Communications on Applied Nonlinear Analysis
ISSN: 1074-133X
Vol 32 No. 8s (2025)

Artificial Neural Network Approach to Multi-Response Prediction of Transesterification

Rohit Khatri[1*], Om Prakash Jakhar[1]
Department of Mechanical Engineering, Engineering College Bikaner, India
[*]Corresponding Author: rohit_me_mania@yahoo.co.in

Article History:

Received: *22-10-2024*

Revised: *25-11-2024*

Accepted: *26-12-2024*

Abstract:

This study investigates the impact of transesterification parameters on biodiesel yield and kinematic viscosity, using an Artificial Neural Network (ANN) with the Levenberg-Marquardt algorithm to predict these outcomes. Predictions are validated against experimental results using established metrics like RMSE, MAPE, and R2. The experiments follow a Design of Experiment (DOE) approach, enabling accurate yield and viscosity measurements for each biodiesel sample. Results show that the ANN model strongly aligns with experimental results, showing lower RMSE and MAPE and higher R^2, outperforming RSM. Consequently, the ANN model is recommended for reliable biodiesel yield and viscosity prediction.

Keywords: ANN, Regression, Optimization, Prediction.

1. Introduction

The transportation sector has been utilizing about three-fourths of the total petroleum consumption in the country [1]. Transport contributes 12% of India's energy-related CO_2 emissions. To address these challenges, sustainable and renewable fuel alternatives like biodiesel must be explored [2], [3], [4]. The environmentally friendly fuel known as biodiesel stands out as a very promising substitute because of its biodegradability and lack of sulphur oxides in the exhaust [5] [6], [7]. Biodiesel can be obtained from edible and non-edible crops, algae, etc. WCO is obtained after frying or cooking, and this is a third-generation feedstock to produce biodiesel [8]. Transesterification is the most suitable and cost-effective method to manufacture high-quality biodiesel, which has qualities similar to diesel. The process aims to reduce oil viscosity and mimic petrochemical diesel's physical properties [9], [10], [11]. Furthermore, the existing literature has shown that biodiesel meets the ASTM D6751 and EN 14214 fuel specifications [12]. ANNs are widely used for predicting and optimizing parameters and responses in biodiesel production, often outperforming traditional methods. Studies have shown ANN models yield higher accuracy, with better R^2 values and lower MSE than RSM models [13], [14] [15]. [16] ANN provided more accurate predictions than RSM based on RMSE and R^2 metrics.

This study optimizes transesterification variables to maximize biodiesel yield and minimize viscosity. It performs multi-response optimization, predicts outcomes, and compares results with ANN.

2. Materials and Methods

2.1 Feedstock and chemicals

Waste cooking oil was collected from a vendor in Bikaner, Rajasthan, filtered with sieves to remove microparticles and heated to 110°C approx. for 30 minutes to eliminate moisture. The methanol and ethanol are used as alcohols, and KOH as catalysts.

2.2 Design of Experiment & Transesterification

The design of the experiment is done using RSM, Design Expert 13 software using the BBD approach[17]. Five process parameters were selected: reaction temperature (A), reaction duration (B), oil: alcohol ratio (C), catalyst amount (D), and methanol to ethanol Ratio (E). The number of trials (N_T) with different conditions is determined using the Box-Behnken design (BBD) as described in Equation (1).

$$N_T = 2k(k-1) + N_C \quad (1)$$

where k represents the number of variables studied and Nc denotes the number of replicas for central points.

Biodiesel was generated utilizing WCO as feedstock, methanol, ethanol as alcohol, and KOH as a catalyst by Hot plate mode of heating the reactants. The speed of hot plate stirrer was constant. Following a specific time, the reaction mixture was dumped into a separating funnel and left for one day to separate biodiesel and glycerol via gravity. After separating glycerol, the WCO-derived biodiesel is water-washed to remove any pollutants.

The yield conversion and kinematic viscosity was evaluated based on eq. (1) & (2) respectively.

$$\text{Yield}(\%) = \frac{amount\ of\ biodiesel\ produced}{amount\ of\ waste\ cooking\ oil\ sample} * 100 \quad (2)$$

$$\text{Kinematic viscosity } (\nu) = (C_1 * \text{t}) - \frac{C_2}{t} \quad (3)$$

Where, ν represents Kinematic viscosity in centi-stokes, C_1 shows the Viscometer constant, which can be determined by equipment and C_2 denotes the Coefficient of kinetic energy, and t in equation represents Time of flow in seconds[18].

2.3 Modelling of ANN network

Artificial Neural Networks (ANNs) have become a pivotal tool in research, offering significant advancements in prediction and optimization. ANN models have shown superior performance in predicting and optimizing biodiesel yields & kinematic viscosity compared to traditional method [19], [20]. MATLAB 2023 MathWorks was used for modelling of ANN. Levenberg-Marquardt (trainlm) algorithm was used to train model. The network was created by dividing 80% of the data for training and validation, and 20% was used for testing [21]. 5–10–2 architecture was framed as it contains 5 inputs, 2 outputs, and 10 neurons. The metrics employed for assessing the performance of the employed models include RMSE, MAPE, and R^2 [22].

3. Results and Discussion

3.1 RSM analysis

Signification of model was evaluated by lack of fit, analysis of variance and coefficient of determination (R^2). 2FI model was suggested by model due to high F-value & lesser p value (Table1)[13]. ANOVA also helps to recognize the most influential parameter[23][24]. According to ANOVA, the amount of catalyst (D) has the most significant effect, and the reaction time (B) has the least effect on biodiesel yield, whereas for kinematic viscosity, oil to alcohol ratio(C) has the most significant effect, and the reaction temperature (A) has the least effect.

3.2 Artificial Neural Network (ANN):

The study utilized an artificial neural network to forecast biodiesel yield and kinematic viscosity, demonstrating its superior effectiveness to other statistical tools. Model was trained for minimum mean square error and maximum coefficient of determination. Model validation used R^2, root mean square error (RMSE), and MAPE.

Figures 1 & 2 illustrate the performance evaluation of an ANN model used to predict the kinematic viscosity & yield of biodiesel. High value of R and data trend near the mean line show the adequacy of model training and model can predict a new data set.

Table 1 ANOVA analysis

Biodiesel Yield						**Kinematic Viscosity**						
Source	**Sum of Squares**	**df**	**Mean Square**	**F-value**	**p-value**	**Source**	**Sum of Squares**	**df**	**Mean Square**	**F-value**	**p-value**	
Model	**498.49**	**11**	**45.32**	**117.39**	**< 0.0001**	**Model**	**17.72**	**8**	**2.22**	**67.19**	**< 0.0001**	**significant**
A-Temp	39.31	1	39.31	101.84	< 0.0001	A-Temp	0.1406	1	0.1406	4.27	0.046	
B-Time	4.04	1	4.04	10.47	0.0027	B-Time	6.48	1	6.48	196.53	< 0.0001	
C-O:M/E	8.24	1	8.24	21.34	< 0.0001	C-O:M/E	8.17	1	8.17	247.66	< 0.0001	
D-catalyst	389.37	1	389.37	1008.65	< 0.0001	D-catalyst	1.01	1	1.01	30.66	< 0.0001	
E-M:E	10.91	1	10.91	28.25	< 0.0001	E-M:E	0.1914	1	0.1914	5.81	0.0211	
AB	1.12	1	1.12	2.91	0.0971	AC	0.648	1	0.648	19.65	< 0.0001	
AC	5.22	1	5.22	13.53	0.0008	BD	0.2314	1	0.2314	7.02	0.0118	
AE	30.47	1	30.47	78.93	< 0.0001	BE	0.8556	1	0.8556	25.95	< 0.0001	
BD	2.81	1	2.81	7.27	0.0108							
BE	5.09	1	5.09	13.17	0.0009							
CE	1.92	1	1.92	4.97	0.0325							
Residual	13.13	34	0.386			**Residual**	1.22	37	0.033			
Lack of Fit	**12.34**	**29**	**0.4255**	**2.7**	**0.1349**	**Lack of Fit**	**1.06**	**32**	**0.0331**	**1.03**	**0.5513**	**not significant**
Pure Error	0.7865	5	0.1573			Pure Error	0.1611	5	0.0322			
Cor Total	511.62	45				**Cor Total**	18.94	45				

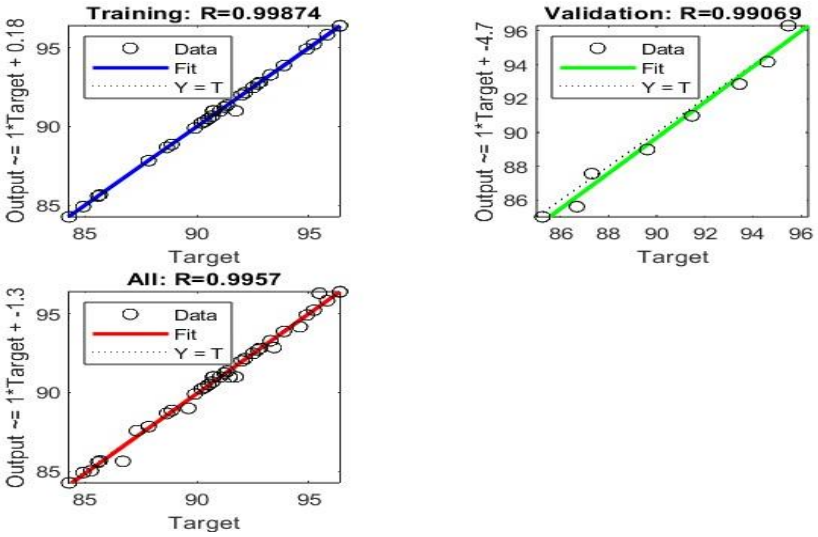


Figure1 Regression curves for biodiesel yield

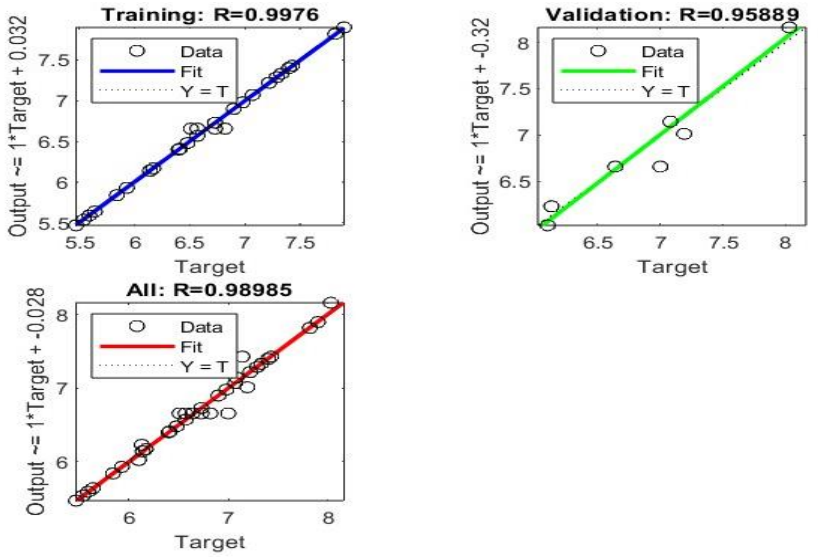


Figure2 Regression curves for biodiesel Kinematic viscosity

In training phase, high value of correlation coefficient (R) 0.99874 & 0.9976 and alignment of Regression line with data for yield and kinematic viscosity respectively, indicates model's capability to establish relationship between predicted and actual values. Similarly, for validation, plot R-values of 0.99069 & 0.95889 for yield and kinematic viscosity, respectively, signifying the predictive capability of the trained model and trend of the curve showing that the model predicted well without overfitting. This high overall correlation for Figures 5 and 6 indicates that the ANN model is highly effective in predicting biodiesel's kinematic viscosity and yield, with minimal deviation from the experimental values. This highlights the capability of ANN models in complex nonlinear regression tasks. Further prediction is made for the complete data set and compared with RSM based on evaluation metrics RMSE, MAPE & R^2.

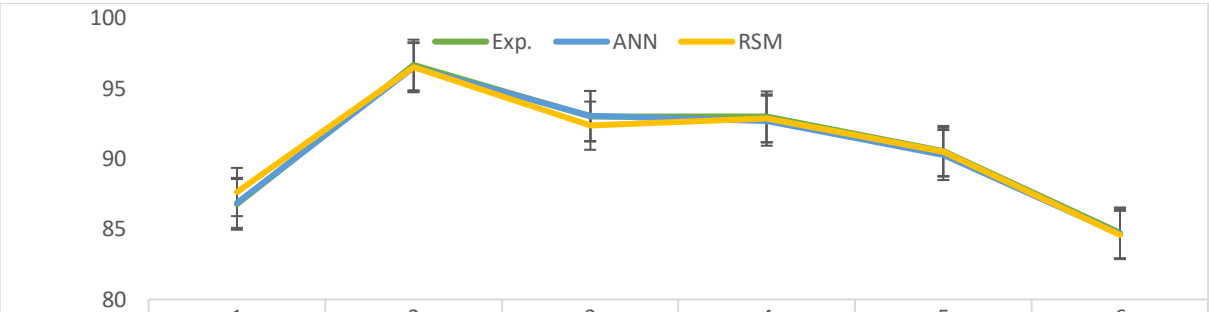
3.3 Comparative Analysis:

In this section, ANN and RSM results were compared with experimental results. Comparison was made in two separate phases:

In first phase, ANN and RSM results were compared with experimental results for the complete data set as shown in Figure (3-4).

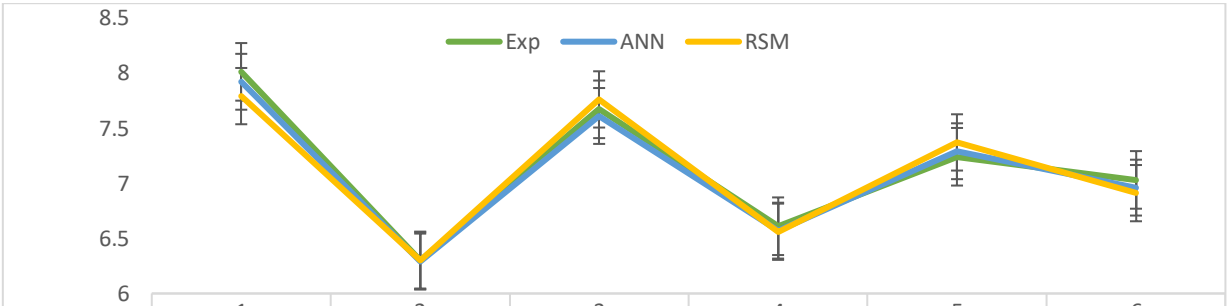
In second phase, a comparison of ANN and RSM model results was made based on RMSE, MAPE & R^2 to find the most accurate model (Figure 5).

Figure 3&4 shows the comparative illustration of experimental, ANN & RSM values for yield and kinematic viscosity, respectively. The data shows that the values predicted by the ANN closely match the experimental results. Metrics for biodiesel yield and kinematic viscosity supports this. Predictions were also compared with experimental results and RSM. (Fig3).



	1	2	3	4	5	6
Exp.	86.75	96.65	93.01	92.97	90.52	84.73
ANN	86.8595	96.4852	93.0258	92.6898	90.2568	84.6405
RSM	87.627912	96.493522	92.337222	92.850712	90.473212	84.581417

Figure 3 comparative chart of Experimental, ANN & RSM yield values for testing data



	1	2	3	4	5	6
Exp	8.01	6.3	7.67	6.61	7.24	7.03
ANN	7.92	6.29	7.61	6.57	7.29	6.96
RSM	7.79	6.3	7.76	6.56	7.37	6.91

Figure 4 comparative chart of Experimental, ANN & RSM kinematic viscosity values for Testing data

The figure 4 compares experimental data with predictions from an Artificial Neural Network (ANN) and a Response Surface Methodology (RSM) model for the kinematic viscosity and yield of biodiesel. It presents forty-six data points, with the experimental results shown as a green line, ANN predictions in blue, and RSM predictions in yellow.

The experimental data serve as a reference, and error bars indicate measurement uncertainty. Both ANN and RSM models closely track the experimental results and demonstrate their effectiveness in capturing the non-linear trend.

The slight deviations between the models and experimental data indicate minimal discrepancies, with the ANN model consistently aligning more closely to experimental values than the RSM model. This suggests that the ANN model better handles the complexities of predicting biodiesel yield and kinematic viscosity.

This comparison underscores the ANN model's suitability for capturing complex non-linear relationships. Meanwhile, the RSM model also performs satisfactorily, but its predictive accuracy slightly lags compared to the ANN model, particularly in regions with higher variance.

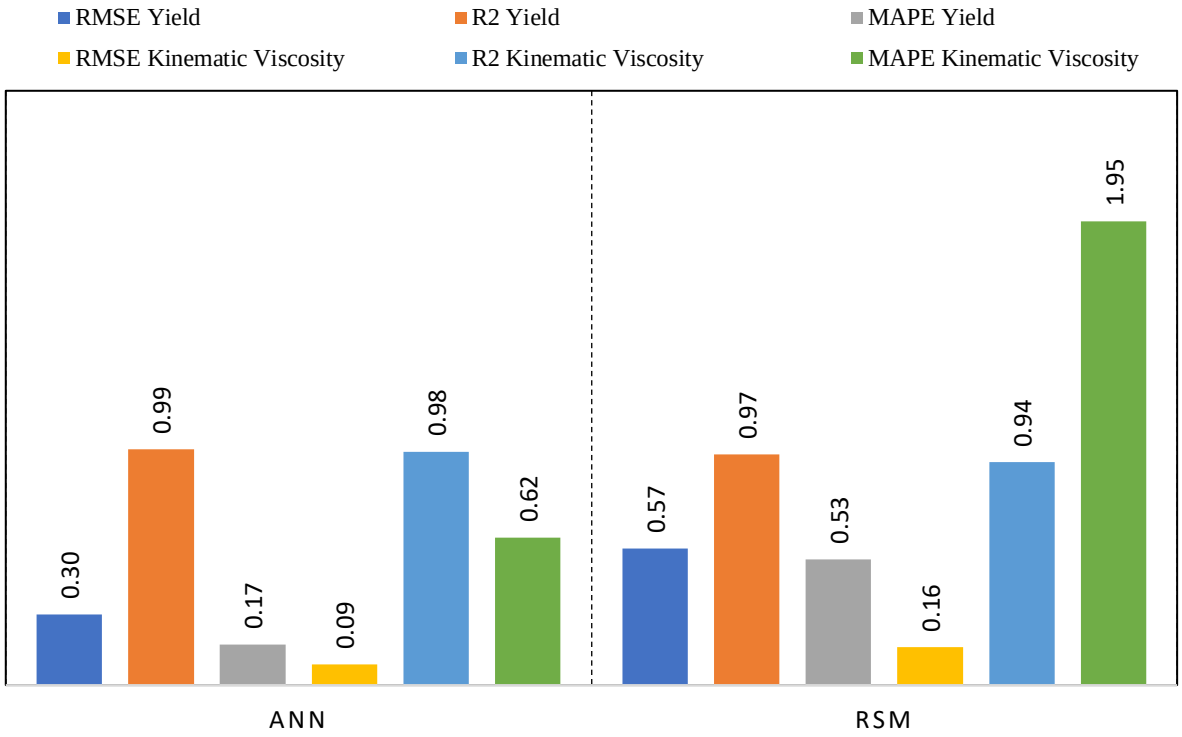


Figure5: R^2, MAPE & RMSE comparison for ANN & RSM

The graph shows that the ANN significantly outperforms the RSM. The ANN's root mean square error (RMSE) for yield is 0.30, 47% lower than the RSM's 0.57. The ANN's mean absolute percentage error (MAPE) for viscosity is 0.09, 95% lower than the RSM's 1.95. Additionally, the ANN achieves higher R^2 values for yield (0.99 vs. 0.97) and viscosity (0.98 vs. 0.94), indicating superior predictive accuracy.

4. Conclusion

The study demonstrates that implementing response surface methodology and an artificial neural network approach can significantly reduce experimental work in finding the combination of process parameters for a desirable response. The experimental and predicted results can be summarized as follows:

a) A maximum biodiesel yield of 96.65% and a kinematic viscosity of 5.467cSt were observed for an oil-to-alcohol ratio (WCO Molar ratio) of 9.99876:1 mol/mol, a catalyst dosage of 0.751004, a reaction time of 68.7703, a reaction temperature of 59.9689, and a methanol-to-ethanol ratio of 95.0148± 0.5.

b) The Levenberg-Marquardt algorithm was more accurate, and the optimized architecture and hidden layers were (5-10-2) and 10, respectively.

c) Finally, the root mean square error for yield and kinematic viscosity was 47% and 43.75% lower, respectively, and the value of R^2 for yield and kinematic viscosity was higher for the artificial neural network compared to response surface methodology.

These findings suggest that the artificial neural network-developed model has better capability than response surface methodology in predicting the response and the effect of process parameters. Future research could expand to develop a deep learning model that can predict it more accurately. Hence, this research concludes that the artificial neural network could be a promising technique for predicting biodiesel properties.

5. References

[1] S. Rakesh and R. S. Subramaniyam, "An experimental investigation of the performance of single cylinder CI engine fueled with biodiesel and hydrogen," in AIP Conference Proceedings, American Institute of Physics Inc., Jul. 2019. doi: 10.1063/1.5117986.

[2] K. Raj Bukkarapu and A. Krishnasamy, "Support vector regression approach to optimize the biodiesel composition for improved engine performance and lower exhaust emissions," Fuel, vol. 348, p. 128604, Sep. 2023, doi: 10.1016/j.fuel.2023.128604.

[3] D. Singh et al., "A comprehensive review of physicochemical properties, production process, performance and emissions characteristics of 2nd generation biodiesel feedstock: Jatropha curcas," Fuel, vol. 285, p. 119110, Feb. 2021, doi: 10.1016/j.fuel.2020.119110.

[4] B. Maleki and S. S. Ashraf Talesh, "Cold flow properties and CI engine parameters synchronic improvement of biodiesel/diesel/ C3 and C4 alcohol blends: Mixture design approach," Process Safety and Environmental Protection, vol. 160, pp. 310–326, Apr. 2022, doi: 10.1016/j.psep.2022.02.026.

[5] G. M. Lionus Leo, R. Jayabal, D. Srinivasan, M. Chrispin Das, M. Ganesh, and T. Gavaskar, "Predicting the performance and emissions of an HCCI-DI engine powered by waste cooking oil biodiesel with Al2O3 and FeCl3 nano additives and gasoline injection – A random forest machine learning approach," Fuel, vol. 357, p. 129914, Feb. 2024, doi: 10.1016/j.fuel.2023.129914.

[6] M. I. El-Galad, K. M. El-Khatib, and F. A. Zaher, "Economic feasibility study of biodiesel production by direct esterification of fatty acids from the oil and soap industrial sector," Egyptian Journal of Petroleum, vol. 24, no. 4, pp. 455–460, Dec. 2015, doi: 10.1016/j.ejpe.2015.06.002.

[7] C. A. Osagiede and F. A. Aisien, "Biochar-based bi-functional catalyst derived from rubber seed shell and eggshell for biodiesel production from waste cooking oil," Fuel, vol. 358, p. 130076, Feb. 2024, doi: 10.1016/j.fuel.2023.130076.

[8] Z. Hu et al., "Waste cooking oil biodiesel and petroleum diesel soot from diesel bus: A comparison of morphology, nanostructure, functional group composition and oxidation reactivity," Fuel, vol. 321, p. 124019, Aug. 2022, doi: 10.1016/j.fuel.2022.124019.

[9] D. Singh, D. Sharma, S. L. Soni, S. Sharma, P. Kumar Sharma, and A. Jhalani, "A review on feedstocks, production processes, and yield for different generations of biodiesel," Fuel, vol. 262, p. 116553, Feb. 2020, doi: 10.1016/j.fuel.2019.116553.

[10] M. Mohadesi, B. Aghel, M. Maleki, and A. Ansari, "The use of KOH/Clinoptilolite catalyst in pilot of microreactor for biodiesel production from waste cooking oil," Fuel, vol. 263, p. 116659, Mar. 2020, doi: 10.1016/j.fuel.2019.116659.

[11] E. Soria-Figueroa, V. Y. Mena-Cervantes, M. García-Solares, R. Hernández-Altamirano, and J. Vazquez-Arenas, "Statistical optimization of biodiesel production from waste cooking oil using CaO as catalyst in a Robinson-Mahoney type reactor," Fuel, vol. 282, p. 118853, Dec. 2020, doi: 10.1016/j.fuel.2020.118853.

[12] B. Maleki, S. S. Ashraf Talesh, and M. Mansouri, "Comparison of catalysts types performance in the generation of sustainable biodiesel via transesterification of various oil sources: a review study," Materials Today Sustainability, vol. 18, p. 100157, Jun. 2022, doi: 10.1016/j.mtsust.2022.100157.

[13] B. Dharmalingam et al., "Comparison of neural network and response surface methodology techniques on optimization of biodiesel production from mixed waste cooking oil using heterogeneous biocatalyst," Fuel, vol. 340, p. 127503, May 2023, doi: 10.1016/j.fuel.2023.127503.

[14] B. Maleki, B. Singh, H. Eamaeili, Y. K. Venkatesh, S. S. A. Talesh, and S. Seetharaman, "Transesterification of waste cooking oil to biodiesel by walnut shell/sawdust as a novel, low-cost and green heterogeneous catalyst: Optimization via RSM and ANN," Ind Crops Prod, vol. 193, p. 116261, Mar. 2023, doi: 10.1016/j.indcrop.2023.116261.

[15] A. Kolakoti and G. Satish, "Biodiesel production from low-grade oil using heterogeneous catalyst: an optimisation and ANN modelling," Australian Journal of Mechanical Engineering, vol. 21, no. 1, pp. 316–328, Jan. 2023, doi: 10.1080/14484846.2020.1842298.

[16] A. Garg and S. Jain, "Process parameter optimization of biodiesel production from algal oil by response surface methodology and artificial neural networks," Fuel, vol. 277, p. 118254, Oct. 2020, doi: 10.1016/j.fuel.2020.118254.

[17] B. Maleki and H. Esmaeili, "Ultrasound-assisted conversion of waste frying oil into biodiesel using Al-doped ZnO nanocatalyst: Box-Behnken design-based optimization," Renew Energy, vol. 209, pp. 10–26, Jun. 2023, doi: 10.1016/J.RENENE.2023.03.119.

[18] Z. Yaakob, M. Mohammad, M. Alherbawi, Z. Alam, and K. Sopian, "Overview of the production of biodiesel from Waste cooking oil," Renewable and Sustainable Energy Reviews, vol. 18, pp. 184–193, Feb. 2013, doi: 10.1016/j.rser.2012.10.016.

[19] N. Pirmoradi, M. T. Ghaneian, M. H. Ehrampoush, M. H. Salmani, and B. Hatami, "The conversion of poultry slaughterhouse wastewater sludge into biodiesel: Process modeling and optimization," Renew Energy, vol. 178, pp. 1236–1249, Nov. 2021, doi: 10.1016/j.renene.2021.07.016.

[20] O. D. Samuel and M. O. Okwu, "Comparison of Response Surface Methodology (RSM) and Artificial Neural Network (ANN) in modelling of waste coconut oil ethyl esters production," Energy Sources, Part A: Recovery, Utilization, and Environmental Effects, vol. 41, no. 9, pp. 1049–1061, May 2019, doi: 10.1080/15567036.2018.1539138.

[21] S. N. Selamat, N. Abd Majid, and A. Mohd Taib, "A Comparative Assessment of Sampling Ratios Using Artificial Neural Network (ANN) for Landslide Predictive Model in Langat River Basin, Selangor, Malaysia," Sustainability, vol. 15, no. 1, p. 861, Jan. 2023, doi: 10.3390/su15010861.

[22] D. Babu, V. Thangarasu, and A. Ramanathan, "Artificial neural network approach on forecasting diesel engine characteristics fuelled with waste frying oil biodiesel," Appl Energy, vol. 263, p. 114612, Apr. 2020, doi: 10.1016/j.apenergy.2020.114612.

[23] W.-H. Chen et al., "Optimization and analysis of syngas production from methane and CO2 via Taguchi approach, response surface methodology (RSM) and analysis of variance (ANOVA)," Fuel, vol. 296, p. 120642, Jul. 2021, doi: 10.1016/j.fuel.2021.120642.

[24] O. M. Olatunji, I. T. Horsfall, and E. V. Ubom, "Response surface optimization approach to predict the maximum %biodiesel yield via transesterification of esterified shea butter oil by utilizing bio-catalysts," Current Research in Green and Sustainable Chemistry, vol. 4, p. 100167, 2021, doi: 10.1016/j.crgsc.2021.100167.