



Original Research Article

Modelling of the Homogeneous Transesterification of *Jatropha Curcas* Seed Oil

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ABSTRACT

Transesterification of Jatropha seed oil with methanol using sodium hydroxide as a catalyst was carried out in an improvised batch reactor. Molar ratio of methanol to oil of 8:1 was used for the reaction. From the start of the reaction, aliquots of the reaction mixture were withdrawn at every 15 minutes interval of time for Gas Chromatographic analysis to determine percentage fatty acid methyl ester formed. Kinetic equations were used to model the system in the LabView software environment. The rate constants were computed by directly evaluating the system of first-order differential equations using mole concentration values obtained during the experiment. The rate constants (k_1 , k_2 and k_4) at 60 °C were found to be 3.12, 2.03 and 0.06 L mol⁻¹min⁻¹ respectively.

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1. INTRODUCTION

The global world atmospheric temperature is increasing steadily and causing damage to the ecosystem. This problem is largely attributed to global warming caused by the emission of oxides of Carbon, Nitrogen and Sulphur from the usage of fossil fuels in internal combustion engine of various automobiles (Das, 2008; Refaat, 2010). The usage of bio-diesel produced from renewable feedstock such as *Jatropha curcas* seed oils or animal fats by transesterification offers a solution.

Transesterification is a chemical reaction between a raw renewable oil such as *Jatropha* seed oil and an alcohol such as methanol or ethanol in the presence of a catalyst such as sodium hydroxide, potassium hydroxide, calcium oxide or zeolite to chemically break the triglyceride molecule in the oil into fatty acid methyl or ethyl esters (biodiesel) with glycerol as a by product (Das, 2008; Pisarello *et al.*, 2010; Refaat, 2010). It is necessary therefore to produce bio-diesel from *Jatropha* seed oil for use in diesel engines either as neat bio-diesel or as a blend with petrol diesel (Das, 2008; Refaat, 2009; Akhihiero *et al.*, 2010). There is also the need to investigate the reaction kinetics and process variables affecting the reaction. *Jatropha curcas* seed oil is a non-edible oil and its usage as feed stock will not compete with food. Various authors have written on the homogeneous transesterification of *Jatropha* seed oil but the knowledge of the reaction kinetics and the variables such as temperature, time, molar ratio affecting the reaction are scarce in literature.

The knowledge of the reaction kinetics will aid in the design of a suitable reactor for bio-diesel processing from *Jatropha curcas* seed oil. This paper reports the reaction kinetics of the biodiesel produced from local *Jatropha* seed oil with methanol using sodium hydroxide as catalyst. The LabView Software was used to model the kinetics results obtained from experiments.

2. MATERIALS AND METHOD

2.1. Materials

Materials used in this research work include *Jatropha* seed oil extracted from fresh *Jatropha* seeds using a hydraulic crude press, methanol of high grade (HPLC grade), sodium hydroxide (Sigma Aldrich Company Germany), hot plate with a magnetic stirrer and temperature regulation system, an improvised reactor (500ml beaker), a mercury thermometer and cotton wool. The LabView software was used to model the reaction kinetic results obtained from experiment.

2.2. Experimental Method

Jatropha seed oil and methanol of equivalent of a molar ratio of methanol to oil 8:1 were weighed and placed each in two beakers, A and B respectively. Beaker A, containing the oil was heated to a temperature of 60-70°C to drive off any moisture that may be present in the oil. The free fatty acid of the oil was tested and found to be approximately 0.8%, hence suitable for transesterification to occur. One percent sodium hydroxide by weight of oil was dissolved in beaker B containing the methanol. The heated oil was allowed to cool to about 30°C. The oil was transesterified with the sodium methoxide solution by adding the solution slowly to the oil to avoid clogging while stirring on the hot plate at 450 rpm. The temperature of the reaction mixture was kept at 32°C and also at 60°C. Aliquots of the reaction mixture were withdrawn at 15 minutes' intervals of time for Gas chromatography analysis to determine concentrations of fatty acid methyl ester (FAME) and other glycerides formed. The reaction was carried out at atmospheric pressure.

2.3. Kinetic Modelling

According to Nouredini and Zhu (1997), transesterification reaction of TG with methanol in the presence of an alkaline catalyst would yield esters of fatty acids and GL, MG, and DG as intermediate products. The overall reaction steps are shown in Equations 1-4.



Where GL, MG, DG and TG represents Glycerol, Monoglycerides, Diglycerides and Triglycerides. The constants $K_1 - k_6$ are the rate constants. The characteristics of the stepwise reactions in Equations 1-4 were modelled using the set of differential equations shown in Equations 5-10.

$$\frac{d[TG]}{dt} = -k_1[TG][A] + k_2[DG][E] \quad (5)$$

$$\frac{d[DG]}{dt} = -k_1[DG][A] + k_2[DG][E] - k_3[DG][A] + k_4[MG][E] \quad (6)$$

$$\frac{d[DG]}{dt} = -k_3[TG][A] + k_4[DG][E] - k_5[DG][A] + k_6[MG][E] \quad (7)$$

$$\frac{d[GL]}{dt} = -k_5[MG][A] + k_6[GL][E] \quad (8)$$

$$\frac{d[E]}{dt} = -k_1[TG][A] + k_2[DG][E] + k_3[DG][A] + k_4[MG][E] + k_5[MG][A] \quad (9)$$

$$\frac{d[A]}{dt} = -\frac{d[E]}{dt} \quad (10)$$

Where A and E denote the alcohol and esters concentrations respectively.

The LabVIEW software was used to model the system of differential equations (Equations 5-10). A coefficient matrix was computed by obtaining the concentration products as presented in Table 1. Values were obtained for the terms on the left-hand side of Equations 5-10 from experimental data and inputted to a virtual instrument (VI) created in LabView.

Table 1: Coefficient matrix at 32 °C

[TG][ROH]	[DG][ME]	[DG][ROH]	[MG][ME]	[MG][ROH]	[GL][ME]
-0.002136	0.00585	0	0	0	0
0.002136	-0.00585	-0.000018	1.8993	0	0
0	0	0.000018	-1.8993	-0.005844	0.0117
0	0	0	0	0.005844	-0.0117
0.002136	-0.00585	0.000018	-1.8993	0.005844	-0.0117
-0.002136	0.00585	-0.000018	1.8993	-0.005844	0.0117

3. RESULTS AND DISCUSSION

3.1. Rate Constants

At 32 °C, the mole concentration derived at 75 minutes was used for the simulation. The initial conditions at room temperature (32 °C) for C_{A0} and C_{B0} were 2.4 mol. L⁻¹ and 19.2 Mol. L⁻¹ respectively. Where C_{A0} is the mole concentration of triglycerides and C_{A0} is the mole concentration of Alcohol. The rate constants are presented in Tables 2 and 3. The simple average of the rate constants obtained over the entire reaction duration was used as a basis for comparison with results from other studies. Table 4 shows the rate constants obtained using the method outlined in this paper and rate constants obtained by Nouredini and Zhu (1997) for soybean oil. Nouredini and Zhu (1997) generated rate constants for temperature of 50 °C. The differences in the results of Nouredini and Zhu (1997) obtained for soybean and that obtained in this study for *Jatropha* could be due to differences in reaction conditions and nature of oil. Although the biodiesel was formed at 32 °C probably because the oil has very low free fatty acid, the reaction in most cases will go to completion at temperature of 60 °C for 60 minutes and above.

Table 2: Rate constant obtained at 32°C

Time (mins)	k1	k2	k3	k4	k5	k6
0	2.4	0	0	0	19.2	0
7.5	2.5	-0.9	0.8	-0.1	19.7	-0.5
15	2.7	-1.8	1.9	-0.4	20.1	-0.9
22.5	2.9	-2.3	2.8	-1	19.6	-0.4
30	3.2	-0.6	1.9	-2.1	16.2	3
37.5	3.7	7.7	-5.4	-3.6	5.1	14.1
45	4.4	31.6	-28.7	-4.9	-21.3	40.5
52.5	4.7	85.1	-84.5	-3	-73.6	92.8
60	3	184.6	-194.9	9.7	-156.7	175.9
67.5	-4.9	329.3	-370.8	48.8	-246.6	265.8

Table 3: Rate constant obtained at 60°C

Time (mins)	k1	k2	k3	k4	k5	k6
0	2.4	0	0	0	19.2	0
7.5	2.6	5.7	-6.1	0.2	13.3	5.9
15	3	1.8	-2	-0.4	15.8	3.4
22.5	2.9	-1	0.2	0.3	19.6	-0.4
30	3.2	7.6	-8.3	0	10.1	9.1
37.5	3.4	-3.8	3.3	-0.4	20.6	-1.4
45	3.1	2.3	-3.7	0.7	16.2	3
52.5	3.7	6.7	-7.4	-0.6	9.2	10
60	3.5	-9.5	8.4	0	26.5	-7.3
67.5	3.4	10.5	-12.2	0.8	7.5	11.7
Average	3.12	2.03	-2.78	0.06	15.8	3.4

Table 4: Comparison of rate constant with previous studies

Glycerides	Rate constant	Value for Soybean oil (Noureddini and Zhu 1997) (Wt.%. min ⁻¹)	Values for <i>Jatropha</i> oil from the current research (L mol ⁻¹ min ⁻¹)
TG > DG	k1	0.050	3.12
DG > MG	k2	0.110	2.03
MG > GL	k4	1.228	0.06

4. CONCLUSION

The kinetics of the homogeneous base catalysed transesterification of *Jatropha curcas* seed oil has been studied. Some of the rate constants at the temperatures specified in this paper are negative and others are large. This could be due to reaction irregularities arising from improper stirring of reaction mixture.

5. CONFLICT OF INTEREST

There is no conflict of interest associated with this work.

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