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Modeling and Optimization of Microwave-Based Bio-Jet Fuel from Coconut Oil: Investigation of Response Surface Methodology (RSM) and Artificial Neural Network Methodology (ANN)

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Abstract: In this study, coconut oils have been transesterified with ethanol using microwave technology. The product obtained (biodiesel and FAEE) was then fractional distillated under vacuum to collect bio-kerosene or bio-jet fuel, which is a renewable fuel to operate a gas turbine engine. This process was modeled using RSM and ANN for optimization purposes. The developed models were proved to be reliable and accurate through different statistical tests and the results showed that ANN modeling was better than RSM. Based on the study, the optimum bio-jet fuel production yield of 74.45 wt% could be achieved with an ethanol–oil molar ratio of 9.25:1 under microwave irradiation with a power of 163.69 W for 12.66 min. This predicted value was obtained from the ANN model that has been optimized with ACO. Besides that, the sensitivity analysis indicated that microwave power offers a dominant impact on the results, followed by the reaction time and lastly ethanol–oil molar ratio. The properties of the bio-jet fuel obtained in this work was also measured and compared with American Society for Testing and Materials (ASTM) D1655 standard.

Keywords: bio-jet fuel; microwave-assisted transesterification; RSM; ANN; optimization; coconut oil

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1. Introduction

Amongst renewable energy technologies the current trend is technology which aims to optimally utilize clean and sustainable energy sources, based on current and future economic and societal needs. Social and economic development is always followed with an increase in energy demand. Currently, most of the energy demand is fulfilled by non-renewable fossil fuels, including natural gas, coal, and petroleum. The formation of fossil fuels took hundreds of million years. It is predicted that with the current consumption rate, fossil fuel will deplete in the near future [1,2]. Furthermore, the burning of fossil fuels results in negative environmental impacts, such as global warming, acid rain, climate change, and others. Hence, it is crucial to look for alternative energy resources that are clean and sustainable to replace the non-renewable fossil fuel.

There are a series of studies that have been done in exploring renewable energy technologies, such as solar energy, wind energy, tidal energy, and biofuels [3–8]. Among the available renewable energy, liquid biofuel from biomass resources has received a lot of attention [9–11], especially in the transportation sector, as it offers an opportunity to replace petroleum in operating the combustion engine with little to no modification [12,13]. In fact, over 90% of transportation nowadays is still dependent on non-renewable fossil fuel [14]. Therefore, many works have been done to enhance and improve the biofuel production technologies, especially biodiesel, a renewable replacement of diesel fuel [15–18]. Nevertheless, there is only a little information about the production of bio-kerosene (bio-jet fuel). Bio-jet fuel is a promising alternative fuel for a jet engine. Other than the aviation sector, bio-jet fuel also can be used in the power generation sector to operate the gas turbine engine. Hence, the bio-jet fuel production technologies should be further explored and investigated in obtaining a comparable renewable replacement for petroleum-based kerosene at sufficient volume.

Based on the statistical report, flights produced 859 Mt of carbon dioxide (CO_2) globally in 2017. In the other words, approximately 2% of the CO_2 emitted through human activities is contributed by the global aviation sector. In addition, this 859 Mt of CO_2 is responsible for 12% of CO_2 emission from all transports sources [19,20]. CO_2 is one of the greenhouse gases that will trap heat within the Earth's atmosphere, causing global warming and climate change. In order to mitigate the CO_2 emissions from air transport and, at the same time, to address the global challenge of climate change, the International Air Transport Association (IATA) has adopted a set of targets and approaches. One of the ambitious targets is to achieve 50% reduction in net aviation carbon emissions by 2050 as compared to 2005, through the deployment of sustainable low-carbon fuels, such as bio-jet fuel [19].

Generally, aviation liquid fuel can be produced from different biomass feedstock with different methods [21–23]. Currently, transesterification and hydrotreating are the main production method of bio-jet fuel [24]. Unlike the hydrotreating process, transesterification requires an upgrading process to separate bio-jet fuel from the product of transesterification (biodiesel). Although an additional downstream process is required, however, the transesterification process operates under milder condition as compared to the hydrotreating process. Hence, its operating cost are relatively lower. The transesterification process involves three consecutive and reversible reactions (refer to Equations (1)–(3)) that react triglyceride with alcohol in the presence or absence of a catalyst and produce a mixture of fatty acid alkyl ester (FAAE or biodiesel) and glycerol as a by-product. In overall, transesterification requires 1 mole of triglyceride and 3 moles of alcohol to produce 3 moles of biodiesel, as shown in Equation (4). However, practically, the excess amount of alcohol is usually used to shift the equilibrium to the product side and allow the phase separation of biodiesel from the glycerol [25].

$$Triglyceride\ (oil\ or\ fat) + ROH\ (alcohol) \leftrightarrow Diglyceride + R\prime COOR \tag{1}$$

$$Diglyceride + ROH \leftrightarrow Monoglyceride + R\prime COOR \tag{2}$$

$$Monoglyceride + ROH \leftrightarrow Glycerol + R\prime COOR \tag{3}$$

$$Triglyceride\ (oil\ or\ fat) + 3ROH\ (alcohol) \leftrightarrow Glycerol + 3R'COOR\ (FAAE) \tag{4}$$

Commonly, methanol is used for biodiesel production via transesterification reactions. This is because methanol is cheaper, allows phase separation to be conducted more easily, and permits the transesterification process to be conducted under milder conditions [26]. However, methanol is very toxic to humans, as in the body methanol is metabolized into formaldehyde and then formic acid. Therefore, there is the scope of using ethanol for producing biodiesel. Ethanol has several advantages to methanol, such as offering better solvent properties and low toxicity relative to methanol [27,28] Furthermore, there is a study reported that the biodiesel formed using ethanol, the fatty acid ethyl ester (FAEE) present a higher cetane number, calorific value, oxidation stability, lubricant characteristics, lower cloud and pour points, and also have lower tailpipe emissions in comparison to the product collected using methanol, fatty acid methyl ester (FAME) [29,30].

In addition, microwave technology is deployed to replace conventional heating in this study. Microwave technology is a green processing method that offers several advantages, such as by being more environmental-friendly, in terms of lower energy consumption. Furthermore, the volumetric heating mechanism of microwave heating also allows rapid heating, enhances chemical reaction rate and selectivity, and improves the production quality and yield [25]. Microwave heating has received a lot of attention since the 1970s, especially in the chemical research. Conventional heating transfers heat into the reactant through the reactant vessel via conduction and convection (wall heating). However, microwave heating is highly dependent on the dielectric properties of the reactant [25,31]. It allows direct heating of the material without heat-up of the reactant vessel [32]. Hence, microwave heating allows selective and rapid heating, as mentioned previously.

Numerous studies have been done on the microwave-assisted transesterification process for biodiesel production [25,33,34]. Compared to other approaches, transesterification is the simplest and a widely-accepted method to reduce oil viscosity because it is cost-effective. Therefore, modeling the process and optimizing the process input variables involved are important in order to save time, achieve high product yield and reduce the overall cost to produce biodiesel. Response surface methodology (RSM) and artificial neural network (ANN) are one of the mathematical methods for modeling transesterification processes [35–38]. Some of the advantages that RSM has are the durability under optimal setting conditions and the ability to minimize the number of trials required to provide sufficient evidence for statistically acceptable results [37].

Artificial neural network (ANN) is an information processing system that has characteristics such as biological neural networks that imitates the behaviour and learning process of the human brain. An interesting characteristic of this ANN is its ability to learn (learning and training). The training process at ANN aims to find convergent weights between layers so that the weights obtained to produce the desired output. ANNs are universal approximators and their predictions are based on prior available data, have shown great ability in solving complex nonlinear systems [39].

Ant colony optimization (ACO) is a swarm intelligence technique which is inspired by natural metaphors, namely communication and cooperation between ants to find the shortest path from the nest ants to the food. It is desirable to integrate ACO with ANN model since ACO is capable of optimizing complex process parameters [15,40]. Coupling ACO with the ANN is desirable since the ACO algorithm is capable of optimizing complex process parameters [41].

This study proposed the production of bio-jet fuel through microwave-assisted catalytic transesterification from coconut oil. Coconut oil was selected as the raw feedstock as it consists of a high percentage of medium-chain triglycerides, which made it suitable to be used for bio-jet fuel production [22,42]. An optimization study was conducted in this work based on three parameters, including oil to ethanol molar ratio, reaction time and microwave power, using response surface methodology (RSM) and artificial neural network (ANN) coupled with ant colony optimization (ACO) algorithm. Additionally, the relevant characterizations of coconut oil through the application of gas chromatographic-mass spectrometry and Fourier transform infrared spectrometry analyses of the coconut oil, FAEE, and bio-jet fuel were conducted and reported. The physicochemical properties of the bio-jet fuel collected and their comparison with the ASTM standard are also reported in this paper.

2. Materials and Methods

2.1. Materials and Equipment

Coconut oil was purchased from the local market in Selangor, Malaysia. The coconut oil was then analyzed using gas chromatography, GC (Agilent, 7890A, Wilmington, DE, USA) to obtain its fatty acid profile, as reported in Table 1. Ethanol (C_2H_5OH) and potassium hydroxide (KOH) were purchased from Sigma–Aldrich (St. Louis, MO, USA).

Table 1. Fatty acid composition of coconut oil.

Fatty Acid	Composition (wt%)
Caprylic acid, C8:0	6.0
Capric acid, C10:0	5.1
Lauric acid, C12:0	48.5
Myristic acid, C14:0	16.9
Palmitic acid, C16:0	9.6
Stearic acid, C18:0	2.3
Oleic acid, C18:1	8.2
Linoleic acid, C18:2	3.4

2.2. *Microwave-Assisted Catalytic Transesterification*

The experiments of this work involve the catalytic transesterification of coconut oil under microwave irradiation. Firstly, coconut oil and ethanol at a specific molar ratio with 0.5 wt% of potassium hydroxide (KOH) catalyst concentration was prepared. Then, the mixture (reactant) was poured into a 250 mL round bottom flask with a magnetic stirrer bar and put into the microwave reactor. Next, the reflux system was attached, and the reactant was then subjected to microwave irradiation with different power settings under different reaction times at a stirring speed of 200 rpm. At the same time, the temperature of the reflux system was maintained at −4 °C by using a chiller to condense back the vaporized reactant. After completion, the product of this transesterification process was cooled to room temperature. The equipment used in producing bio-jet fuel via transesterification was a modified microwave oven equipped with a reflux system, as shown in Figure 1.

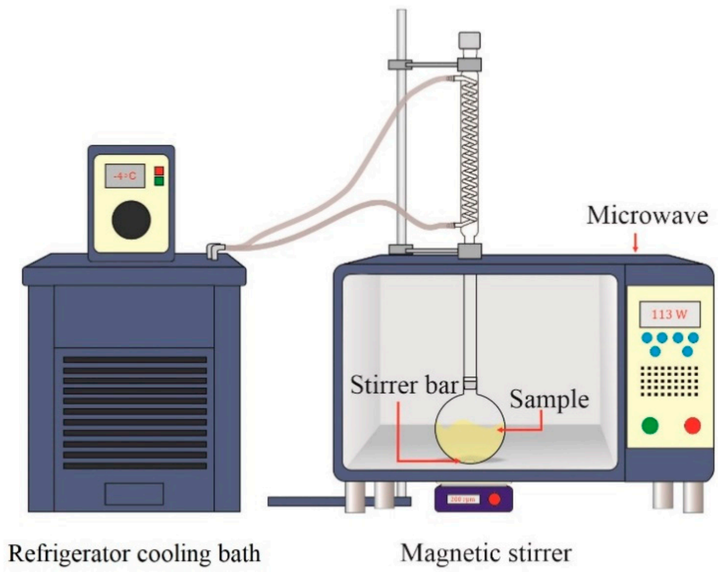

Figure 1. Experimental setup for microwave-assisted catalytic transesterification.

Then, the product was left in a separating funnel to split the liquid phases. The upper layer, which is the fatty acid ethyl ester (FAEE), was washed using warm water three times and dried at 100 °C for 1 h in the conventional oven to remove the moisture.

2.3. *Distillation*

The bio-jet fuel fraction of the FAEE was obtained by fractional distillation process, which was carried out as shown in Figure 2. The bio-jet fuel with a lower boiling point (C8-C14 of FAEE) was separated from the FAEE by using a rotary evaporator at 165 °C and

25 mbar for 120 min. The bio-jet fuel was collected, and the percentage yield of bio-jet fuel was calculated by using the equation below:

$$\%yield\ of\ biojet\ fuel = \frac{amount\ of\ biojet\ fuel\ obtained\ (g)}{amount\ of\ coconut\ oil\ feedstock\ (g)} \times 100\% \quad (5)$$

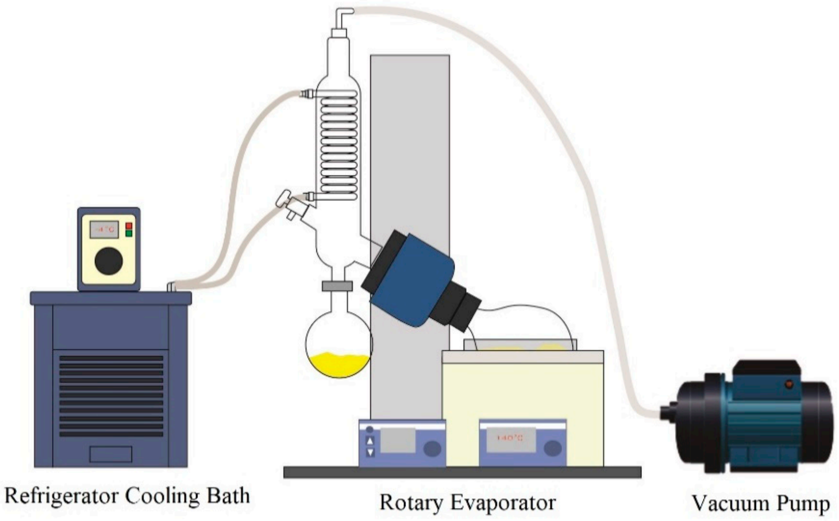

Figure 2. Experimental setup for distillation.

2.4. Response Surface Methodology (RSM)

To investigate the optimal condition for bio-jet fuel production through microwave-assisted catalytic transesterification, response surface methodology (RSM) was applied by using Design Expert 11 software (Stat-Ease, Minneapolis, MN, USA). RSM was normally used to optimize an experiment based on the selected variables [43–45]. Traditionally, the one-factor-at-a-time (OFAT) methodology, which varies one variable at a time while maintaining the others as constant, is time-consuming and expensive because many experimental runs are required to evaluate the relationship between the studied variables. Hence, RSM is recommended as the optimization can be achieved with less experimental runs as compared to OFAT by varying different parameters at a time. Moreover, a mathematical model can be generated to describe the experiments by using a polynomial function that fitted by the least square method:

$$Y = \beta_0 + \sum \beta_i X_i + \sum \beta_{ij} X_i X_j + \sum \beta_i \beta_i X_i X_i + e \quad (6)$$

where X_i indicates the studied variable, while Y symbolize the results to be optimized. β_0, β_i, and β_{ij}, however, are the regression coefficient. Finally, e represents the random error.

In this project, the Box–Behnken design was selected as it able to estimate the regression coefficient of a second-degree quadratic equation with less experimental runs in comparison to central composite design. In this optimization study, three parameters were considered, namely, coconut oil to ethanol molar ratio, reaction time, and microwave power. The respective levels of different parameters are summarized in Table 2 and note that the center point was repeated three times to determine the experimental errors. The 3-levels-3-parameters Box–Behnken Design was implemented and showed that a total 15 experimental runs with different reaction conditions (refer to Table 3) are required to conduct the optimization study. From there, bio-jet fuel was produced, and the result obtained was inserted into software for further analysis. Analysis of variance (ANOVA) was conducted to generate a mathematical model for the studied response, in this case, the biokerosene yield.

Table 2. Experimental level of studied parameters.

Experimental Level	Coconut Oil to Ethanol Molar Ratio, F_1	Reaction Time, F_2 (min)	Microwave Power, F_3 (W)
Low level, L (−1)	1:6	5	100
Medium level, M (0)	1:9	10	300
High level, H (+1)	1:12	15	500

Table 3. Fit summary table.

Source	Sequential *p*-Value	Lack of Fit *p*-Value	Adjusted R-Squared	Predicted R-Squared	Remarks
Linear	0.0418	0.0211	0.3787	0.2289	
2 Factors Interaction	0.9898	0.0143	0.1574	−0.4111	
Quadratic	<0.0001	0.4277	0.9792	0.9130	Suggested
Cubic	0.4277		0.9839		Aliased

2.5. Artificial Neural Network (ANN)

MATLAB's Neural Network in MATLAB R2011b (MathWorks Inc., Natick, MA, USA) was used to train the backpropagation ANN developed in this study. The hyperbolic *tangent sigmoid* (Equation (7)) and the *purelin* (Equation (8)) transfer function was used for the input layer to the hidden layer and the hidden layer to the output layer, respectively.

$$tangent\ sigmoid\ (x) = \frac{2}{(1+\ e^{-2x})} - 1 \tag{7}$$

$$A = purelin\ (x) = x \tag{8}$$

The proposed ANN has an input layer with three neurons (coconut oil to ethanol molar ratio, reaction time and microwave power), a hidden layer and an output layer with one neuron (bio-jet fuel yield). The ANN model was trained until the mean square error (MSE) was minimized and the average correlation coefficient was close or equal to 1. The optimum number of hidden neurons was selected by heuristic procedure. The dataset containing the bio-jet fuel yield and the process input variables were divided into three subsets: training (70%), validating (15%), and testing (15%).

2.6. Ant Colony Optimization (ACO)

Ant colony optimization (ACO) is also known as a swarm intelligence technique, which is inspired by the foraging pattern of ant colonies. Ants can find the shortest path from a food source to their nest, without having to see it directly. The ants have a unique and very advanced solution, namely using a pheromone trail on a path to communicate and building a solution, the more pheromone traces are left, the other ants will follow that path. These pheromones too relate to the previous good element solutions formed by the ants. Equation (9) describes the probability of an ant move from one node (*i*) to another (*j*):

$$P_{i,j} = \frac{\left(\tau_{i,j}^{\alpha}\right)\left(\mathrm{n}_{i,j}^{\beta}\right)}{\sum\left(\tau_{i,j}^{\alpha}\right)\left(\mathrm{n}_{i,j}^{\beta}\right)} \tag{9}$$

where $\tau_{i,j}$ indicates the amount of pheromone on edge *i,j* (refer to Equation (10)) and the α symbolizes the factors selected to regulate the impact of $\tau_{i,j}$. $\tau_{i,j}$. Meanwhile, $n_{i,j}$ is the desirability of edge *i,j* (commonly $1/\mathrm{d}_{i,j}$) and the β implies the factors selected to regulate the impact of $n_{i,j}$.

$$\tau_{i,j} = 1 - \rho\tau_{i,j} + \Delta\tau_{i,j} \tag{10}$$

where ρ is the rate of pheromone evaporation and $\Delta\tau_{i,j}$ is the amount of pheromone deposited.

If ant k travels on edge i,j, the amount of pheromone deposited is given by Equation (11):

$$\Delta\tau_{i,j}^{k} = \begin{cases} \frac{1}{L_k}, & \text{if ant k travels on edge } i,j \\ 0, & \text{Otherwise} \end{cases} \tag{11}$$

where L_k is the cost of the kth ant's tour (typically length).

2.7. Statistical Evaluation of the Developed Models

Different statistical measures, including correlation coefficient (R), coefficient of determination (R^2), root mean absolute error (RMSE), standard error of prediction (SEP), mean absolute error (MAE) and Chi-square were used to test the developed models, as described in Equations (12)–(17) [39]:

$$\mathrm{R} = \frac{\sum_{i=1}^{n}\left(M_p - M_{p,avg}\right) \times \left(M_e - M_{e,avg}\right)}{\sqrt{\left[\sum_{i=1}^{n}\left(M_p - M_{p.avg}\right)^2\right]\left[\sum_{i=1}^{n}\left(M_e - M_{e.avg}\right)^2\right]}} \tag{12}$$

$$\mathrm{R}^2 = 1 - \frac{\sum_{i=1}^{n}\left(M_e - M_p\right)^2}{\sum_{i=1}^{n}\left(M_{e,avg} - M_p\right)^2} \tag{13}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(M_e - M_p\right)^2} \tag{14}$$

$$\mathrm{SEP} = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(M_e - M_p\right)^2}}{M_{e,avg}} \times 100 \tag{15}$$

$$\mathrm{MAE} = \frac{1}{n}\left(\sum_{i=1}^{n}\left|\left(M_e - M_p\right)\right|\right) \tag{16}$$

$$\mathrm{Chi-square} = \sum_{i=1}^{n}\frac{\left(M_e - M_p\right)^2}{M_e} \tag{17}$$

where n shows the number of points, and M_p, M_e, $M_{p,avg}$ and $M_{e,avg}$ are the predicted value, experimental value and the average of the predicted and experimental values, respectively.

2.8. Sensitivity Analysis

The importance of the studied variables (coconut oil to ethanol molar ratio, reaction time, and microwave power) was explored through conducting the sensitivity analysis. In this analysis, Equation (18) is used with the "sum of squares" values obtained from the ANOVA table generated from response surface methodology (RSM).

$$sensitivity\% = \frac{S_x}{S_y} \times 100 \tag{18}$$

where S_x and S_y indicate the sum of square of the individual variable and total sum of squares of all the variables, correspondingly.

The significance input variables for ANN, were calculated based on Equation (19) [37]:

$$F_k = \frac{\sum_{j=1}^{j=M_o}\left(\left(\frac{\left|W_{kj}^{ag}\right|}{\sum_{h=1}^{M_y}\left|W_{hj}^{ac}\right|}\right) \times \left|W_{jm}^{gl}\right|\right)}{\sum_{h=1}^{h=M_y}\left\{\sum_{j=1}^{j=M_o}\left(\left(\left|W_{qr}^{an}\right|\frac{\left|W_{hj}^{ag}\right|}{\sum_{d=1}^{M_p}\left|W_{hj}^{ag}\right|}\right) \times \left|W_{jm}^{gl}\right|\right)\right\}} \tag{19}$$

where, F_k is the relative significance of the kth input variable on the output variable. M_o is the number of input neurons and M_y is the number of hidden neurons. W is the connection weight. The superscript a, g, and l represent the input, output, and hidden layer, respectively, whereas the subscript h, j, and m represent the input, output, and hidden neuron, respectively.

2.9. Optimization of Transesterification Process Variables

RSM and ANN-ACO were used to evaluate the optimal value of the three respective studied parameters in order to obtain the highest bio-jet fuel yield. The bio-jet fuel yield and the studied parameters were set at "maximum" and "in the range" individually in the case of RSM. ACO was used to determine the optimal values with the maximum bio-jet fuel yield for ANN. By conducting triplicate experiments, the optimal values determined by each approach were validated and the average values obtained were compared with the expected values.

2.10. Bio-Jet Fuel Properties

The bio-jet fuel isolated from biodiesel (FAEE) was then analyzed and compared with the standard requirements for aviation turbine fuels (ASTM D1655) of the American Society for Testing and Materials. In this work, according to the respective ASTM test process, physicochemical properties including density at 15 °C, kinetic viscosity at −20 °C, flash point, and freezing point were calculated. Using a bomb calorimeter, the lower heating factor, also known as calorific value, was calculated as well.

3. Results

3.1. RSM

Based on this result, a fit summary table was generated to evaluate the suitable model for the optimization study. The fit summary table is shown in Table 3, and the outcomes indicate that the quadratic model is adequate to model the studied response (bio-jet fuel yield). This finding is based on the sequential p-value of the quadratic model, which is less than 0.05. In other words, the quadratic model consists of more than 95% confidence in modeling the experiments. Besides that, inclusion of cubic model terms might cause the model to be aliased and hence, the quadratic model is the best with the highest polynomial order.

The model used in this quadratic equation using a notation such as F_1 for the coconut oil ethanol molar ratio, F_2 for the reaction time, and F_3 for microwave power. The experimental and predicted results in this work are summarized in Table 4 and the uncoded quadratic equation is shown in the following equation:

$$\begin{aligned}\text{Bio} - \text{jet fuel yield } (\%) &= 21.84\mathrm{F}_1 + 2.419\mathrm{F}_2 + 0.0416\mathrm{F}_3 - 0.00717\mathrm{F}_1\mathrm{F}_2 + 0.00227\mathrm{F}_1\mathrm{F}_3 - 0.000165\mathrm{F}_2\mathrm{F}_3 \\ &\quad -1.18644\mathrm{F}_1^2 - 0.082917\mathrm{F}_2^2 - 0.00016\mathrm{F}_3^2 - 50.84552\end{aligned} \tag{20}$$

Table 4. Experimental runs in RSM design with the different operating conditions and their respective experimental and predicted bio-jet fuel yield.

Experimental Run	Coconut Oil to Ethanol Molar Ratio, F_1	Reaction Time, F_2 (min)	Microwave Power, F_3 (W)	Experimental Bio-Jet Fuel Yield (%)	Predicted Bio-Jet Fuel Yield (%) RSM	Predicted Bio-Jet Fuel Yield (%) ANN
1	1:6	10	500	40.92	40.07	41.10
2	1:9	15	100	70.86	71.12	70.73
3	1:12	5	300	56.05	56.11	56.18
4	1:6	5	300	48.21	49.32	47.97
5	1:12	15	300	63.88	62.77	64.13
6	1:9	15	500	55.73	56.64	55.69
7	1:9	5	100	64.83	63.92	64.84
8	1:9	5	500	50.36	50.10	50.38

Table 4. *Cont.*

Experimental Run	Coconut Oil to Ethanol Molar Ratio, F_1	Reaction Time, F_2 (min)	Microwave Power, F_3 (W)	Experimental Bio-Jet Fuel Yield (%)	Predicted Bio-Jet Fuel Yield (%) RSM	Predicted Bio-Jet Fuel Yield (%) ANN
9	1:6	10	100	57.14	56.94	56.64
10	1:12	10	500	49.16	49.36	49.19
11	1:12	10	100	59.94	60.79	59.96
12 *	1:9	10	300	69.82	68.85	69.81
13	1:6	15	300	56.47	56.41	55.96
14 *	1:9	10	300	69.15	68.85	69.81
15 *	1:9	10	300	67.59	68.85	69.81

* The center points of the experiments are replicated for 3 times.

The effect of the studied parameters as linear, quadratic, and interaction coefficients on the studied responses was determined for their significance through analysis of variance (ANOVA). The ANOVA results of this work are reported in Table 5. The studied parameters coconut oil to ethanol molar ratio, reaction time and microwave power represent as F_1, F_2, and F_3 terms particularly. It is noted that the model used was statistically significant with a confidence level of 95%. From the table, it observed that parameters F_1, F_2, and F_3 have a significant influence on bio-jet fuel production (p-values < 0.0500). Furthermore, note that the "lack of fit" of the model consists of a p-value of 0.4227 (not significant as >0.05). In the other words, the model is fit to be used for further analysis.

Table 5. Analysis of Variance for the modeling of bio-jet fuel production.

Source	Sum of Squares	df	Mean Square	*F*-Value *	*p*-Value	Remarks
Model	1127.25	9	125.25	74.3	<0.0001	significant
F_1-Ethanol	86.4	1	86.4	51.25	0.0008	
F_2-Time	94.46	1	94.46	56.04	0.0007	
F_3-Power	400.45	1	400.45	237.55	<0.0001	
F_1F_2	0.0462	1	0.0462	0.0274	0.875	
F_1F_3	7.4	1	7.4	4.39	0.0903	
F_2F_3	0.1089	1	0.1089	0.0646	0.8095	
F_1^2	420.99	1	420.99	249.74	<0.0001	
F_2^2	15.11	1	15.11	8.96	0.0303	
F_3^2	150.55	1	150.55	89.31	0.0002	
Residual	8.43	5	1.69			
Lack of Fit	5.81	3	1.94	1.48	0.4277	not significant
Pure Error	2.62	2	1.31			
Cor Total	1135.68	14				

* The F value for a term shows the test in order to compare the variance of that particular term with the residual variance.

Effect of the Parameter

Effect of the Ethanol to Oil Molar Ratio

Figure 3a shows the effect of ethanol to oil molar ratio and reaction time for the bio-jet fuel production. It is shown, from the ANOVA analysis (Table 5), that ethanol to oil molar ratio has the positive effect for bio-jet fuel production (p value < 0.05). Increasing the ethanol to oil molar ratio from 1:6 to 1:9.36, the bio-jet fuel yield increases until an optimal point and then decreases. Similar trends have been reported in several studies [46]. As stated before, the stoichiometry of the transesterification requires three moles of alcohol to react with one mole of triglyceride. However, since it involves a reversible reaction, so, an excessive amount of alcohol is usually needed to shift the reaction equilibrium toward the production of biodiesel. In the work done by Encinar et al. [47], the conventional alkali-catalyzed transesterification was reported to be incomplete for the molar ratio of methanol to Cynara oil that was less than 4.05. As expected, the methyl esters yield increases with the methanol molar ratio and achieve an optimal yield at a molar ratio of 5.67. However, for the methanol molar ratio higher than 5.67, the methyl esters yield drops. This result tallies with current work. This phenomenon is observed because the separation and recovery process of glycerol has been interfered by the high alcohol molar ratio [48]. The high amount of ethanol, in this case, has increased the solubility of the glycerol in the ester phase and shifts the reaction equilibrium towards the reactant side. As the result, biodiesel yield decreases as well as bio-jet fuel.

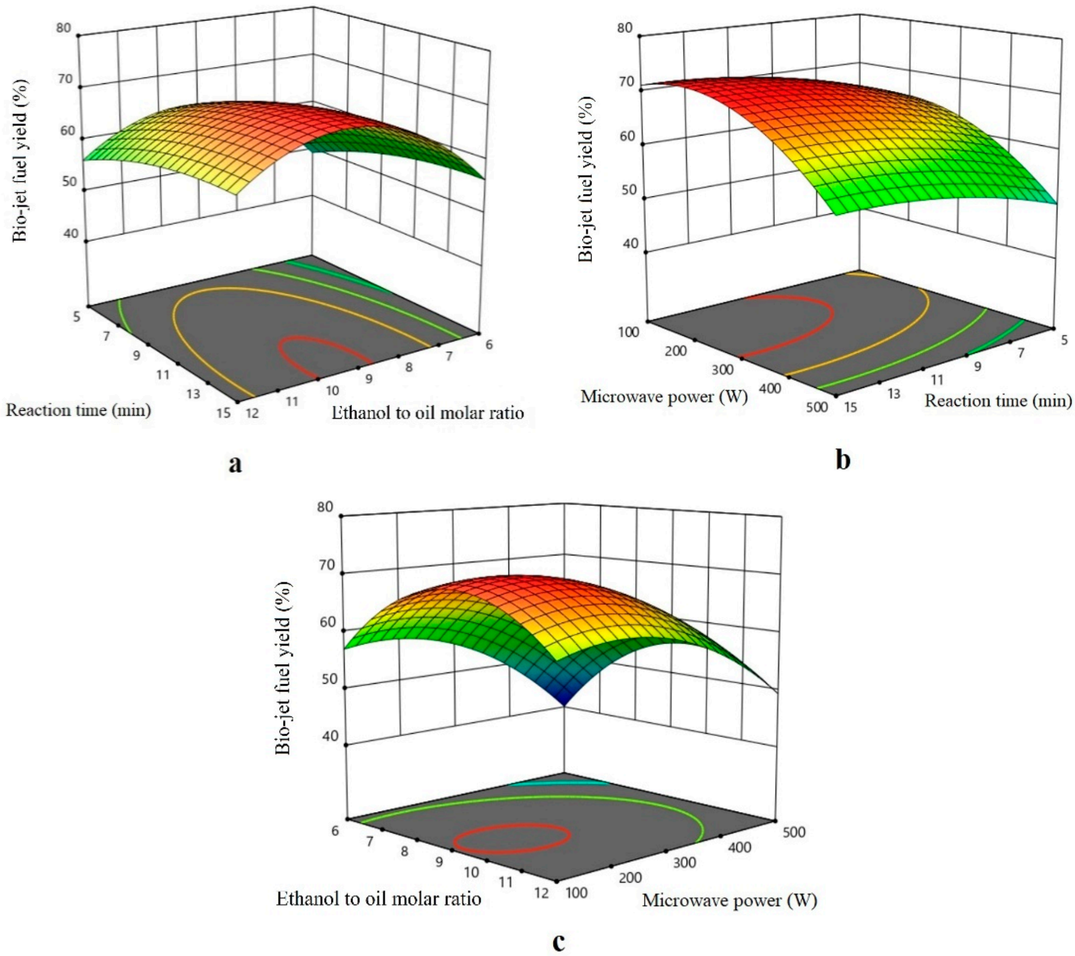

Figure 3. Three-dimensional response for the interaction on bio-jet fuel yield between (**a**) reaction time and ethanol to oil molar ratio, (**b**) microwave power and reaction time and, (**c**) ethanol to oil molar ratio and microwave power.

Effect of the Reaction Time

The relationship between reaction time and microwave power is shown in Figure 3b. The p-value = 0.0007 of the reaction time parameter suggested that there was a reasonably large impact of reaction time on the production of bio-jet fuel yield (Table 5). With the increase in reaction time from 5 to 14.34 min followed by the increase in microwave power from 100–189.53 W, bio-jet fuel yield improved, which may be due to the explanation that more reaction time causes a more productive reaction time. It can be noticed that the bio-jet fuel yield increases as the reaction time increases, similar to the studies done by other researchers [42].

Effect of the Microwave Power

It is observed that the interaction of the microwave power and ethanol molar ratio have positively approached the bio-jet fuel yield. From Figure 3c, it observed that increasing the microwave power from 100 to 189.53 W, and the ethanol to oil molar ratio from 1:6 to 1:9.36, will increase the bio-jet fuel into maximum point and then it will decrease. The bio-jet fuel yield was decreasing when the microwave power reached above 189.53 W, with an ethanol molar ratio of more than 1:9.36. This might be due to the possibility of high microwave power causes the destruction of triglycerides [49]. Hence, less triglycerides were reacted with alcohol, and resulting in lower yield.

3.2. Analysis of the Developed ANN Model

The design of the ANN architecture chosen for this work was based on the minimum mean square error (MSE) and the highest coefficient correlation value (R). The ANN network modeling output plots (predicted values) versus target (actual values) for training, validation, testing and entire datasets with R values of 0.997, 1, 1, and 0.99785, respectively, are shown in Figure 4. In this study, the best topology was found to be 3-8-1, (Figure 5). The architecture consists of a three-neuron input layer.

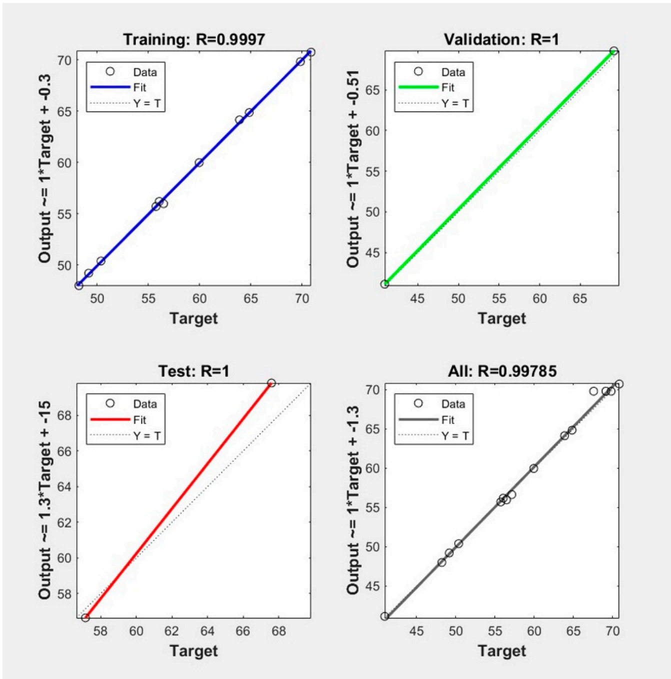

Figure 4. Artificial neural network modeling.

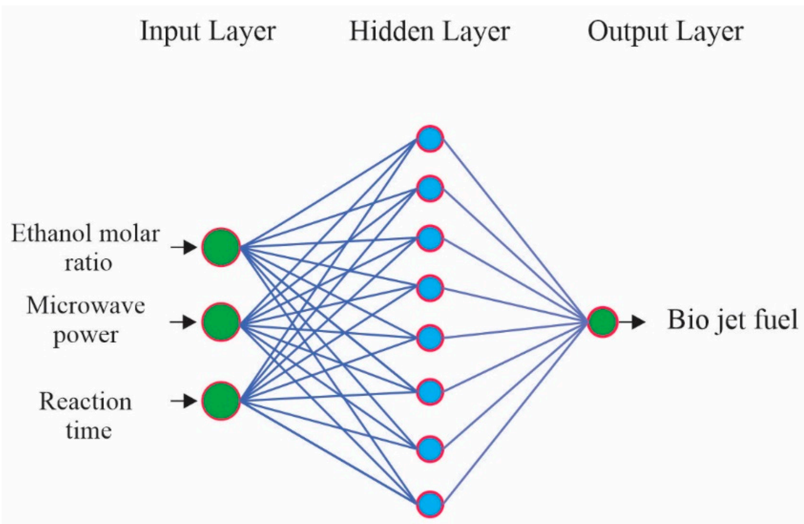

Figure 5. Artificial neural network architecture.

3.3. Comparison of the Predictive Capability of Models

Table 6 displays the findings obtained from different statistical metrics used to test the built models. For both developed models (RSM and ANN), the high R values (Table 6) indicate that there is a strong link between the real and the predicted yields of bio-jet fuel. For both RSM and ANN, the R and R^2, were 0.9963, 0.9926, and 0.9979,0.9957, respectively.

Table 6. Statistical analysis.

Statistical Analysis	RSM	ANN
R	0.9963	0.9979
R^2	0.9926	0.9957
RSME	0.5619	0.4048
SEP (%)	0.9563	0.6889
MAE	0.0414	0.0220
Chi-square	0.0096	0.0061

The good fit of the models is representative of these high values. RMSE is a test of the dataset adherence to the regression line. For both RSM and ANN models, the values of RMSE that were obtained were all low, confirming the models' good fit. To calculate the residuals (deviation from actual objective) of the built models, SEP (percent) and MAE were used. The ANN model had less divergence from experimental values of SEP (0.6889 percent) and MAE (0.022) than the RSM model, as seen in Table 6. In comparison, lower chi-square (0.782) values confirmed that the most reliable was the ANN model with the lowest error term values and highest R and R^2 values. It was noted in this analysis that ANN was found to be superior than RSM.

3.4. Sensitivity Analysis Results of the Input Variables on the Developed Models

The sensitivity analysis findings for both RSM and ANN are shown in Figure 6. The result for both models have the same pattern in that the most influential response input variable (bio-jet fuel yield) was seen to be microwave power, followed by reaction time and finally by ethanol to oil molar ratio. The degrees of significance distributions, however, differed between the methods of modeling. The significance level of 68.89% microwave power, 16.25% reaction time and 14.86% ethanol to the molar ratio for RSM. While for ANN, the important microwave power rating was 42.29%, the reaction time was 29.03% and the ethanol oil molar ratio was 28.68%.

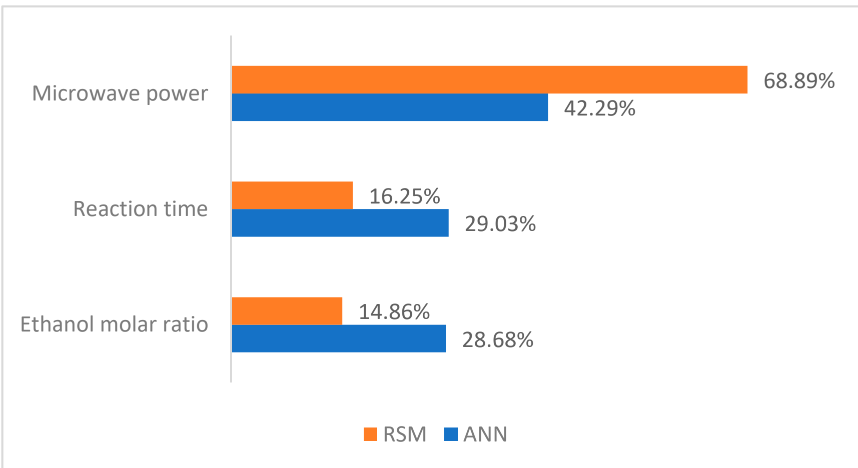

Figure 6. Sensitivity analysis for bio-jet fuel production.

3.5. Optimization of the Process Variables for Bio-Jet Fuel

To obtain the highest value of bio-jet fuel yield, the optimization of the studied variables was carried out using RSM and ANN-ACO. In the case of RSM, the in-build optimization method in the Design Expert software was used for the optimisation study. On the other hand, the ANN models acted as the fitness functions when combined with ACO in the case of optimization using the ANN-ACO method. Table 7 shows the optimum values expected by each system. For each model bio-jet fuel validated by triplicate experiments in the laboratory, the expected optimal condition and the average bio-jet fuel yields were reported (Table 7). From the result, it was observed that RSM predicted 72.49% of bio-fuel jet yield. While for ANN-ACO, the predicted yield was 74.45% with process variables (9.25:1 ethanol oil molar ratio, 12.66 min reaction time and 163.69% microwave power) was higher than most RSM values.

Table 7. Optimization of RSM and ANN-ACO.

Modeling Method	Ethanol	Time	Power	Predicted	Observed
RSM	9.35	14.34	189.53	72.49	73.02
ANN	9.25	12.66	163.69	74.8	74.45

3.6. FTIR

The results obtained from the FTIR study of the spectrum of coconut oil, FAEE and bio-jet fuel are given in Figure 7. The peaks shown in between 3000 to 2800 cm^{-1} indicate the stretching vibration of = C-H (alkene) and C-H (alkane) functional groups [50], which contributed by the esters chain of the samples. The characteristics peak at wavenumber of 1743 cm^{-1}, 1742 cm^{-1}, and 1740 cm^{-1} in the spectrum of coconut oil, FAEE and bio-jet fuel, respectively, show the occurrence of C=O stretching. Although this peak is shorter in the bio-jet fuel as compared to FAEE, however, the presence of this peak showing that there is a need for deoxygenation process to remove the oxygen content in the jet fuel. Besides, blending of the bio-jet fuel with the conventional fossil-based jet fuel is also recommended to balance the bio-jet fuel property deficiency. Furthermore, it is noted that an extra peak at 1437 cm^{-1} in the spectrum of FAEE and bio-jet fuel in comparison to the spectrum of coconut oil. This peak can be explained by the bending vibration of C-H groups in the samples. In addition, it confirms the transesterification process was successfully conducted and converted triglycerides in the coconut oil into ethyl esters in biodiesel (FAEE) and bio-jet fuel [44,51,52].

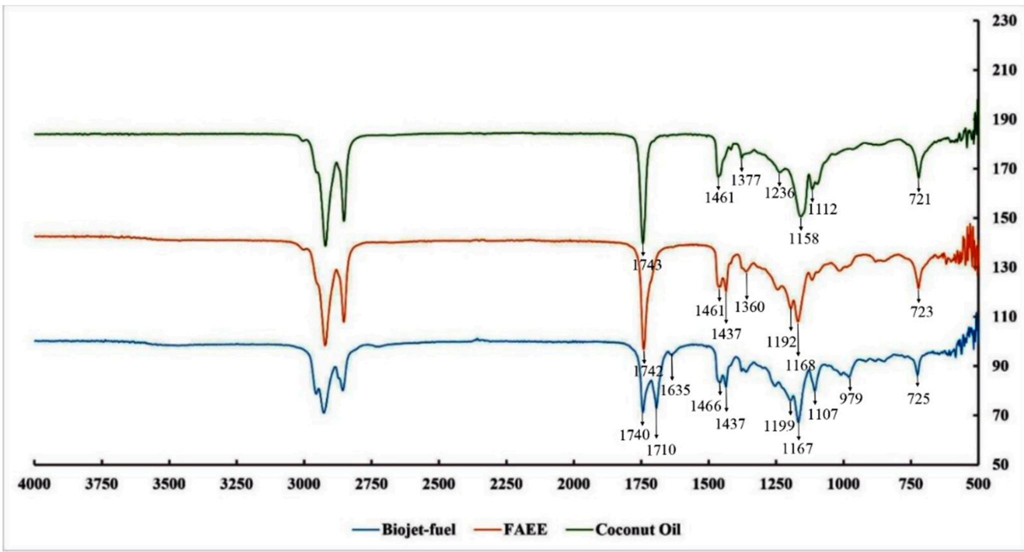

Figure 7. FTIR spectrum for coconut oil, FAEE, and bio-jet fuel.

3.7. Bio-Jet Fuel Properties

To evaluate the suitability of the bio-jet fuel produced in this work as alternative jet fuel, some of the major properties of bio-jet fuel were analyzed and compared with American Society for Testing and Materials (ASTM) D1655, the standard specification for aviation turbine fuels. The test results and the standard limit are summarized in Table 8.

Table 8. Comparison of properties between bio-jet fuel of the current work with ASTM D1655 standard.

Properties	Unit	ASTM D1655	This Work	Soybean [53]	Palm [42]
Density at 15 °C	kg/m^3	775–840	788	776	866.3
Kinetic viscosity at −20 °C	cSt	<8	6.52	3.30	-
Flash point	°C	>38	55	48.5	105
Freezing point	°C	<−47	−16	-	−50
Lower heating value	MJ/kg	>42.8	43.5	-	-

It can be seen that the kinematic viscosities and densities of the bio-jet fuel is lower than the maximum value provided by the ASTM D1655 standard (<8 cSt and 775–840 kg/m^3, respectively). The measurement of kinematic viscosity and density of fuel are important and should be within the acceptable limits established in the standard to avoid clogging in the fuel injectors and to achieve good fuel atomization. From the table, it is noticed that the density and kinematic viscosity of the bio-jet fuel in this study is higher compared to soybean, but lower than palm. The lower heating value of the bio-jet fuel in this study is 43.5 MJ/kg, which is well below the limit given in the ASTM D1655 standard, slightly lower than that for diesel (>42.8 MJ/kg). The flashpoint of the bio-jet fuel from FAEE coconut oil is 55 °C, which is significantly higher than the limit given in the ASTM D1655 (>38 °C). The flashpoint is higher than soybean, and much lower than the palm. As shown, bio-jet fuel obtained in the current study does not meet the criteria for the freezing point. A similar result has been reported by [42]. This showed that freezing point is the biggest challenge for bio-jet fuel technologies. This might be because bio-jet fuel consists of nearly no aromatics or cycloalkanes that are required for jet fuel [54]. Freezing point is one of the properties that affects the operability of bio-jet fuel at low temperature. Hence, further upgrading or blending is needed to bring down the freezing point and improve its jet fuel characteristics. Cheng and Brewer [55] suggested that blending of bio-jet fuel with alkyl-benzens might be the best, as it has a low molecular weight and emit less soot combustion as compared to other aromatics compounds. However, the effect of different aromatic compounds on the freezing point of bio-jet fuel has not been explored. As this objective is beyond the scope of this paper, it is suggested as a future work.

4. Conclusions

Other than the depletion issue of non-renewable fossil fuel, the increasing greenhouse gas emission has also driven the aviation industry toward sustainable development, such as exploration and commercialization of alternative renewable aviation fuels. This paper has investigated the effect of three parameters, including coconut oil to ethanol molar ratio, reaction time, and microwave power, on bio-jet fuel production. Bio-jet fuel production data was modeled using RSM and ANN. Statistical analysis proved that the ANN modeling was better than RSM. The optimal parameters predicted using ANN- ACO were, ethanol to oil molar ratio: 1:9.25, reaction time: 12.66 min and microwave power 74.8 W. Optimal yield of 74.45% were obtained experimentally in this optimal parameter conditions. Lastly, it was found that the bio-jet fuel collected in this work had comparable properties with the ASTM D1655, except freezing point. Hence, the aromatic additive is suggested to be added for properties enhancement. Besides, future work on evaluating the effect of catalyst and deoxygenation method on the improvement of bio-jet fuel properties will be conducted.

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