

A Study on Optimal Control Strategy For The Production of Biodiesel By Using AVK Method

R.Prabakaran¹, S. Palaniammal², D. Anandakumar³

¹Department of Mathematics, Coimbatore Institute of Technology, Coimbatore, India.

²Department of Mathematics, Sri Krishna College of Technology, Coimbatore, India.

³Department of Mathematics, Sri Krishna College of Engineering & Technology, Coimbatore, India.

Abstract- In this paper, we consider a system of biodiesel production with no initial mass transfer resistance. We find an optimal control strategy for smooth production of biodiesel using AVK Method.

Keywords- optimal control, Biodiesel, Jatropha Curcas oil, Transesterification, Reaction parameter, Maximum principal, AVK Method

I. INTRODUCTION

Biodiesel is a clean burning renewable fuel made using natural vegetable oils and fats. The utilization of liquid fuels such as biodiesel produced from Jatropha oil by transesterification process represents one of the most promising options for the use of conventional fossil fuels. 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.

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.

In this paper, we study a optimal control problem [26] in biodiesel production. For this problem, we are going to find a temperature control policy that can change with time using the AVK Method.

II. 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 modeling, 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.

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



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]:

$$k_s = \frac{a}{1+e^{-bN+c}} \tag{2.2}$$

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

The term is used in our model by the expression $k_s x_B \left[1 - \frac{x_B}{B_{max}} \right]$

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.

$$\begin{aligned}
 \frac{dx_B}{dt} &= k_1 x_T x_A - k_2 x_D x_B + k_3 x_D x_A - k_4 x_M x_A + k_5 x_G x_B + k_s x_B \left[1 - \frac{x_B}{B_{max}} \right] \\
 \frac{dx_T}{dt} &= -k_1 x_T x_A + k_2 x_D x_B \\
 \frac{dx_D}{dt} &= k_1 x_T x_A - k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_A \\
 \frac{dx_M}{dt} &= k_3 x_D x_A + k_4 x_M x_A - k_5 x_G x_B + k_6 x_G x_B \\
 \frac{dx_A}{dt} &= -k_1 x_T x_A + k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_A - k_5 x_G x_B + k_6 x_G x_B \\
 \frac{dx_G}{dt} &= k_3 x_D x_A + k_6 x_G x_B
 \end{aligned}
 \tag{2.3}$$

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]:

$$k_i = \alpha_i e^{-\frac{\beta_i}{T}} \tag{2.4}$$

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)

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
	0.098e10		7366.64
	5.35e3		3231.18
	2.15e4		4824.87

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 solve 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,

$$\begin{aligned} &\text{Maximize } J = x_B(t_f) \\ &\text{Subject to the following system} \\ &\frac{dx_B}{dt} = k_1 x_T x_A - k_2 x_D x_B + k_3 x_D x_A - k_4 x_M x_A + k_5 x_G x_B + k_6 x_G x_B \left[1 - \frac{x_B}{B_{max}} \right] \\ &\frac{dx_T}{dt} = -k_1 x_T x_A + k_2 x_D x_B \end{aligned}$$

$$\begin{aligned} \frac{dx_D}{dt} &= k_1 x_T x_A - k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_A \\ \frac{dx_M}{dt} &= k_3 x_D x_A + k_4 x_M x_A - k_5 x_G x_B + k_6 x_G x_B \\ \frac{dx_A}{dt} &= -k_1 x_T x_A + k_2 x_D x_B - k_3 x_D x_A + k_4 x_M x_A - k_5 x_G x_B + k_6 x_G x_B \\ \frac{dx_G}{dt} &= k_5 x_D x_A + k_6 x_G x_B \end{aligned} \tag{2.5}$$

The initial conditions for this system are,

$$\begin{aligned} x_T(0) &= x_{T_0}, x_B(0) = x_{D_0} = 0 \\ x_m(0) &= x_G(0) = 0, x_A(0) = x_{A_0} \end{aligned}$$

The system (2.3) can be written in compact form as

$$\frac{dx_i}{dt} = f_i(t, x, T) \tag{2.6}$$

Where $f_i (i = 1, \dots, 6)$ are the right sides of system (2.5) 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.

III. DISCRETIZATION METHOD

We show the effect of molar ratio and temperature on the system in a fixed stipulated time. Transformation of the model was carried out using ordinary differential equations and analysis performed by a numerical method solved on the basis of a special discretization method called AVK method.

In AVK method, for solving the optimal control problem [26]

$$\text{Maximize } J(x, T) = x_B(t_f)$$

Subject to

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

with initial values of state variables given:

$$x_T(0) = x_{T_0}, x_B(0) = x_D(0) =$$

$$x_m(0) = x_G(0) = 0, x_A(0) = x_{A_0}$$

$$x_T(0) = x_{T_0}, x_B(0) = x_D(0) =$$

$$x_m(0) = x_G(0) = 0, x_A(0) = x_{A_0}$$

Control variable T is bounded by: $\alpha \leq T \leq \beta$

the following steps should be applied:

Step 1. Form the total error function E_1 as:

$$E_1 = \left\| \frac{dx_i}{dt} - f_i(t, x, T) \right\|$$

Step 2. Combine the total error function with the objective functional as follows:

$$\text{Maximize } J(x, T) = \lambda_1 x_B(t_f) + \lambda_2$$

$$\left\| \frac{dx_i}{dt} - f_i(t, x, T) \right\|$$

Subject to the initial values of state variables given:

$$x_T(0) = x_{T_0}, x_B(0) = x_D(0) =$$

$$x_m(0) = x_G(0) = 0, x_A(0) = x_{A_0}$$

where nonnegative numbers λ_1 and λ_2 are two given weights and $\lambda_1 + \lambda_2 = 1$

Step 3. Induce error control measure called the constraint to the error,

$$\text{i.e. } E(x, T) \leq \epsilon$$

to the optimal control problem in step 2.

Therefore, the modified optimal problem arising from equations (2.14)-(2.15), is reformulated as:

$$\text{Maximize } \lambda_1 x_B(t_f) + \lambda_2$$

$$\left\| \frac{dx_i}{dt} - f_i(t, x, T) \right\|$$

$$\text{Subject to } \left\| \frac{dx_i}{dt} - f_i(t, x, T) \right\| \leq \epsilon$$

(2.7)

Step 4. Calculate $T(t_i)$ by maximizing the optimal control problem (2.17), using discretization method. Let the norm function $\|\cdot\|$ be given as norm 1, and then we can solve the optimization problem that follows :

$$\text{Maximize}$$

$$g \sum_{g=0}^{r-1} \left\{ \lambda_1 x_B(t_f) + \lambda_2 \left\| \frac{dx_i}{dt} - f_i(t, x, T) \right\| \right\}$$

$$\text{Subject to } g \sum_{g=0}^{r-1} \left\| \frac{dx_i}{dt} - f_i(t, x, T) \right\| \leq \epsilon$$

(2.8)

$$x_T(0) = x_{T_0}, x_B(0) = x_D(0) =$$

$$x_m(0) = x_G(0) = 0, x_A(0) = x_{A_0}$$

$$\text{Where } g = \frac{x_{A_0} - x_{T_0}}{r}, t_i = t_0 + ig,$$

$$x_i = x_i(t_i), T_i = T_i(t_i)$$

$$\frac{dx_i}{dt} = \dot{x}_i \approx \frac{x_{i+1} - x_i}{g} \text{ for } i=0,1,2,\dots,r-1$$

IV. CONCLUSIONS

We use AVK technique to solve the above control problem. This method represents a very attractive way for determination of optimal control policies of chemical processes. The method will be helpful for computer performances. This will be useful for upcoming researchers.

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