $r_{\min}(t)$ of the Initial value problem $\frac{dx_i}{dt} = f_i(t,x,T)$, $i=1,2,3,4,5,6$ with the initial values

$$x_T(0) = x_{T_0}\; x_B(0) = x_D(0) = x_m(0) = x_G(0) = 0, x_A(0) = x_{A_0}$$

on $t_0 \le t \le t_0 + a$ guarantees the existence of a solution $x(t)$ of the Initial value problem in sufficiently small interval.

Optimal control theoretic approach is applied on in and around of temperature boundaries. This approach may be useful for real time situations and doing some simulation works. These results are useful for examining the indigenous temperature effects and other control parameters on the effects of transfer of mass for quick rate in the biodiesel extraction.

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