# Artificial Neural Network Approach to Predict Biodiesel Production using Algae-Based Heterogeneous Catalyst

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**Abstract.** The rising dependence on fossil fuels has intensified environmental issues such as greenhouse gas emissions and resource depletion. Biodiesel offers a renewable alternative with lower emissions. However, conventional biodiesel production are sensitive to free fatty acids and water, causing soap. Heterogeneous catalysts derived from biomass provide a cleaner and reusable alternative. In this study, *Ulva lactuca*, a green macroalga with rapid growth and no need for arable land or fertilizers, was used as a sustainable source for catalyst preparation. This research integrates an *U. lactuca*-based heterogeneous catalyst with an Artificial Neural Network (ANN) to predict biodiesel yield under different process conditions. The objective was to develop a robust predictive model for biodiesel production from waste cooking oil. Transesterification was performed at 50–70 °C, catalyst loadings of 2–5 wt%, and reaction times of 60–180 min, with a fixed methanol-to-oil ratio of 6:1. The ANN, trained using the Levenberg–Marquardt algorithm in MATLAB R2022a, achieved an optimal architecture of 4–18–1. The model showed excellent predictive accuracy, with R values of 0.9989, 0.9969, 0.9980, and 0.9987 for training, validation, testing, and overall datasets, and minimum MSE values of 2.81 × $10^{-4}$. The highest experimental biodiesel yield of 0.96 mol $mol^{-1}$ closely matched the ANN-predicted yield of 0.97 mol $mol^{-1}$ at 60 °C, 90 min, and 4 wt% catalyst loading. These results confirm the ANN's strong predictive capability and demonstrate its potential for optimizing biodiesel production using sustainable algae-based catalysts.

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# 1 Introduction

Energy is a fundamental necessity that sustains human life and drives economic development, industrial progress, and transportation systems [1]. Currently, fossil fuels remain the dominant global energy source; however, their continued use has raised serious environmental and sustainability concerns. The combustion of fossil fuels releases large quantities of greenhouse gases, leading to global warming, air pollution, and the depletion of natural resources. Moreover, the finite nature of fossil reserves poses an urgent challenge for future energy security. To address these issues, renewable and sustainable energy alternatives are essential [2–4]. Among various renewable options, biodiesel has emerged as a promising candidate due to its biodegradability, renewability, and compatibility with existing diesel engines [5].

Biodiesel offers several advantages over conventional petroleum diesel, including lower emissions of carbon monoxide, sulfur oxides, and unburned hydrocarbons [5]. It also provides superior lubricity and a higher flash point, making it safer to handle and store. Despite these benefits, the production of biodiesel still faces technological and economic challenges, particularly regarding catalyst selection. Conventional biodiesel production typically relies on homogeneous catalysts such as sodium hydroxide or potassium hydroxide. While these catalysts are effective, they are highly sensitive to free fatty acids (FFA) and water content in the feedstock, which can cause unwanted side reactions like saponification [6]. This leads to soap formation, complicating product purification and reducing overall process efficiency .

To overcome these limitations, heterogeneous catalysts have gained increasing attention due to their ease of separation, reusability, and reduced wastewater generation. In recent years, the use of biomass-derived heterogeneous catalysts has grown rapidly as a sustainable alternative. These catalysts not only provide a cost-effective solution but also promote waste valorization by utilizing naturally available materials. One particularly promising biomass source is *Ulva lactuca*, a green macroalgae species. *U. lactuca* is advantageous because it grows rapidly without the need for arable land, fertilizers, or fresh water. Moreover, its high ash content provides a natural precursor for catalyst synthesis, making it an environmentally benign and renewable resource for biodiesel production [7,8].

In parallel with experimental research, mathematical modeling has become an invaluable approach for predicting biodiesel yield and optimizing process conditions. Among various modeling techniques, the Artificial Neural Network (ANN) has proven highly effective in simulating nonlinear and complex relationships between input and output parameters in chemical processes [9,10]. ANNs can learn from experimental data, adaptively improve prediction accuracy, and eliminate the need for extensive experimental trials, saving both time and resources.

Several studies have successfully applied ANN models to predict biodiesel production using different feedstocks and catalytic systems. However, the application of ANN to predict biodiesel yield using algae-based heterogeneous catalysts remains limited. Most existing works focus on conventional catalysts or plant-based biomass sources, leaving a research gap in understanding the predictive capability of ANN models for marine biomass-derived catalysts such as *U. lactuca*.

The novelty of this study lies in integrating an ANN-based modeling approach with an algae-derived heterogeneous catalyst system for biodiesel production. By combining experimental data with predictive analytics, this research provides new insights into optimizing process parameters and improving biodiesel yield prediction accuracy. The objective of this work is to develop and validate an Artificial Neural Network model capable of accurately predicting biodiesel yield produced from waste cooking oil using an U. lactuca-based heterogeneous catalyst. This study aims to establish a reliable predictive framework

that supports process optimization and contributes to the advancement of sustainable biofuel technologies.

## 2 Materials and methodology

### 2.1 Materials

The waste cooking oil used as the feedstock for biodiesel production was purchased from Pasar Bogor, Indonesia. The catalyst utilized in this research was produced from *Ulva lactuca*, a species of green macroalgae, which was harvested from Ekas Beach in Lombok Island, Indonesia. The methanol and potassium hydroxide (KOH) used in this experiment, each with a purity of 99.5%, were obtained from Sigma-Aldrich Indonesia. A standard biodiesel mixture (≥90.0%, Supelco brand) was also supplied by Sigma-Aldrich Indonesia, while the phenolphthalein indicator (≥99.5%) was procured from CV. Mulya Jaya.

### 2.2 Biodiesel synthesis

Biodiesel was produced through a single-step transesterification process using waste cooking oil and a catalyst derived from *Ulva lactuca*. The experimental setup, illustrated in **Fig. 1**, followed the configuration described in our earlier study [11]. The reaction was carried out under various conditions, including temperatures of 50, 60, and 70 °C; reaction times of 60, 90, 120, 150, and 180 minutes; and catalyst loadings of 2, 3, 4, and 5 wt%. The molar ratio of methanol to oil was fixed at 6:1 throughout the experiments.

Initially, a predetermined volume of waste cooking oil was placed into a reactor equipped with a condenser. Methanol and the prepared catalyst were then combined and added to a three-necked glass reactor. The mixture was heated to the target temperature to initiate the transesterification. Upon completion, the reaction system was cooled and immersed in an ice bath to terminate the process. This step ensured that the transesterification ceased completely.

The cooled mixture was allowed to separate into two distinct layers: the upper biodiesel phase and the lower glycerol phase. The biodiesel layer was subsequently washed to remove residual catalyst and other impurities, followed by a drying step to eliminate moisture before storage or further use. All transesterification experiments were performed in triplicate to ensure reproducibility.

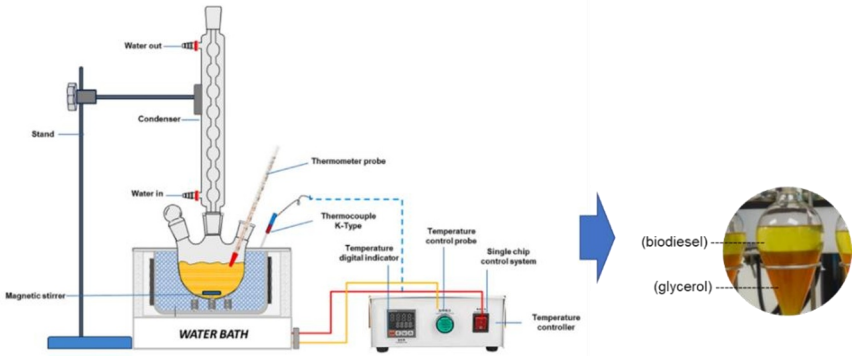


**Fig. 1.** Experimental apparatus for biodiesel synthesis using algae-based catalyst.

### 2.3 Biodiesel analysis

Biodiesel characterization was conducted using an HP-6890 gas chromatograph (GC) with helium as the carrier gas. The analytical procedure followed the method described in our earlier publication [11]. In summary, the GC column temperature was programmed in three stages: initially maintained at 50 °C for 1 minute, then increased to 250 °C at a rate of 15 °C $min^{-1}$ over 15 minutes, and finally ramped to 300 °C at 5 °C $min^{-1}$ for an additional 10 minutes. Each analysis involved the injection of a 1 mL biodiesel sample, and all measurements were performed in triplicate to ensure reproducibility.

The biodiesel yield was calculated based on the molar ratio of the fatty acid methyl esters (FAMEs) produced to the total moles of fatty acid groups originally present in the triglycerides, as expressed in Eq. (1). This yield determination approach was consistent with methodologies reported in previous studies [11].

$$\text{Product yield [\%]} = \frac{\text{mol of biodiesel product}}{\text{mol of a fatty acid in the feedstock}} \times 100 \qquad (1)$$

### 2.4 ANN modeling

The artificial neural network (ANN) model was developed to predict biodiesel yield based on the experimental results obtained from the transesterification process. The modeling and training were performed using MATLAB R2022a (MathWorks, USA), employing the Levenberg–Marquardt backpropagation algorithm due to its proven efficiency in achieving high accuracy, characterized by a strong coefficient of determination ($R^2$) and low mean squared error (MSE). The dataset, consisting of input variables such as reaction temperature, catalyst loading, methanol-to-oil molar ratio, and reaction time, along with corresponding biodiesel yields, was randomly divided into three subsets: 70% for training, 15% for validation, and 15% for testing. During the training phase, the ANN iteratively adjusted the connection weights to minimize the MSE between the predicted and experimental yields. The validation data were used to monitor network performance and prevent overfitting, while the testing dataset was applied to evaluate the model's predictive capability using the final set of trained weights. The model's performance was assessed using both the coefficient of determination (R) and mean squared error (MSE), ensuring that the trained ANN could accurately and reliably estimate biodiesel yield with minimal deviation from experimental data.

## 3 Result and discussion

### 3.1 Effect of temperature and catalyst loading on biodiesel yield

The effect of calcination temperature on biodiesel yield was examined under optimized transesterification conditions, namely, a reaction temperature of 60 °C, a methanol-to-oil molar ratio of 6:1, and a reaction time of 90 minutes. As presented in **Figure 2**, the relationship between the calcination temperature of the *U. lactuca*-derived catalyst and the biodiesel yield reveals a distinct influence of thermal treatment on catalytic performance. When the calcination temperature was increased from 550 °C to 650 °C, the biodiesel yield rose markedly, suggesting that moderate heating enhances catalyst activity. This improvement can be attributed to better decomposition of organic residues and the formation of more active catalytic sites, resulting in increased surface area and improved basicity that promote the transesterification reaction [12].

However, a further rise in calcination temperature to 750 °C led to a slight decrease in biodiesel yield. The reduction is likely due to sintering and agglomeration of the catalyst particles at higher temperatures, which causes a loss of active surface area and diminishes catalytic efficiency. Excessive thermal exposure can also alter the crystalline structure of the catalyst, thereby reducing the accessibility of active sites required for methanol–oil interaction. Overall, the findings indicate that 650 °C is the optimal calcination temperature for preparing U. lactuca-derived catalysts, balancing structural stability and catalytic reactivity to achieve the highest biodiesel yield.

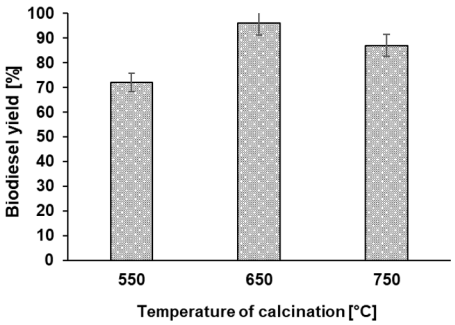


**Fig. 2.** The effect of calcination temperature on biodiesel yield.

The effect of reaction temperature and time on biodiesel yield was examined using a U. lactuca-derived catalyst at a fixed catalyst loading of 4 wt% and a methanol-to-oil molar ratio of 6:1. As illustrated in **Figure 3**, both parameters significantly influenced the transesterification performance. At a reaction time of 60 minutes, increasing the temperature from 50 °C to 60 °C markedly enhanced the biodiesel yield from 0.48 to 0.87. This improvement can be attributed to the endothermic nature of the transesterification reaction, where higher temperatures provide sufficient activation energy to accelerate molecular collisions between methanol and triglycerides, resulting in a greater conversion rate. However, when the temperature was further increased to 70 °C, a slight decline in biodiesel yield (0.67) was observed. This reduction is likely due to methanol evaporation at higher temperatures, which lowers its availability in the reaction medium and consequently slows down the transesterification rate [13]. Therefore, a reaction temperature of 60 °C was identified as the optimum condition for achieving the maximum biodiesel yield.

Reaction time also played a critical role in determining the overall conversion efficiency. As the reaction duration increased from 60 to 180 minutes, the biodiesel yield generally improved across all temperatures, particularly at 50 °C, indicating that longer reaction times allow for more complete conversion of triglycerides to methyl esters. Nevertheless, at higher temperatures (60–70 °C), extending the reaction beyond 90 minutes resulted in a gradual decrease in yield. This phenomenon may be associated with the reversible nature of transesterification and potential hydrolysis of methyl esters, which can lead to soap formation and interfere with phase separation. The highest biodiesel yield, approximately 0.96, was achieved at 60 °C after 90 minutes of reaction, demonstrating that optimal thermal and temporal conditions are essential to balance reaction kinetics and stability of the produced esters.

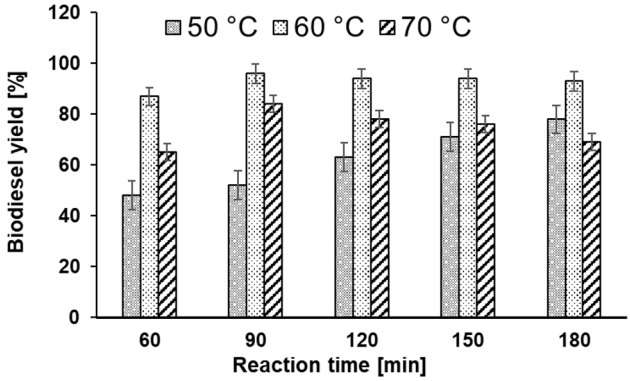


**Fig. 3.** The effect of calcination temperature on biodiesel yield.

The influence of catalyst loading on biodiesel yield was evaluated under constant reaction conditions to determine the optimal amount of *U. lactuca*-derived catalyst required for efficient conversion. As illustrated in **Figure 4**, catalyst loading had a significant impact on the transesterification process. Increasing the catalyst concentration from 2 wt% to 4 wt% led to a clear improvement in biodiesel yield, rising from 0.78 to 0.96. This enhancement can be attributed to the greater availability of active catalytic sites, which facilitates more effective contact between methanol and triglycerides, thereby accelerating the transesterification reaction and improving the overall conversion of waste cooking oil into biodiesel.

However, when the catalyst loading was further increased to 5 wt%, no substantial improvement in yield was observed. This behavior may result from the excessive presence of catalyst particles in the reaction mixture, which can promote side reactions such as saponification, leading to soap formation that interferes with phase separation and reduces product recovery. Additionally, a higher catalyst concentration may increase the viscosity of the mixture, hindering mass transfer between the oil and methanol phases. These findings are consistent with previous reports suggesting that beyond a certain catalyst threshold, the biodiesel yield tends to plateau or even decline due to these secondary effects [14].

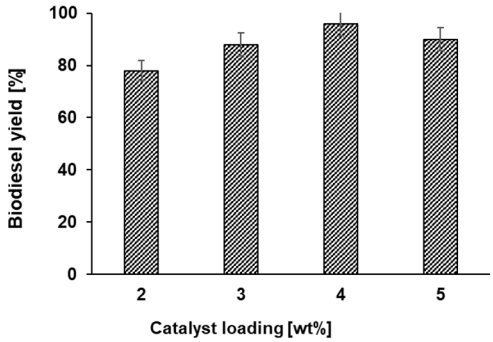


**Fig. 4.** The effect of catalyst loading on biodiesel yield.

## 3.2 ANN modeling

The optimum number of neurons in the hidden layer of the artificial neural network (ANN) was determined using a heuristic approach, which involves evaluating model performance across several network configurations to identify the structure that best balances prediction

accuracy and computational efficiency. As illustrated in **Figure 5**, this procedure examined the effect of varying neuron numbers on both the coefficient of determination (R) and mean squared error (MSE). The results show clear variations in performance as the number of hidden neurons increased, emphasizing that both underfitting and overfitting can occur if the hidden layer is not properly optimized.

Among the tested configurations, the network with 18 hidden neurons demonstrated the best predictive performance, yielding the highest correlation coefficients (R) for the training, validation, and testing datasets, 0.9969, 0.9899, and 0.9658, respectively, and the lowest MSE values of $1.07 \times 10^{-3}$, $2.81 \times 10^{-4}$, and $2.35 \times 10^{-3}$, respectively. These results indicate that this configuration offers the best balance between learning and generalization capabilities, effectively minimizing prediction errors while maintaining strong consistency between experimental and modeled biodiesel yields.

Based on this optimization, the selected ANN architecture was established as 4–18–1, corresponding to four neurons in the input layer (representing process parameters), eighteen neurons in the hidden layer, and one neuron in the output layer (biodiesel yield). The strong agreement between predicted and experimental results confirms the robustness of the developed ANN model and validates its suitability for accurately modeling the nonlinear relationships in the transesterification process.

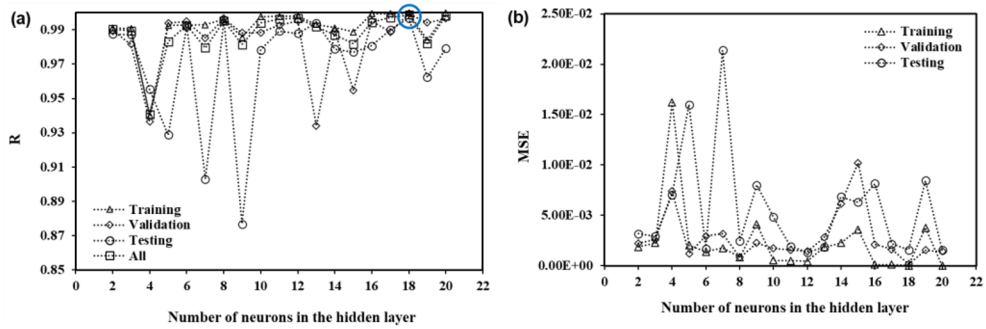


**Fig. 5.** Heuristic determination of the optimum number of hidden neurons: (a) coefficient of determination (R) and (b) mean squared error (MSE).

### 3.3 Prediction of biodiesel yield by ANN

The predictive capability of the developed artificial neural network (ANN) model for estimating biodiesel yield was evaluated by comparing the experimental and predicted values of fatty acid methyl ester (FAME) yield. The coefficient of determination (R) between these two datasets serves as a key indicator of the model's validity and accuracy. As illustrated in **Figure 6**, the ANN model with a 4–18–1 topology demonstrated excellent agreement between predicted and experimental data across all phases of training, validation, and testing. The obtained R values were 0.9989, 0.9969, 0.9980, and 0.9987 for the training, validation, testing, and overall datasets, respectively.

These exceptionally high R values, all exceeding 0.99, confirm that the developed ANN model effectively captures the nonlinear relationships among the process parameters influencing biodiesel production. The close alignment between the experimental and predicted data points, as observed in the plots, indicates that the model possesses strong generalization ability with minimal deviation from actual measurements. Moreover, the near-unity slope of the regression lines suggests that the ANN predictions are not only accurate but also unbiased across the entire data range. Therefore, the established ANN model can be considered a reliable and robust tool for predicting biodiesel yield under various operating conditions, offering a precise alternative to extensive experimental trials. This study aligns

with previous research on the application of artificial neural networks (ANN) to enhance Aspergillus flavipes lipase synthesis for green biodiesel production, confirming that ANN was more accurate and outperformed the BBD model [15].

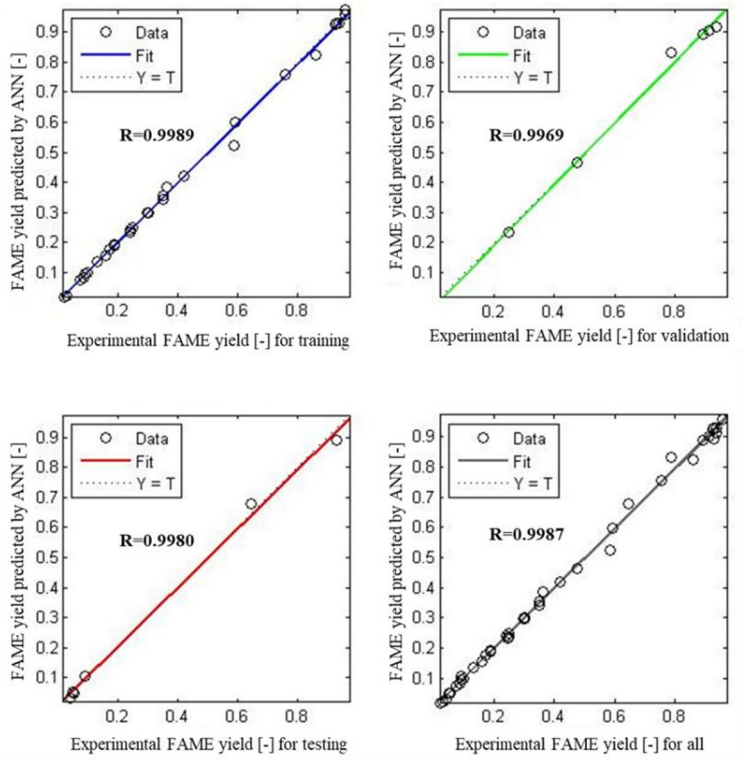


**Fig. 6.** Comparison between the experimental values and biodiesel yield predicted by ANN.

The predictive performance of the artificial neural network (ANN) for estimating biodiesel yield in supercritical methanol was evaluated by comparing the experimental and predicted results obtained using the Levenberg–Marquardt backpropagation algorithm. As summarized in **Table 1**, the ANN model demonstrated a strong agreement between predicted and experimental biodiesel yields under various operating conditions. The model effectively captured the nonlinear interactions between process parameters, including calcination temperature, reaction temperature, reaction time, and catalyst loading.

The results indicate that the highest predicted biodiesel yield of 0.97 mol/mol closely corresponded to the experimental yield of 0.96 mol/mol. This optimum yield was achieved at a reaction temperature of 60 °C, a reaction time of 90 minutes, and a catalyst loading of 4 wt%. Such close agreement between experimental and predicted values confirms the robustness and reliability of the developed ANN model. The small prediction errors observed across the dataset further suggest that the ANN was capable of accurately generalizing from the training data to unseen conditions. These findings demonstrate that the ANN, trained with the Levenberg–Marquardt algorithm, can serve as a powerful predictive tool for modeling biodiesel production in supercritical methanol systems. It allows for precise yield estimation without requiring exhaustive experimental trials, thus optimizing process efficiency and reducing the need for extensive laboratory experimentation.

Table 1. Experimental versus predicted yield of biodiesel over algae-derived catalyst by neural network using Lavenberg-Marquardt back propagation

| Run | Variables | | | | Experimental Yield [%] | Predicted Yield [%] | Error |
|---|---|---|---|---|---|---|---|
| | Temperature of calcination [°C] | Temperature of reaction [°C] | Reaction time [min] | Catalyst [wt%] | | | |
| 1 | 550 | 50 | 60 | 2 | 2.15 | 1.95 | 0.0020 |
| 2 | 550 | 50 | 90 | 2 | 4.30 | 2.99 | 0.0131 |
| 3 | 550 | 50 | 120 | 2 | 8.65 | 8.09 | 0.0056 |
| 4 | 550 | 50 | 150 | 2 | 13.02 | 13.63 | 0.0061 |
| 5 | 550 | 50 | 180 | 2 | 17.33 | 17.69 | 0.0036 |
| 6 | 550 | 60 | 60 | 2 | 24.28 | 23.17 | 0.0111 |
| 7 | 550 | 60 | 90 | 2 | 29.69 | 29.72 | 0.0003 |
| 8 | 550 | 60 | 120 | 2 | 5.32 | 4.83 | 0.0049 |
| 9 | 550 | 60 | 150 | 2 | 9.16 | 9.60 | 0.0044 |
| 10 | 550 | 60 | 180 | 2 | 23.95 | 23.95 | 0.0000 |
| 11 | 550 | 70 | 60 | 2 | 35.02 | 34.23 | 0.0079 |
| 12 | 550 | 70 | 90 | 2 | 47.75 | 46.48 | 0.0127 |
| 13 | 550 | 70 | 120 | 2 | 59.29 | 59.9 | 0.0061 |
| 14 | 550 | 70 | 150 | 2 | 64.45 | 67.85 | 0.0340 |
| 15 | 550 | 70 | 180 | 2 | 36.31 | 38.60 | 0.0229 |
| 16 | 650 | 50 | 60 | 2 | 58.69 | 52.30 | 0.0639 |
| 17 | 650 | 50 | 90 | 2 | 75.69 | 75.71 | 0.0002 |
| 18 | 650 | 50 | 120 | 2 | 78.93 | 83.09 | 0.0416 |
| 19 | 650 | 50 | 150 | 2 | 89.43 | 89.14 | 0.0029 |
| 20 | 650 | 50 | 180 | 2 | 92.87 | 92.82 | 0.0005 |
| 21 | 650 | 60 | 60 | 2 | 92.97 | 89.18 | 0.0379 |
| 22 | 650 | 60 | 90 | 2 | **95.88** | **97.26** | **0.0138** |
| 23 | 650 | 60 | 120 | 2 | 93.83 | 92.87 | 0.0096 |
| 24 | 650 | 60 | 150 | 2 | 95.85 | 95.68 | 0.0017 |
| 25 | 650 | 60 | 180 | 2 | 93.68 | 91.54 | 0.0214 |
| 26 | 650 | 70 | 60 | 2 | 86.04 | 82.27 | 0.0377 |
| 27 | 650 | 70 | 90 | 2 | 91.29 | 90.24 | 0.0105 |
| 28 | 650 | 70 | 120 | 2 | 92.73 | 92.51 | 0.0022 |
| 29 | 650 | 70 | 150 | 2 | 2.91 | 2.25 | 0.0066 |
| 30 | 650 | 70 | 180 | 2 | 5.01 | 5.13 | 0.0012 |
| 31 | 750 | 50 | 60 | 2 | 9.98 | 10.02 | 0.0004 |
| 32 | 750 | 50 | 90 | 2 | 16.01 | 15.70 | 0.0031 |
| 33 | 750 | 50 | 120 | 2 | 18.95 | 19.12 | 0.0017 |
| 34 | 750 | 50 | 150 | 2 | 24.96 | 23.45 | 0.0151 |
| 35 | 750 | 50 | 180 | 2 | 30.05 | 29.97 | 0.0008 |
| 36 | 750 | 60 | 60 | 2 | 7.61 | 7.50 | 0.0011 |
| 37 | 750 | 60 | 90 | 2 | 8.99 | 10.50 | 0.0151 |
| 38 | 750 | 60 | 120 | 2 | 18.74 | 18.76 | 0.0002 |
| 39 | 750 | 60 | 150 | 2 | 25.01 | 24.96 | 0.0005 |
| 40 | 750 | 60 | 180 | 2 | 30.15 | 29.89 | 0.0026 |
| 41 | 750 | 70 | 60 | 2 | 35.01 | 35.49 | 0.0048 |
| 42 | 750 | 70 | 90 | 2 | 42.05 | 41.91 | 0.0014 |
| 43 | 650 | 60 | 90 | 3 | 88.01 | 88.15 | 0.0014 |
| 44 | 650 | 60 | 90 | 5 | 89.99 | 90.04 | 0.0005 |

## 4 Conclusion

This study successfully developed an Artificial Neural Network (ANN) model to predict biodiesel production using an Ulva lactuca-based heterogeneous catalyst. The primary objective, to establish a reliable predictive framework for estimating biodiesel yield under

varying reaction conditions, was effectively achieved. The ANN model, trained using the Levenberg–Marquardt backpropagation algorithm, demonstrated excellent predictive accuracy with an optimized network architecture of 4–18–1. The high correlation coefficients ($R > 0.99$) and low mean squared errors confirmed the robustness and reliability of the model in capturing the nonlinear relationships among process parameters such as temperature, catalyst loading, and reaction time. Experimentally, the U. lactuca-derived catalyst exhibited strong catalytic performance, achieving a maximum biodiesel yield of 95.88% at 60 °C, 90 minutes, and 4 wt% catalyst loading, which closely matched the ANN-predicted value of 97.26% mol $mol^{-1}$. The results also revealed that moderate calcination temperature (650 °C) and optimal reaction conditions enhanced catalytic activity and yield, while excessive catalyst loading or temperature reduced performance due to side reactions and methanol evaporation.

## Acknowledgments

We gratefully acknowledge the support from the Directorate General of Higher Education, Research, and Technology, Ministry of Education, Culture, Research, and Technology of Indonesia, for providing financial assistance for this study through the Regular Fundamental Research Scheme, Grant No. 006/C3/DT.05.00/PL/2025.

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