



College of Engineering

ISSN: 1813-162X (Print) ; 2312-7589 (Online)

Tikrit Journal of Engineering Sciences

available online at: <http://www.tj-es.com>

TJES
Tikrit Journal of
Engineering Sciences

Owolabi RU, Usman MA, Anuoluwapo AD, Oguamanam OP. Modelling, Optimization and Green Metrics Evaluation of Bio-Catalytic Synthesis of Biodiesel. *Tikrit Journal of Engineering Sciences* 2020; 27(3): 17- 30.

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Keywords:

Response Surface Methodology, Central
Composite Design, Analysis of Variance,
Biodiesel

ARTICLE INFO

Article history:

Received 14 Jan. 2020
Accepted 15 Aug. 2020
Available online 01 Sep. 2020

Tikrit Journal of Engineering Sciences Tikrit Journal of Engineering Sciences Tikrit Journal of Engineering Sciences

Modelling, Optimization and Green Metrics Evaluation of Bio-Catalytic Synthesis of Biodiesel

ABSTRACT

The response surface methodology (RSM) was adopted in this study to evaluate the influence, interplay and interaction of various process variables on the biodiesel yield using methanol and castor oil as feedstocks in the presence of bovine bones as bio-catalyst. Twenty experimental runs were designed using central composite design (CCD). RSM statistical model of second order was developed. Analysis of variance (ANOVA) tests were performed on the model to find the relative influence of the process variables. An optimum yield of 95.12% was obtained at 60 °C reaction temperature, 120 minutes reaction time, molar to oil ratio 6:1, catalyst concentration of 10 % w and a stirring rate of 900 rpm. The experimental conditions under which biodiesel was synthesized in this study was compared with those of previous studies. It can therefore be inferred that, the conditions herein is competing with prior established conditions. The biodiesel was found to possess fuel properties that fall within acceptable limits and green metrics estimated showed compliance of the process with the dictates of green and sustainable chemistry.

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DOI: <http://dx.doi.org/10.25130/tjes.27.3.03>

1. INTRODUCTION

Fuels derived from biological sources are continuously receiving increasing attention over the years. In the last decade for instance, lengthy list of researchers [1], [2], [3], [4], [5], [6],[7] among others successfully carried out alcoholysis of various bio-sourced oil respectively, with each stressing the need for the synthesis of an alternative fuel called biodiesel referred to herein as green fuel. The dwindling depletion of the fossil fuel reserve and the

campaign to maintain pollution free environment have called for the sourcing of an alternative fuel [8], [9],[10],[11],[12],13,[14]. Biodiesel which can also act as a solvent [15] is characterized with proven positive toxicological records (Table 1) which is a key requirement to operate a green process to maintain a green and sustainable climate and generation. The green initiatives led to the renewed interest in biodiesel as alternative energy sources [5], [16] for reducing

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greenhouse effects in line with the Kyoto principle agreement, and need to further conserve the fossil fuel reserves on the basis of its direct use without any modification in diesel engines, boilers or other combustion engines and equipment. Though till recent time, manufacturers are still associated with limited field experience with biodiesel, few instances of such experience include the first successful trial run on a superfast passenger train which was conducted on December 31, 2002 by Indian railway on Delhi-Amritsar Shatabdi Express with use of 5 % biodiesel [17] and the first trial to test run a fossil diesel generator for hours at the University of Ilorin, Kwara state, Nigeria, Longitude 8.50 °N and Latitude 4.55 °E [18].

Apart from the green nature of the bio- catalyst, its use is an essential component of the present study as it may pave ways for synthesis of more functionalised biodiesel. However, a number of metrics have been proposed almost a decade ago to make chemists aware of the need to change the practice of chemical synthesis so that they become greener and less wasteful [19]. Hudlicky *et al* [20] proposed a metric known as effective mass yield (Eq.1) that is defined ‘as the percentage of the mass of desired product relative to the mass of all non-benign materials used in its synthesis.

$$\text{Effective mass yield} = \frac{\text{mass of product}}{\text{mass of non-benign reagents}} \times 100 \quad (1)$$

Sheldon [21] also proposed a metric known as E-factor (Eq.2) which is defined as

$$E - \text{factor} = \frac{\text{Total waste (kg)}}{\text{kg product}} \quad (2)$$

Curzons *et al* [22] similarly proposed a metric known as

$$\text{Mass Intensity} = \frac{\text{Total mass used in a process or process step (Kg)}}{\text{mass of product (kg)}} \quad (3)$$

Other metrics used in green and sustainable chemistry are shown in (Eq 4 - 6)

$$\% \text{ Carbon Efficiency} = \frac{\text{Amount of carbon in product}}{\text{Total carbon present in reactants}} \times 100 \quad (4)$$

$$\text{Reaction Mass Efficiency} = \frac{\text{mass of product}}{\text{mass of reactant}} \times 100 \quad (5)$$

$$\text{Atom Economy} = \frac{\text{molecular weight of desired product}}{\text{molecular weights of all the reactants or products}} \quad (6)$$

Wang *et al.*, [23] also described and proposed another concept called real atom economy or effective atom economy (Eq.7).

$$\text{Real Atom Economy} = \frac{\text{Actual weight of desired product(kg)}}{\text{Total weight of all raw materials in the product(kg)}} \quad (7)$$

To the best of our knowledge, no study has reported prior to this, the chemical process economy of biodiesel synthesis, the case of which is also been considered in this study.

Table 1

Toxicological Properties of Biodiesel and Organic solvents

Solvents	Toxicity
Toluene ¹	Narcotic, Liver and Kidney damage at high concentration
Benzene ¹	Carcinogenic
EthylBenzene ¹	Carcinogenic
Ethyl Acetate ¹	Narcotic, Liver and Kidney damage at high concentration
Xylene ¹	Narcotic at high concentration
Biodiesel ²	Non-Hazardous material.

1: [24] 2: [25]

The trans-esterification process that transforms the bio-sourced oil into the important green and future fuel should be optimized to improve its performance to obtain the maximum benefit from it by discovering process conditions that produce the best possible yield without compromising product quality and process safety. Traditionally, one-variable-at-a-time optimization technique was the common method among researchers of process optimization studies [26]. This method is prone to error as it does not include the interactive effects among the process variables. The biodiesel synthesis is affected by factors such as; the mode of reaction (homogeneous or heterogeneous), molar ratio of alcohol-to-oil, type of alcohol, type of oil, nature and amount of

catalysts, reaction time, reaction temperature and stirring rate [27]. These factors can be optimized using statistical optimization method of response surface methodology (RSM). Marcos [26] described RSM as a collection of mathematical and statistical techniques based on the fit of a polynomial equation to the experimental data, which must describe the behaviour of data set with the objective of making statistical correlation.

The actual objective is to simultaneously optimize the levels of these variables to attain the best system performance. It was observed from literature [28], [29], [30], [31] that numerous optimization studies on biodiesel synthesis from castor oil especially have been earlier reported, the dissimilarities are in terms of the

experimental design, methodology and alcoholysis. Kumar et al. [13] have optimized three reaction variables viz. catalyst concentration, reaction time and methanol quantity using five-level-three-factor central composite rotatable design (CCRD) based on RSM for the reduction of high FFA in JCO to <1% in 34 experiments. Two variables viz. methanol quantity and reaction time were optimized in 21 experiments to maximize the *Jatropha curcas* biodiesel (JCB) yield to 99%. Some biodiesel research groups have also applied RSM to optimize process variables for biodiesel production, using rapeseed oil, soybean oil, cottonseed oil, and lard [32], [33], [34], [35]. The objective herein is to investigate the effects of process variables (methanol-to-oil molar ratio, bio-catalyst amount reaction time and stirring rate) on the methanolysis of castor oil to biodiesel (fatty acid methyl ester, FAME) in a bio-catalysed environment and to optimize the variables using response surface modeling methodology (RSM) with central composite design (CCD).

2. Materials and Methods

2.1 Process optimization of the green fuel synthesis

A statistical approach was adopted for the process optimization of the green fuel production. This is to **Table 2**

Experimental variables and their coded levels for central composite design

Variables	Symbols	Units	Coded Variables Level		
			-1	0	1
Catalyst Concentration	X ₁	Weight % of oil	5	10	15
Reaction Time	X ₂	mins	40	80	120
Stirring Speed	X ₃	Rotation per minute	800	900	1000

The central level chosen for the reactions were the 5 % weight catalyst concentration, 80 minutes reaction time and a stirring speed of 900 rotation per minute. The reaction temperature and methanol to oil molar ratio of 6:1 in were chosen to be constant. Other levels were chosen based on prior experience.

The response for this experiment was the yield of biodiesel (Y %). The response was used to develop an algebraic model of the form of (Eq.9) that correlated the response to the process parameters.

$$Y = b_o + \sum_{i=1}^n b_i X_i + \sum_{i=1}^n b_{ii} X_{ii} + \sum_{i=1}^{n-1} \sum_{j=i+1}^n b_{ij} X_i X_j \tag{9}$$

where Y is the predicted response, b_o is a constant coefficient, b_i is a linear coefficient, b_{ii} is the quadratic equation, b_{ij} is an interaction coefficient, and X_i and

enable us to have a statistical understanding of the parametric on the yield of the biodiesel. Application of the statistical approach requires appropriate selection of the response, factors or variables and level. For the limitation of complexities, some other reaction parameters such as agitation speed and reactants molar ratio were made constant and reactions were conducted at atmospheric pressure.

2.2 Design of Experiment

The green fuel productions were carried out following the design of the RSM tool (Table 3) after prior selection of factors or variables and ranges based on prior experience [30], [36],[37],[38], [39]. The variables studied were the catalyst concentration (X₁), reaction time (X₂) and stirring speed (X₃). Table 2 shows all variables and their corresponding ranges on the basis of preliminary studies as earlier said. A five-level-three-factor central composite design (CCD) which requires 20 experimental runs (calculated based on Eq.8 with the following distributions; 8 factorial runs, 6 axial runs and 6 replicates runs at the centre was employed.

$$N = 2^{n*} + 2n* + N_c \tag{8}$$

where N is the total experimental runs, n* is the number of variables and N_c is the centre point replication.

X_j are the coded values of the process variables. Table 3 and Table 4 (standard experimentation matrix) shows the run order and experimental design. Columns 2 to 4 represent the variable levels coded in the dimensionless coordinate while columns 5 to 7 represent the dimensional variable levels.

Experimental design tool (MINITAB 16.1) was used for RSM regression analysis. The statistical analysis, significance and testing of the regression model were done by ANOVA analysis with F-test to obtain the statistical correlation between the process variables. To determine the soundness of fit of the model, each term of model was statistically tested to confirm the significance of F - values with 95% confidence level (i.e p ≤ 0.05). The p values indicate the significance of the coefficients in the algebraic model. The influence of the term is significant if the value of the critical level p < 0.05 [40]. The values of R² (Coefficient of Determination), adjusted

R², and predicted R², lack of fit and adequate precision of models were also obtained to check the soundness, adequacy and limitations or shortcomings of the **Table 3**

Experimental design matrix for the green fuel synthesis.

Run	Coded Factor			Actual Factor		
	X ₁	X ₂	X ₃	X ₁ (% w)	X ₂ (mins)	X ₃ (rpm)
1	-1	-1	-1	5	40	800
2	-1	1	1	5	120	1000
3	0	0	0	10	80	900
4	-1	0	0	5	80	900
5	1	-1	1	15	40	1000
6	0	0	-1	10	80	800
7	-1	1	-1	5	120	800
8	1	1	-1	15	120	800
9	0	0	0	10	80	900
10	0	0	0	10	80	900
11	1	-1	0	15	40	800
12	-1	-1	1	5	40	1000
13	0	0	-1	10	80	900
14	1	1	1	15	120	1000
15	0	0	-1	10	80	900
16	0	0	1	10	80	1000
17	0	1	0	10	120	900
18	0	0	0	10	80	900
19	0	-1	0	10	40	900
20	1	0	0	15	80	900

presented model. The response surface plots and contour plots were also drawn to visualize relationships between the process variables.

2.3 Greenness parameters of the fuel production

The green metrics of the green fuel production were estimated based on the correlations as contained in Eq 1 to 7 for the evaluation of effective mass yield, e-factor, mass intensity, % carbon efficiency, reaction mass efficiency, atom economy and real atom economy.

3. Results and Discussions

3.1 Process optimization of the green fuel synthesis

The CCD component of the response surface methodology was used to established a statistical relationship between the trans-esterification process parameters and the biodiesel yield through a designed experimental model to determine the optimal point [41] herein referred to as set of process parameters that yield highest biodiesel yield. Experimental run 17 gave the optimum conditions with the highest biodiesel yield of 95.12 % at 10 wt% catalyst concentration, 120 reaction time and stirring speed of 900 rpm. The same experimental run was repeated for further verification and validation and obtained a yield of 95.74 %. The optimum yield was obtained at constant temperature of 60 °C and methanol to oil molar ratio of 6:1 [3]. One

key difference between the process conditions herein and that of others, particularly for homogeneous catalyst is that larger amount of biocatalyst (≥ 5 wt %) was required compared to homogeneous catalyst which required ≤ 1 wt% catalyst concentration [3], [41].

3.2 Validation of the statistical model

Various kinetic models of the trans-esterification process have been developed where we observed intricacies and mathematical rigours which can pose a serious challenge to model routine usage. There is therefore a strong need to obtain a more user friendly model suitable for industrial applications. The present study proffered solution in this regard by generating an algebraic model in terms of the trans-esterification process parameters through the RSM software application (Minitab). A polynomial regression equation of order 2 was fitted between biodiesel yield and the process variables such as catalyst concentration (X₁), reaction time (X₂) and stirring speed (X₃) to obtain Eq.10

$$\begin{aligned}
 \text{Yield \%} = & 209 + 9.70X_1 + 0.645X_2 - 0.452X_3 - \\
 & 0.3792X_1^2 - 0.00103X_2^2 + 0.000265X_3^2 - 0.01144X_1X_2 - \\
 & 0.00071X_1X_3 - 0.000194X_2X_3
 \end{aligned} \tag{10}$$

A positive coefficients is an indication of a synergetic effect while a negative one indicates an antagonistic effect. A high value of coefficient also indicates the extent of synergetic or antagonistic effect and vice versa. From the model, stirring speed does not have much effect compared to the catalyst concentration and the reaction time at constant temperature of 60 °C methanol to oil molar ratio of 6:1. From the regression model (Eq.10), the catalyst has the highest and most positive coefficient. This implies that increase in the bio-catalyst

concentration will accelerate the trans-esterification rates. Bouaid *et al* [43] in their optimization studies of biodiesel production from waste canola oil obtained similar results and in another scenario for waste cooking oil. Yuan *et al.*[44] also presented similar observation. Still, a reduction in biodiesel yield is possible if much of the catalyst is loaded and when reactions are further prolonged. Similar observation for the catalyst loading was recorded by Charoenchaitrakool and Thienmethangkoon [45].

Table 4
Experimental design matrix for the green fuel synthesis.

	Coded Factor			Actual Factor			Observed response	Predicted Response	Residuals
	X ₁	X ₂	X ₃	X ₁ (% w)	X ₂ (mins)	X ₃ (rpm)			
1	-1	-1	-1	5	40	800	70.42	68.84	1.58
2	-1	1	1	5	120	1000	92.28	89.89	2.39
3	0	0	0	10	80	900	93.64	91.43	2.21
4	-1	0	0	5	80	900	74.26	79.14	-4.88
5	1	-1	1	15	40	1000	80.40	81.06	-0.66
6	0	0	-1	10	80	800	93.22	93.84	-0.62
7	-1	1	-1	5	120	800	91.60	90.26	1.34
8	1	1	-1	15	120	800	92.38	92.01	0.39
9	0	0	0	10	80	900	93.38	91.43	1.95
10	0	0	0	10	80	900	90.42	91.43	-1.01
11	1	-1	0	15	40	800	78.02	79.74	-1.72
12	-1	-1	1	5	40	1000	71.88	71.57	0.31
13	0	0	-1	10	80	900	95.02	91.43	3.59
14	1	1	1	15	120	1000	89.32	90.23	-0.91
15	0	0	-1	10	80	900	92.86	91.43	1.43
16	0	0	1	10	80	1000	94.12	94.31	-0.20
17	0	1	0	10	120	900	95.12	97.43	-2.31
18	0	0	0	10	80	900	94.12	91.43	2.69
19	0	-1	0	10	40	900	83.28	82.13	1.15
20	1	0	0	15	80	900	88.46	84.76	3.70

3.3 Analysis of variance

Table 5 shows the analysis of variance to further ascertain the adequacy of the model for the prediction of biodiesel yield. From the analysis, it can be inferred which of the trans-esterification process variables significantly affected the biodiesel yield. For instance, the linear terms were found to be significant with special emphasis on the catalyst concentration and the reaction time. None of the quadratic terms was found to be significant. This implies

that the excess amount of the catalyst concentration, prolonged reaction time and agitation in excess will reduce the biodiesel production. In support of this, Vicente *et al* [33] reported that, the excessive amount of catalyst increases emulsion formation. In another report, Leung and Guo [46] reported the influence of excess reaction time on trans-esterification process. According to them, it does not enhance the biodiesel yield but favour the reverse reaction of transesterification. Though, the two major feedstocks (castor oil and

methanol) showed strong immiscibility calling for a high mixing rate to increase the contact surface area of the reactants and to overcome the likely mass transfer limitation, still, the agitation should not be in excess to disallow the reverse reaction.

As depicted by the small probability (p) value (<0.05) and insignificant lack of fit, the adequacy of the model is guaranteed. The significance and adequacy of the established model was further ascertained by the coefficient of determination (R²) value of 0.9354 and adj. R² value of 0.8772. This implies that the model explains 93.54% of the variation in the experimental data.

Table 5.

Analysis of variance (ANOVA) for biodiesel yield

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Regression Model	9	1201.18	1130.46	125.607	16.08	0.000
Linear	3	667.83	668.21	222.738	28.51	0.000
catalyst concentration	1	79.30	79.19	79.186	10.14	0.010
reaction time	1	588.98	588.29	588.289	75.30	0.000
stirring speed	1	0.55	0.74	0.740	0.09	0.765
Square	3	485.73	414.56	138.186	17.69	0.000
catalyst concentration*catalyst concentration	1	465.42	247.19	247.191	31.64	0.000
reaction time*reaction time	1	4.09	7.40	7.405	0.95	0.353
stirring speed*stirring speed	1	16.23	19.30	19.299	2.47	0.147
Interaction	3	47.62	47.69	15.897	2.03	0.173
catalyst concentration*reaction time	1	41.77	41.86	41.861	5.36	0.043
catalyst concentration*stirring speed	1	0.98	0.99	0.994	0.13	0.729
reaction time*stirring speed	1	0.98	4.84	4.836	0.62	0.450
Residual Error	10	83.01	78.12	7.812		
Lack-of-Fit	5	70.18	61.57	12.315	3.72	0.088
Pure Error	5	12.82	16.55	3.310		
Total	19	1208.59				

$S = 2.79508$ $R^2 = 93.54\%$ $R^2(\text{pred}) = 56.66\%$, $R^2(\text{adj}) = 87.72\%$

Three dimensional surface plots were obtained using the minitab software to study the interactive effects of the process variables on the biodiesel yield. This was done by plotting three dimensional surface curves against any two independent variables, while maintaining other variables at their central (0) level. The surface plots are shown in Fig 2-4.

The surface curves provides indepth understanding of the interaction of variables and identifies the optimum level of each variable for maximum response also referred to as biodiesel yield. Elliptical curves indicates a good interaction of the two process variables while

The bio-catalyst concentration (both linear and quadratic) has the smallest p –values and largest F-values. This informed that among the process parameters, the bio-catalyst concentration is the most important under the conditions considered [47].

The residual plots associated with the regression model (Eq.10) were analysed as depicted on Fig 1 for the model accuracy. The points on Fig 1 are well distributed on the line of best fit which is an indication of the adequacy of the generated model.

cyclical one denotes an evidence of no interaction between the variables. For this study, all the curves obtained showed that there are some level of interaction between all the variables.

In Fig 2, the catalyst loading and stirring speed increases with increase in biodiesel yield up to a level (10 % wt catalyst concentration and 900 rpm) otherwise, it decreases at constant reaction time of 80 minutes. Most related optimization studies unlike the present one remain silent particularly on the interactive effects of stirring rate with other process variables as observed in the work of Goli and Sahu [48].

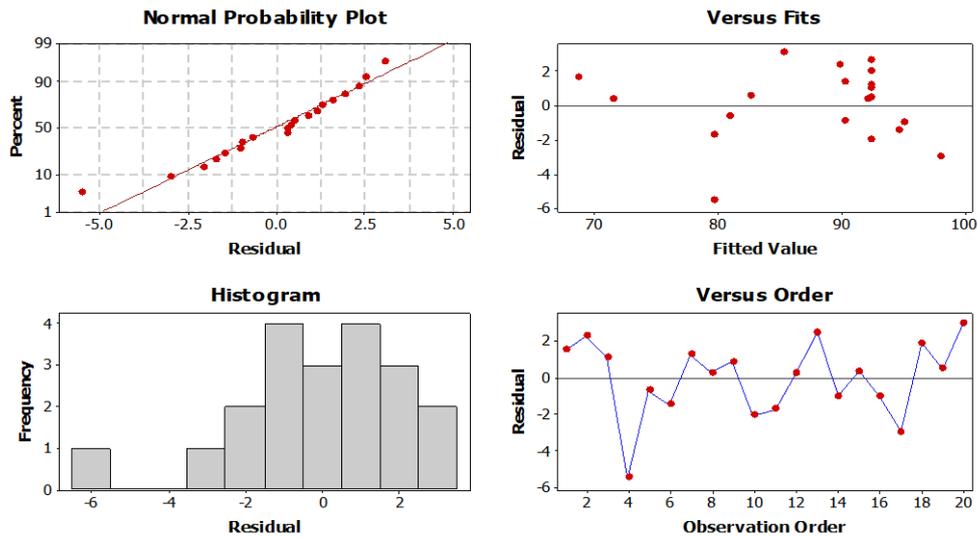


Fig.1. Residual plots for The Biodiesel Yield

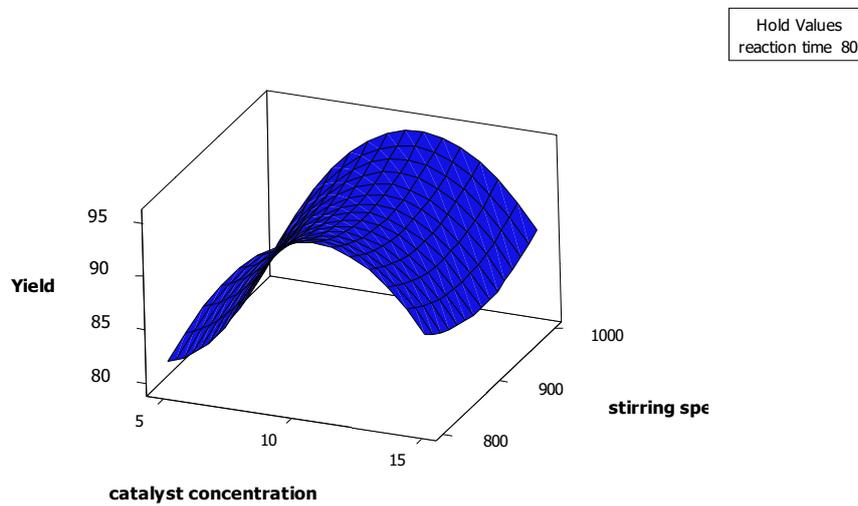


Fig. 2. Surface plot for the biodiesel yield against stirring speed and catalyst concentration at constant reaction Time.

Similarly, in Fig 3, biodiesel yield increases up to a catalyst loading of 10 wt % and with increase in reaction

time at constant stirring speed of 900 rpm. At lower catalyst loading and shorter reaction time, the biodiesel yield drops drastically.

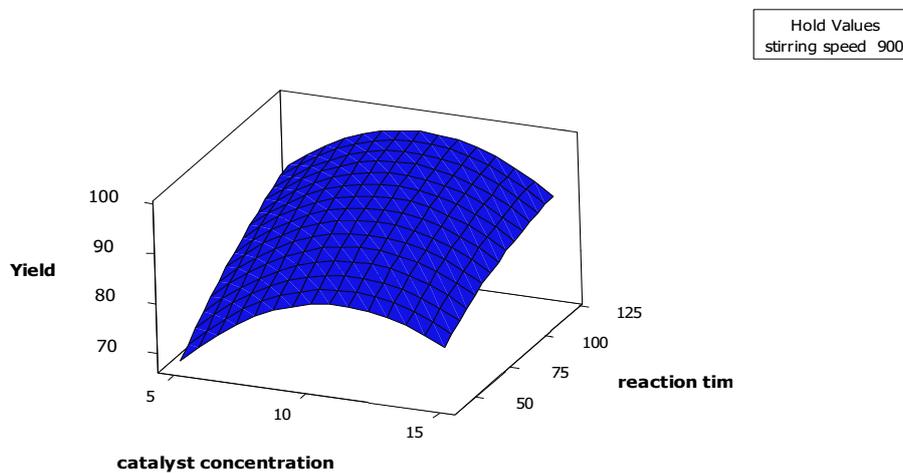


Fig. 3. Surface plot for biodiesel yield against reaction time and catalyst concentration at constant stirring speed

From Fig. 4, no significant interactive effect was observed between reaction time and stirring speed. Biodiesel yield increases with increase in reaction time but the yield remained fairly constant with increase in stirring speed. At low reaction time, the biodiesel yield remains low even at high stirring rate. The effect of reaction time on biodiesel yield is clearly pronounced at constant catalyst loading.

provides clearer explanation on how the yield of biodiesel respond to changes in process conditions. The contour plots specifies optimum conditions and their corresponding responses. Operating at a reaction time of between 100 - 110 mins at any stirring speed between 800 -1000 rpm gives a biodiesel yield > 97.5%. holding catalyst concentration to be 10 wt%. Reduction of the reaction time to about 40 minutes with same stirring speed and catalyst concentration values may result to < 85 % biodiesel yield.

Fig. 5 shows the contour plot of the biodiesel yield with reaction time and stirring speed. The contour regions

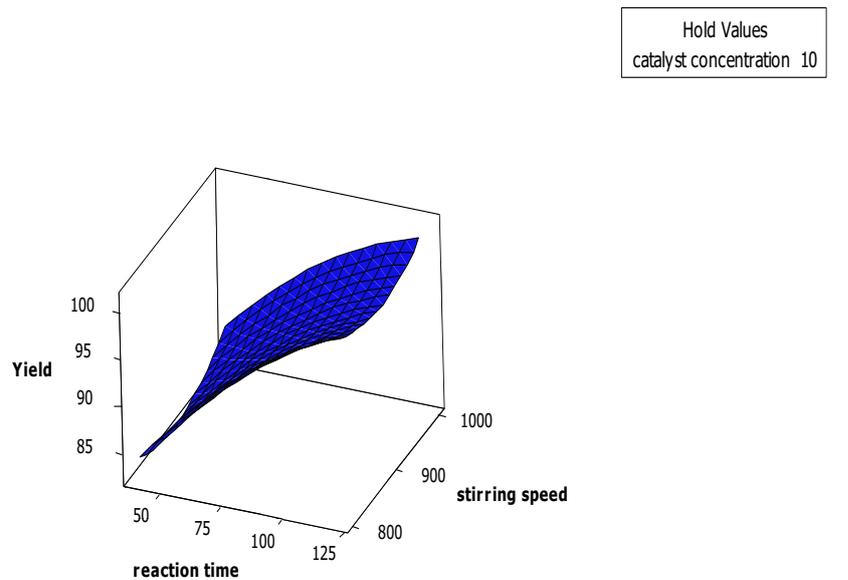


Fig.4. Surface plot for biodiesel yield against stirring speed and reaction time at constant catalyst concentration.

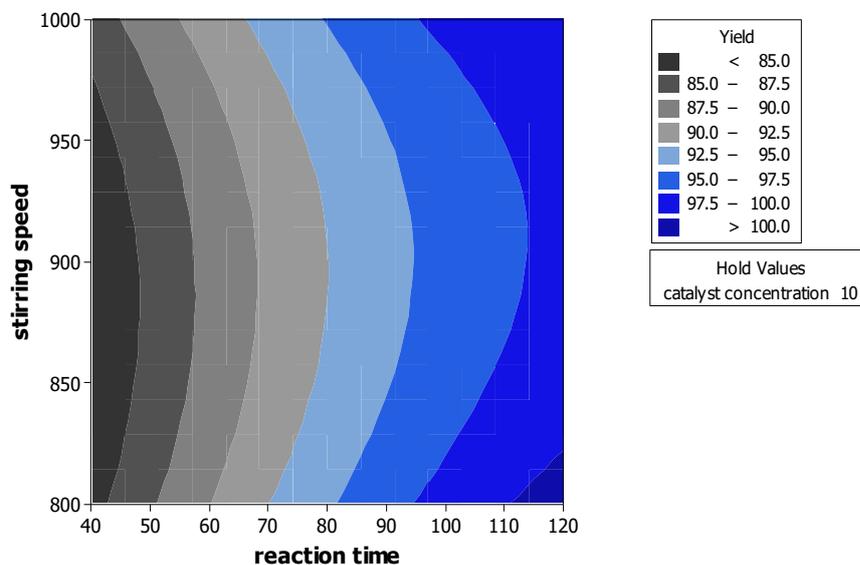


Fig. 5. Contour plots of biodiesel yield with stirring speed and reaction time

Fig. 6 shows the contour plot of biodiesel yield with catalyst concentration and stirring speed at constant reaction time. Operating at a catalyst concentration of about 10 wt % and stirring speed of about 900 rpm will results into biodiesel yield of about 92.5 - 95 %.

Similarly, Fig.7 shows the contour plot of biodiesel yield with reaction time and catalyst concentration at constant reaction time of 80 minutes. Operating at a catalyst concentration of about 10 wt % and reaction time of 100 - 120 minutes will results into biodiesel yield > 95 %. The experimental conditions under which biodiesel was synthesized in this study was compared with those of previous studies (Table.6) .It can therefore be inferred that , the conditions herein is competing with prior established conditions. Low amount of catalyst, shorter

reaction time, milder agitation and low consuming molar ratio were observed for the case of synthetic and homogeneous catalysts compared to others.

Calculated values of green index for biodiesel production are contained in Table 7 For the E-factor, the closer to zero it is, the lesser the waste generated which is an indication of a more sustainable and greener process [54]. The effective mass yield is an indication of the presence of the product (biodiesel) in all other reacting species [20], [21]. Atom economy is an index that provides information about the quantity of the feedstocks that got converted into finished products [55],[56]. The percentage carbon is an index for the carbon re-distribution and accounting.

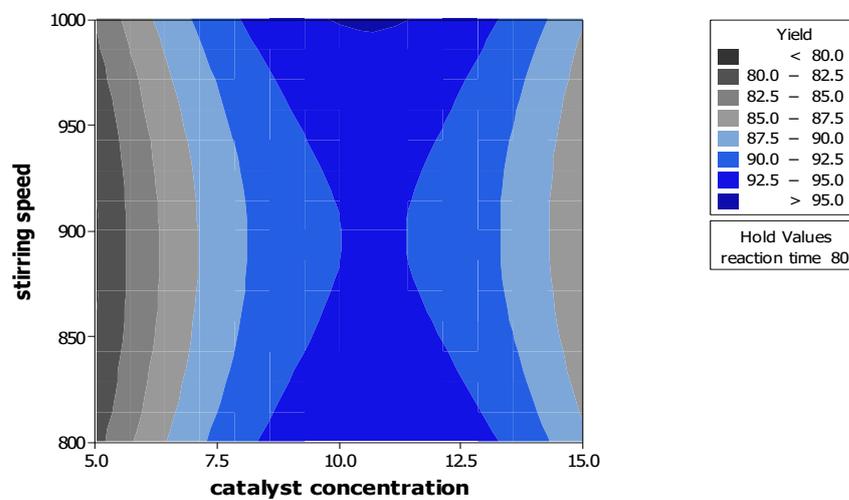


Fig.6. Ccontour plot for biodiesel yield with stirring speed and catalyst concentration

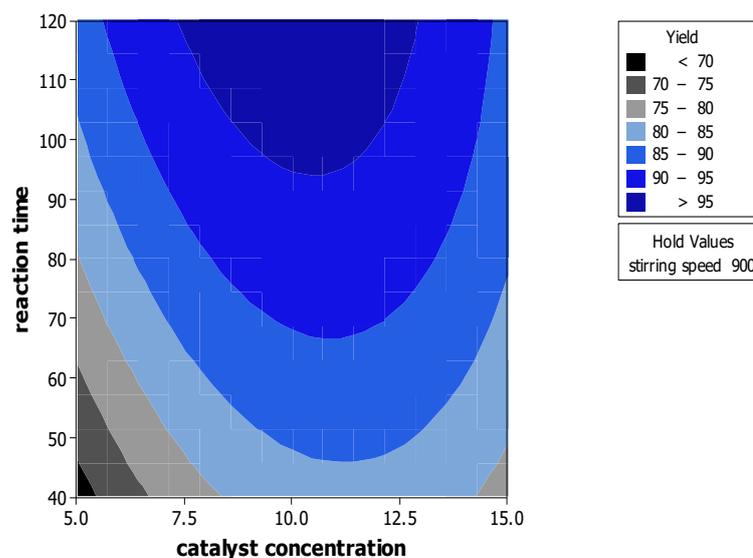


Fig. 7. Contour plots for yield with reaction time, catalyst concentration

Conclusion

The optimization of castor oil methanolysis was carried out using response surface methodology. The RSM designed procedure was adopted to optimize the process variables to determine maximum biodiesel yield and a second-order response equation was obtained for the biodiesel yield as a function of the process variables. All the process variables considered influenced the methanolysis either positively or negatively. The methanol oil molar ratio was the most significant linear effect, no significant squared effects while the reaction time has the least squared negative effect and the reaction temperature/methanol to oil molar ratio was the most significant interactive effect. An optimum yield of 95.12% was obtained at 60 °C reaction temperature, 120 minutes reaction time, molar to oil ratio 6:1, catalyst

concentration of 10 % w and a stirring rate of 900 rpm. The major composition of the castor oil is ricinoleic acid with a content of 85 -95 %. The castor oil biodiesel produced under the optimized conditions meets standard specification. The synthesized green fuel at optimum operating conditions was found to meet the dictates of the green and sustainable chemistry which aimed at saving the earth and preserving the climate for future generation.

Acknowledgement

This research work received full funding from the Professor Ayo Ogunye professorial chair in chemical engineering (Third Edition) through the office of advancement, University of Lagos Ref. No.:VC/OA/E.29/Vol.7.

Table 6

Comparison of the present work with other related studies

S/N	Optimum Conditions	Feedstocks	Biodiesel Yield	Reference
1	Cow bone 10 wt% , 120 mins, 900 rpm, 60 °C, 6:1	Castor oil	95.12%	This Study
2	KOH 1.4 wt % , 60 mins, 500 rpm, 65 °C, 7.5:1	Waste cooking oil (Soya bean and Sun flower)	99.38%	[47]
3	Chicken egg shell 7 wt % , 3 hrs, 57.5 °C, 6:1	Soya bean oil	93%	[48]
4	Animal bone 20 wt % , 4 hrs, 18:1, 200 rpm, 65 °C	Palm oil	96.78%	[49]
5	Animal bone 6 wt % , 3 hrs, 9:1, 70 °C	Jatropha	96.1%	[50]
6	Crab shell 2.5 wt% , 120 mins, 700 rpm, 8:1, 65 °C	Karanja seed oil	94%	[51]
7	CaO derived from Mud Clam Shell 3 wt% , 2 hrs, 60 °C , 14:1,	Castor	96.7%	[52]
8.	River snail shell 5 wt% , 90 mins, 12:1, 65 °C, 10% v/v co- solvent	Palm oil	98.5%	[53]

Table 7

Greeness Parameters of the Fuel Production

S/N	Green Correlation	Metrics	Calculated Values	Remark
1	Environmental Factor		0.201	Close to zero and hence less waste is generated [54]
2	Effective Mass Yield		1.5	This is an indication of presence of the products on other reacting species [20],[21].
3	Atom Economy		90.58 %	An indication of feedstocks that incorporated into products [55],[56].
4	% carbon Efficiency		33.33 %	This is an account of the carbon present in the product compared to the starting material [55],[22].
5	Real Atom Economy		76.6	Relatively High usage of Feedstock
6	Mass Productivity		1.41	Close to 1 which indicates slight wastage.
7	Reaction Efficiency	Mass	84.6	This is an index to identify better reaction routes for waste minimization [22],[57],[58],[59],[60],[61].

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