



Green Nanocatalyst-driven Ultrasonic Synthesis of Biodiesel from *Madhuca longifolia* Oil: Integrated Taguchi, ANN and Genetic Algorithm Optimization

Alok Rajendra Narkhede¹, R. Venkatesh², Amuthakkannan Rajakannu^{3*},
Suvetha Poyyamani Sunddararaj⁴, N. Selvam⁵ and V. V. S. Sasank⁶

¹Department of Mechanical Engineering, Yeshwantrao Chavan College of Engineering, Nagpur, MH, India

²Department of Mechanical Engineering, Vinayaka Mission's Kirupananda Variyar Engineering College, Vinayaka Mission's Research Foundation (Deemed to be University), Salem, TN, India

³Department of Mechanical and Industrial Engineering, College of Engineering, National University of Science and Technology, Muscat, Sultanate of Oman

⁴Department of Electrical and Electronics Engineering, Dayananda Sagar College of Engineering, Bengaluru, KA, India

⁵Department of Electrical and Electronics Engineering, M. Kumarasamy College of Engineering, Karur, TN, India

⁶Department of Computer Science and Engineering, Koneru Lakshmaiah Education Foundation, Guntur, AP, India

Received: 05.05.2026 Accepted: 18.05.2026 Published: 30.06.2026

*kannan.maya1986@gmail.com



ABSTRACT

The swift exhaustion of fossil fuel reserves and increasing demand for sustainable energy have increased the need for eco-friendly alternative fuels. This study investigated biodiesel production from *Madhuca longifolia* (Mahua oil), a cost-effective non-edible feedstock, utilizing an ultrasonic-assisted two-step esterification-transesterification process catalyzed by green-synthesized ZnO nanoparticles. The ZnO nanocatalyst was synthesized utilizing *Moringa oleifera* leaf extract and extensively evaluated by FTIR, XRD, SEM-EDX, and particle size analysis, validating its structural integrity, shape, and nanoscale characteristics. Process parameters, such as ultrasonication duration (30–40 min), catalyst concentration (0.5–1.5 wt%) and methanol-to-oil molar ratio (6–12) were adjusted utilizing Taguchi design in conjunction with ANOVA. The molar ratio was determined to be the primary factor influencing biodiesel yield. Despite the statistical regression model demonstrating substantial predictive power ($R^2 = 98.76\%$), its capacity to depict intricate nonlinear relationships was constrained. An artificial intelligence-based strategy was employed to surmount this limitation. The constructed backpropagation artificial neural network (BP-ANN) model exhibited exceptional predictive efficacy ($R^2 = 0.999$), markedly surpassing Radial Basis Function (RBF) and Random Forest (RF) models regarding accuracy and error reduction. Subsequent optimization employing a hybrid BP-ANN combined with a genetic algorithm (GA) determined the ideal operating conditions to be 40 minutes of ultrasonication, 1.2317 wt% ZnO catalyst loading, and a molar ratio of 12. Under the conditions, maximum anticipated biodiesel yield of 96.042% were attained and experimentally corroborated with a yield of 94.5%, reflecting a minimal deviance of 1.605%. The results indicate that ultrasonication significantly accelerates reaction kinetics by enhancing cavitation and mass transfer, facilitating high conversion efficiency with less catalyst loading. The integration of Taguchi design, ANN modeling, and GA optimization provides a stable and efficient framework for biodiesel synthesis. This study highlights the promise of green nanocatalytic systems combined with modern computational methods for the scalable and sustainable synthesis of biofuels from non-edible oil sources.

Keywords: Green synthesis; *Madhuca longifolia*; ZnO nanocatalyst; *Moringa oleifera*; Biodiesel; Artificial neural network.

1. INTRODUCTION

Growing environmental concerns, depletion of fossil fuels, and stringent emission norms have driven the development of sustainable alternative fuels. Biodiesel derived from non-edible sources like mahua oil and waste cooking oil has gained significant attention because of their renewable nature, compatibility and biodegradability, with existing diesel engines. However, limitations such as lower efficiency and higher emissions necessitate the use of advanced catalysts, nano-additives, and optimization techniques to enhance overall performance. Green synthesis of ZnO nanoparticles using cow dung fuel demonstrated improved biodiesel

properties and engine performance, where the B20 blend with ZnO-GS exhibited enhanced brake thermal efficiency and reduced emissions (Kavalli *et al.* 2022). Incorporation of ZnO nanoparticles (25 ppm) in mahua oil methyl ester blends improved combustion characteristics, supported by Fourier transform infrared (FTIR) and FESEM analyses confirming nanoparticle dispersion (Kumar *et al.* 2022). Enhanced engine efficiency and emission reduction were also observed in ZnO-blended fuels, with optimal results reported for B20 with 50 ppm ZnO (Seela and Ravi, 2020).

Supercritical methanol processes integrated with ZnO catalysts significantly improved biodiesel

conversion efficiency and reduced activation energy, indicating enhanced reaction kinetics (Lamba *et al.* 2019). ZnO nanostructures with controlled morphologies and doping strategies achieved high conversion efficiency up to 99.3%, emphasizing the importance of surface area and catalyst design (Darvishvand *et al.* 2024). ZnO-modified sulfonated biochar catalysts enabled simultaneous esterification and transesterification, improving biodiesel yield and process sustainability (Pratiwi *et al.* 2026). Eco-friendly synthesis of ZnO nanoparticles using biomass-based fuels resulted in materials with tunable bandgap and catalytic efficiency for biodiesel production (Rudreshappa *et al.* 2024). ZnO-based biocatalysts demonstrated efficient biodiesel synthesis from lipid sources with good reusability over multiple cycles (Parthiban and Jambulingam, 2025). High-performance bifunctional catalysts achieved biodiesel yields up to 97.81% with strong kinetic and thermodynamic feasibility (Maleki *et al.* 2023).

Shell-derived CaO–ZnO catalysts exhibited enhanced catalytic activity with biodiesel yields exceeding 90% and significant emission reductions (Chong *et al.* 2023). Zinc-modified anthill catalysts provided a sustainable and cost-effective approach for biodiesel production with high model accuracy and catalyst stability (Yusuff *et al.* 2021b). Similarly, ZnO–coal fly ash composite catalysts demonstrated reliable biodiesel production with high yield and reusability (Yusuff *et al.* 2022). Two-step catalytic systems using ZnO/CuO composites effectively reduced free fatty acids and achieved high biodiesel yields under optimized conditions (Marso *et al.* 2021). Bifunctional CeO₂/ZnO nanocatalysts enabled simultaneous esterification and transesterification with improved stability and conversion efficiency (Vardast *et al.* 2022). Advanced mesoporous carbon-based catalysts such as ZnC1000@SO₃H exhibited high surface area and catalytic performance, achieving biodiesel yields above 97% with strong reusability (Zheng *et al.* 2026).

MOF-based ZnO/Cu-BTC catalysts demonstrated efficient biodiesel conversion with enhanced porosity and catalytic stability (Yusuf *et al.* 2026). Doping strategies such as Al-modified ZnO further improved catalytic efficiency and recyclability, achieving biodiesel yields above 96% (Maleki and Esmacili, 2023). The incorporation of oxygenated additives such as 2-ethylhexyl nitrate significantly enhanced combustion efficiency and reduced emissions in biodiesel blends (Gugulothu *et al.* 2025b). Further investigations on ternary biodiesel blends confirmed improved engine performance and emission characteristics under optimized operating conditions using Response Surface Methodology (RSM) and machine learning techniques (Gugulothu *et al.* 2025a). Multi-objective optimization approaches such as RSM–NSGA-II (Non-dominated Sorting Genetic Algorithm)

provided Pareto-optimal solutions for balancing performance and emission (Dhingra *et al.* 2016). Hybrid optimization techniques combining RSM and Genetic Algorithm achieved biodiesel yields up to 97.54%, validating the effectiveness of advanced modeling approaches (Ahmad *et al.* 2023).

This study presents an innovative hybrid framework for biodiesel synthesis that combines ultrasonic-assisted transesterification with a green-synthesized ZnO nanocatalyst and powerful artificial intelligence optimization techniques. The integration of Taguchi design, BP-ANN modeling, and genetic algorithms facilitates precise prediction and determination of global optimal conditions, in contrast to traditional statistical methods. This method markedly accelerates reaction kinetics by ultrasonication while decreasing catalyst usage, therefore enhancing process efficiency and sustainability. Moreover, the utilization of a plant-mediated nanocatalyst guarantees environmental compatibility. This combined experimental and computational approach offers a dependable, scalable, and high-precision method for sustainable biodiesel generation from non-edible feedstocks.

2. MATERIALS AND METHODS

2.1 Materials

Chemicals like methanol, sulfuric acid, potassium hydroxide, zinc acetate dihydrate [Zn(CH₃COO)₂·2H₂O, purity 99%] and copper sulfate, were procured from Star Scientific Enterprises, Erode, Tamil Nadu, India. Double-distilled water was utilized as required.

2.2 Synthesis of Zinc Oxide Nanoparticles

Fresh ripe leaves of *Moringa oleifera* was harvested from Coimbatore, Tamil Nadu, India, and meticulously rinsed by distilled water to eliminate any sticking contaminants. The cleaned leaves were shade-dried under ambient conditions for 5–7 days to maintain phytochemical integrity, thereafter ground as fine powder by mechanical grinding. About 2 g of the leaf powder was suspended in 100 mL of DI water and heated to 80 °C for 20 minutes to enhance the extraction of bioactive phytoconstituents. The resultant mixture was cooled to ambient temperature, centrifuged at 5000 rpm for 10 mins, and clear supernatant were collected as stabilizing and reducing agent. For nanoparticle synthesis, 100 mL of *Moringa oleifera* leaf extract was incrementally introduced to 100 mL of 1 M zinc acetate dihydrate [Zn(CH₃COO)₂·2H₂O] solution while maintaining continuous magnetic stirring. The reaction mixture was maintained at 70 °C until the color changed from pale yellow to milky white, confirming the formation of ZnO nanoparticles. The product was subsequently centrifuged and thoroughly washed with DI water and ethanol to

eliminate residual contaminants and unreacted components. The filtered precipitate was subjected to drying in a hot air oven at 110 °C for 10 hours to yield fine ZnO nanopowder (Thanikodi and Solairaju, 2026). This environmentally sustainable synthesis method employs phytochemicals, including flavonoids, phenolics, and proteins, as natural reducing and capping agents, hence providing improved stability and biocompatibility of nanoparticles for environmental and catalytic applications. The synthesized ZnO nanoparticles were characterized by FTIR (Bruker – Tensor II FTIR spectrometer), XRD (Shimadzu – XRD-7000), SEM-EDX (ZEISS Gemini), and particle size distribution analysis (Malvern Panalytical – Mastersizer 3000).

2.3 Biodiesel Preparation from Mahua

Mahua oil (MO) derived from *Madhuca longifolia* was used as non-edible feedstock for biodiesel production. The crude oil was first filtered to eliminate suspended contaminants then dried at 105 °C to eliminate residual moisture (Gupta *et al.* 2012). The free fatty acid level was assessed according to ASTM standards, and because it over 1%, a pre-esterification phase were implemented to reduce soap formation during the subsequent transesterification process. Esterification catalyzed by acid was performed utilizing 25 wt% sulfuric acid as a catalyst, under continuous agitation at 60 °C. The reaction was sustained until stable and diminished Free Fatty Acid (FFA) level was attained, validating the efficient transformation of free fatty acids into methyl esters. The transesterification procedure was subsequently performed utilizing methanol with ZnO nanoparticles as heterogeneous catalyst. The reaction mixture was ultrasonicated at 20 kHz and 500 W to improve interfacial mass transfer and speed up the reaction. All the process factors (methanol-to-oil molar ratio, catalyst loading, and ultrasonication duration) were meticulously regulated to attain maximal biodiesel yield. After completion, the reaction mixture was permitted to settle, leading to phase separation into biodiesel (upper layer) and glycerol (lower layer).

The biodiesel layer was carefully decanted, rinsed with warm distilled water to eliminate residual catalyst and contaminants, and then dried to remove moisture. The ultimate biodiesel yield was measured by gas chromatography (GC) following ASTM standards.

Biodiesel yield was calculated using Eqn. (1).

$$\text{Biodiesel yield \%} = \frac{\text{Quantity of methyl esters}}{\text{Quantity of pretreated mahua oil}} \times 100 \dots (1)$$

2.4 Taguchi-based Experimental Design and Process Optimization for Biodiesel Production

This study optimized biodiesel production by Taguchi design of experiments (DoE) due to its efficacy

in reducing experimental runs while accurately determining the impact of process factors. Three essential parameters, ultrasonication duration (30–40 min), ZnO catalyst concentration (0.5–1.5 wt%), and methanol-to-oil molar ratio (6:1–12:1), were chosen due to their substantial impact on transesterification efficiency. An L27 (3³) orthogonal array was utilized to methodically construct the experimental matrix, facilitating a thorough assessment of the individual and synergistic impacts of the chosen factors on biodiesel yield. The Taguchi method enables robust optimization through the minimization of variability and the improvement of process reliability. Signal-to-noise (S/N) ratio analysis, according to the "larger-is-better" criterion, was employed to identify the ideal levels of process parameters, hence maximizing biodiesel yield and minimizing the impact of experimental noise. ANOVA was employed to assess the relevance of process factors, while the general linear model based on the experimental data was used to forecast biodiesel yield under different operating circumstances. The process parameters and their respective levels chosen for the Taguchi experimental design are displayed in Table 1.

Table 1. Process parameters and their levels employed in the Taguchi L27 experimental design for biodiesel production

Factor	Parameter	Unit	Level 1	Level 2	Level 3
A	Ultrasonication time	min	30	35	40
B	ZnO catalyst loading	wt%	0.5	1.0	1.5
C	Molar ratio (MO)		6:1	9:1	12:1

2.5 Artificial Neural Network Modeling

Feedforward artificial neural networks were developed to explain nonlinear relationship among process factors and yield of biodiesel. The input variables selected included ultrasonication time, concentration of ZnO catalyst, molar ratio and biodiesel yield was considered output response. Model construction was based on the experimental data obtained through the experiments conducted. To ensure reliable model generalization, data were randomly divided into training (70%), testing (15%) and validation (15%) sets. The ANN structure consisted of input layer with three neurons corresponding to the process variables, a hidden layer with optimized neurons, and output layer with single neuron, which corresponds to biodiesel yield.

Number of neurons in hidden layers were determined using trial and error approach to minimise prediction error and improve the model accuracy. Nonlinear activation functions were used in hidden layer to effectively capture the complex interactions between variables, whereas linear functions were used in output layer. The statistical measures applied to determine the performance of ANN model were the coefficient of

determination (R^2), Root Mean Square Error (RMSE), and Mean Absolute Error (MAE), therefore, ensuring an accurate predictive ability.

2.6 Optimization by Genetic Algorithm

The proposed ANN was combined with genetic algorithm (GA) to determine optimal process conditions to maximize the yield of biodiesel. The objective (fitness) function used during the optimization process was the trained artificial neural network model. The optimization was performed using the process variables: ultrasonication time (30-40 min), concentration of ZnO catalyst (0.5- 1.5 wt%), and molar ratio (6-12). The GA was implemented using MATLAB optimization toolbox. The GA systematically explored the search space and identified the optimal combination of process parameters that maximizes the expected biodiesel yield.

3. RESULTS AND DISCUSSION

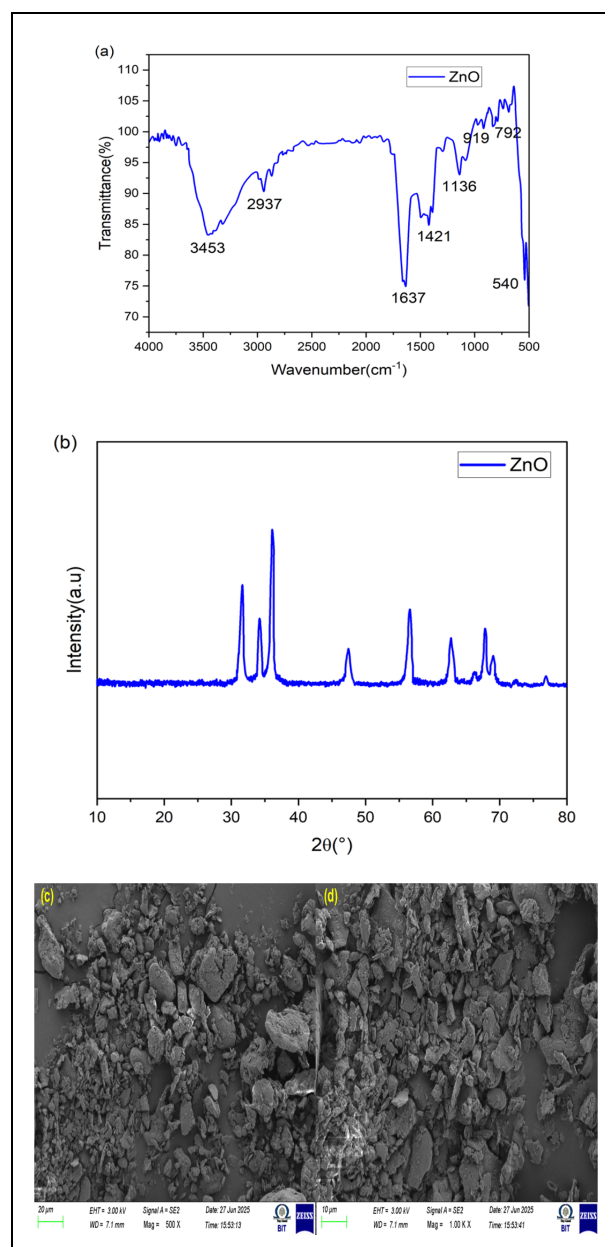
3.1 Characterization of ZnO

Fourier transform infrared of the ZnO nanocatalyst exhibited prominent peaks at 792 cm^{-1} and 540 cm^{-1} , corresponding to metal-oxygen vibrations related to copper incorporation and Zn-O bonding, respectively. These distinctive peaks further corroborate the establishment of a monoclinic ZnO phase. Other peaks observed between 1136 and 1421 cm^{-1} are attributed to Ce-O stretching vibrations, whereas the one observed at 1637 cm^{-1} was ascribed to N-H stretching of amine functional groups. The FTIR analysis indicates that bioactive compounds including phenolics and flavonoids from *Moringa oleifera* leaf extract, served efficiently as stabilizing and capping agents, thus preventing nanoparticle aggregation. As reported in earlier studies, FTIR analysis revealed characteristic absorption bands corresponding to hydroxyl and ZnO functional groups, confirming the successful formation of ZnO nanocatalyst and the presence of surface-active moieties (Rajavel *et al.* 2025).

The X-ray diffraction (XRD) pattern (Fig. 1b) displayed sharp and intense diffraction peaks, indicating a high level of crystallinity in the synthesized nanocatalyst. Significant diffraction peaks with 2θ values of 31.67° , 34.57° , 36.42° , 47.53° , 63.14° , and 68.09° align well with standard data from JCPDS card No. 45-0937, confirming the crystalline structure of ZnO. Earlier findings show that X-ray diffraction analysis confirmed the characteristic crystalline phases of ZnO and the WSA/ZnO/ K_2CO_3 composite. The observed diffraction peaks verified the successful formation of the catalyst and its crystalline structure (Foroutan *et al.* 2022).

Surface morphology study conducted by scanning electron microscopy (SEM) (Fig. 1c and d) revealed that the ZnO nanoparticles primarily exhibit an

irregular shape with a particle size of around 20 nm. Analysis of elemental composition by energy-dispersive X-ray spectroscopy (EDX) confirmed the presence of zinc, oxygen, and trace amounts of sulfur. The presence of sulfur is probably due to residual phytochemical impurities from the plant extract used in the synthesis. Moreover, particle size distribution study revealed that most nanoparticles are concentrated around $\sim 20\text{ nm}$, with an average size of roughly 64 nm, confirming uniform nanoscale formation attained through green synthesis. In previous research, SEM analysis revealed uniformly distributed manganese-doped ZnO nanoparticles with well-defined morphology and nanoscale structure. The observed particle size ($\sim 24.18\text{ nm}$) and homogeneous surface confirmed effective synthesis, contributing to enhanced catalytic activity in biodiesel production (Baskar *et al.* 2017).



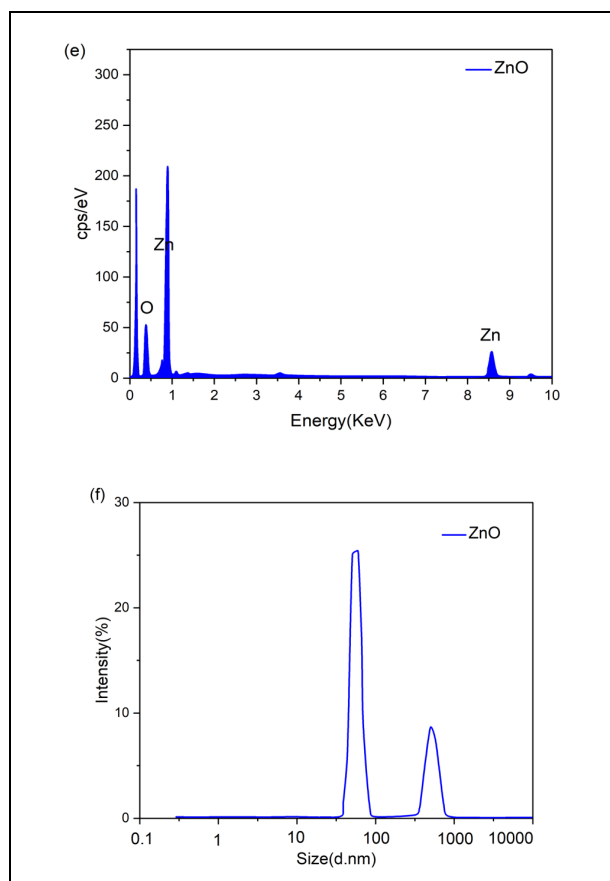


Fig. 1: Characterization of biosynthesized ZnO nanocatalyst (a) FTIR analysis, (b) XRD diffraction pattern, (c,d) Surface morphology by SEM, (e) Elemental composition from EDX, and (f) Particle size distribution profile

Table 2. Composition of mahua oil

Fatty Acid Profile	Carbon Molecules	Retention Time (Minutes)	Mass %
Arachidic (C ₂₀ H ₄₀ O ₂)	C20:0	24.05	1.85
Linoleic (C ₁₈ H ₃₂ O ₂)	C18:2	15.62	5.20
Oleic (C ₁₈ H ₃₄ O ₂)	C18:1	18.21	47.8
Stearic (C ₁₈ H ₃₆ O ₂)	C18:0	20.12	18.7
Heptadecanoic (C ₁₇ H ₃₄ O ₂)	C17:0	29.85	1.35
Palmitoleic (C ₁₆ H ₃₀ O ₂)	C16:1	18.76	3.25
Palmitic (C ₁₆ H ₃₂ O ₂)	C16:0	25.98	22.4
Others	–	–	0.45

Table 3. Physicochemical properties of MO, commercial diesel and biodiesel

Properties	MO	Diesel	Biodiesel	ASTM Norms
Acid value	18.5	-	0.26	-
Methyl ester (%)	96.2	-	99.1	>96.5
Specific gravity	0.912	0.82-0.88	0.88	0.86-0.90
FFA (%)	9.2	-	0.14	-
Saponification value (mg KOH/g oil)	192	-	162.3	-
Viscosity (mm ² /s)	36.8	1.3-5.5	4.53	1.9-6.0
Calorific value (MJ/kg)	36.5	42.7	41.3	-
Cetane number	42	30-40	67	>47
Cloud point (°C)	18	-	2	(-3) – (+12)
Flash point (°C)	215	38-55	178	>130
Sulphur content (mg/kg)	45	10	0.87	±0.4ppm
Pour point (°C)	12	(-15) – (+3)	6	(-15) – (+10)
Total glycerine (wt%)	0.28	-	0.04	<0.24

3.2 Composition of MO and Biodiesel

Fatty acid composition of raw mahua oil indicated that more than 80% consisted of C16 and C18 fatty acids, specifically palmitic, linoleic, oleic, stearic, and palmitoleic acids. The relevant composition is given in Table 2.

Table 3 contains the physicochemical properties of MO, commercial diesel, and the synthesized biodiesel. The produced biodiesel exhibited density and viscosity within acceptable parameters. It exhibited a superior cetane number and calorific value compared to commercial diesel. Furthermore, its diminished sulfur concentration mitigates environmental and engine-related problems, including corrosion and acid rain. These findings validate its appropriateness as an alternate fuel.

3.3 Taguchi Analysis (S/N Ratio)

To evaluate the effect of process parameters of the biodiesel yield quantitatively, and to counteract effects of experimental variability, the Taguchi signal-to-noise (S/N) ratio analysis, where criterion is larger-is-better, was applied. The S/N ratio is an effective way of integrating average performance and variability of the response, hence providing a valuable measure of optimization. The response analysis of S/N ratios (Table 4) revealed that the molar ratio had the highest delta (1.35) with ultrasonication time (0.98) and ZnO catalyst loading (0.89) following it. Higher delta value indicates a stronger effect of the response variable. Thus, the molar ratio was concluded to be the most important factor affecting biodiesel yield. This effect is attributed to the increased availability of methanol molecules, which shifts the transesterification equilibrium toward product formation, thereby enhancing the conversion rate. According to a previous research, coal fly ash-supported ZnO catalyst enabled biodiesel production from used cooking oil with 83.17% yield. Taguchi optimization confirmed the significance of process variables, while catalyst reusability ensured process stability (Yusuff *et al.* 2021a).

The comparatively lower delta values of ultrasonication duration and catalyst concentration suggest their minor yet notable roles in yield improvement.

Table 4. Response table for S/N ratios

Level	US Time (min)	ZnO (wt%)	Molar Ratio (MO)
1	37.40	37.43	37.20
2	37.91	38.32	37.94
3	38.38	37.95	38.55
Delta	0.98	0.89	1.35
Rank	2	3	1

Signal-to-noise ratio and mean main effects plot (Fig. 2) demonstrates how each parameter influences the biodiesel yield. A clear positive correlation with yield was observed as ultrasonication time increased, indicating that prolonged sonication enhances cavitation effects, thereby improving mass transfer and accelerating the reaction rate between immiscible phases. The molar ratio had a dramatic positive impact on the yield, which suggests that excess methanol has a positive impact on the kinetics of the forward reaction and increases ester production. However, at a certain point, the increase in yield with extra methanol might not be significant because of dilution and separation challenge.

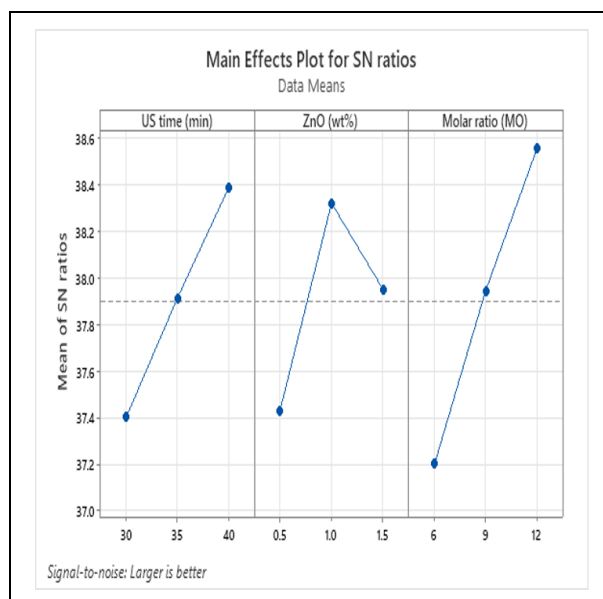


Fig. 2: Main effects plot for S/N ratios

The loading of the ZnO catalyst followed an optimum pattern with the highest yield at 1 wt%. A further addition to 1.5 wt% led to a slight reduction in yield which can be attributed to agglomeration of catalyst particles that reduced the effective surface area and limited active sites of reaction. These trends clearly indicate that there is an optimal operating regime, within which the synergistic effect of the process factors enhance the biodiesel yield and reduce the undesirable consequences of the processes, including, but not limited to, the mass transfer limitation or the deactivation of the catalysts.

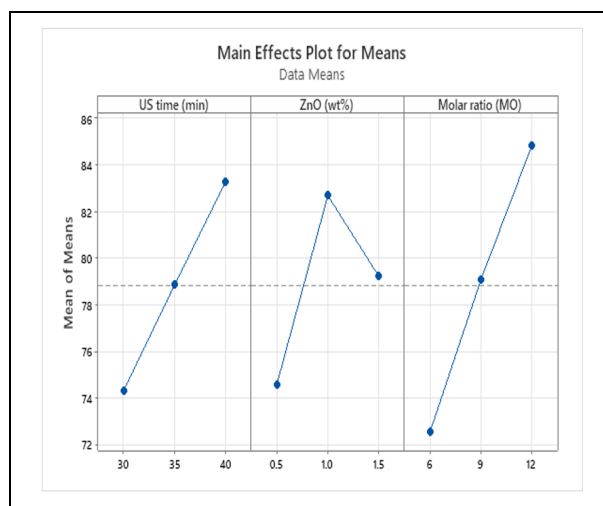


Fig. 3: Main effect plot for means

3.4 ANOVA Analysis

Analysis of variance was conducted to evaluate applicability and effect of process factors on biodiesel yield (Table 5). Results showed that molar ratio was the most dominant factor with 50.21% of total variation followed by ultrasonication time with 26.65% and ZnO catalyst loading with 21.90%. The substantial role of molar ratio also supports its crucial role in controlling the transesterification reaction process. Ultrasonication duration significantly enhances mixing efficiency and reduces diffusion barriers, while the ZnO catalyst further promotes the reaction by providing active sites.

All the parameters had p-values less than 0.05 meaning that they are significant at 95% confidence. The F-values also support the significant influence of the selected parameters. The contribution of error was 1.24%, which indicates that there is a small amount of noise in the experiment and the results were very reproducible. The fact that the residual error is minimal confirms that the selected model is adequately able to explain the differences in biodiesel yield and justifies the effectiveness of the Taguchi-based optimization approach. In prior studies, ANOVA confirmed that Ca/Zn ratio, methanol-to-oil ratio, and reaction time significantly influenced biodiesel yield with nearly equal contributions. The statistical results validated the robustness of the Taguchi optimization, supporting the achievement of 98% methyl ester conversion under optimal conditions (Rahmawati *et al.* 2021).

Table 5. ANOVA results for biodiesel yield

Source	DF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	P-Value
US time (min)	2	361.82	26.65%	361.82	180.910	215.45	0.000
ZnO (wt%)	2	297.29	21.90%	297.29	148.643	177.03	0.000
Molar ratio (MO)	2	681.69	50.21%	681.69	340.843	405.93	0.000
Error	20	16.79	1.24%	16.79	0.840		
Total	26	1357.59	100.00%				

The general linear regression model was developed to quantify relationship among process factors and biodiesel yield. The model summary the coefficient of determination was quite high ($R^2 = 98.76\%$), meaning that about 98.76% of the variability in biodiesel yield was explained by selected factors. The high value of the R^2 and standard error support the high predictive power of model developed. The regression model incorporates overall effect of ultrasonication time, ZnO catalyst concentration, and molar ratio, allowing to accurately predict biodiesel yield under different conditions of operation. This foresight is particularly beneficial to industrial use, as it reduces the need for many experiment trials.

Residual analysis was also used to verify adequacy and reliability of the developed regression model. Normal probability plot of residuals had a fairly linear shape, indicating residuals follow normal distribution. The diagram of the residues *versus* the fitted values showed that such dispersion was purely random, and it did not follow any pattern, thus confirming that no heteroscedasticity was present as well as that assumption of constant variance was accepted. The histogram of residuals was also symmetric around zero, which further supports the soundness of the model. The independence of residuals was further confirmed by the residuals *versus* order plot which showed that there were no time or sequence effects in the experimental data. All these findings confirm that the regression model meets all basic statistical assumptions and is highly reliable to predict and optimize biodiesel yield.

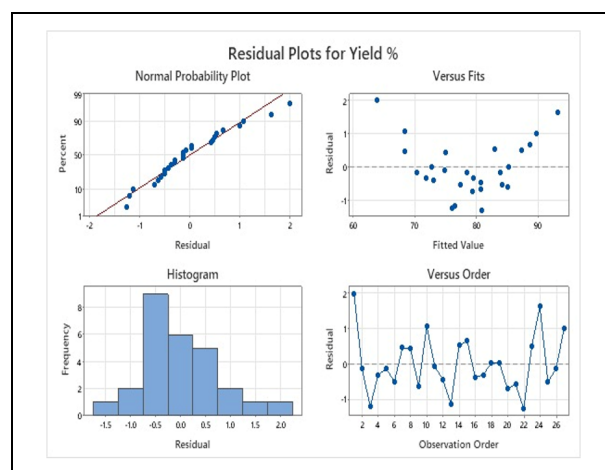


Fig. 4: Residual analysis plots for biodiesel yield prediction model

Despite the regression model exhibiting robust prediction abilities, it may inadequately account for complex nonlinear relationships among process variables. Consequently, models based on artificial intelligence were created to improve prediction accuracy and to execute worldwide optimization of biodiesel yield.

3.5 Artificial Intelligence-based Modeling, Optimization and Validation

3.5.1 ANN Modeling and Performance Evaluation

Regression and performance graphs (Figure 5) were used to evaluate the predictive efficacy of constructed ANN. The regression value of the best ANN model has an excellent correlation among predicted and experimental values of biodiesel yield, and coefficient of determination ($R^2 = 0.99958$). The points are closely concentrated around the 45° line ($Y = X$) showing near-perfect correlation and a very small error in prediction. This confirms that the ANN model has successfully learned the nonlinear relationships between

ultrasonication time, ZnO catalyst concentration, molar ratio and the biodiesel yield.

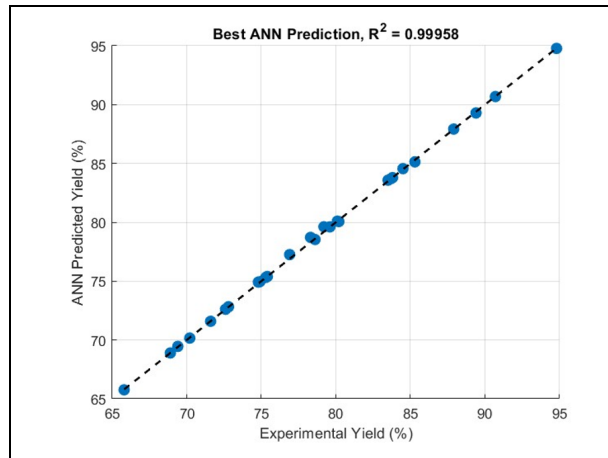


Fig. 5: Experimental Vs ANN prediction

The performance plot gives an idea about the training process, as it shows how mean squared error (MSE) varies with the training epochs. The best validation performance was achieved at an initial epoch (epoch 5), and thereafter, the validation error did not change any further. This action indicates that the model has achieved the best learning without falling to overfitting. This consistency between the training, validation and testing curve further supports the strength and ability of the ANN model to generalize.

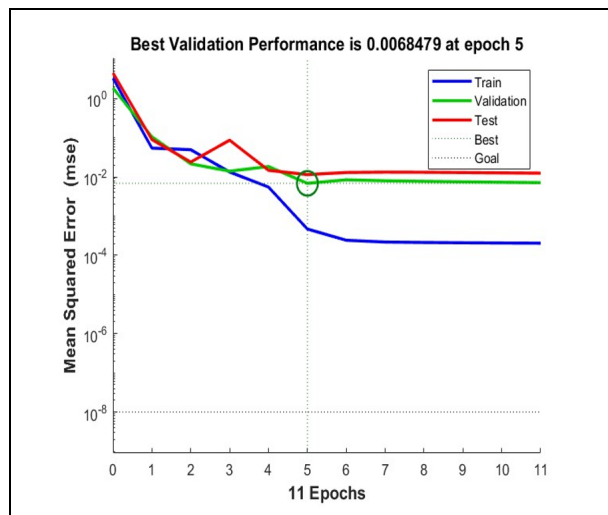


Fig. 6: Regression plot for testing, validation, training and overall dataset

The regression graphs for testing, validation, training and overall datasets demonstrate excellent correlation coefficients, hence affirming the model's dependability. The higher correlation coefficients noted across training, validation, testing, and overall datasets validate robust predictive capacity and generalization efficacy of the ANN model.

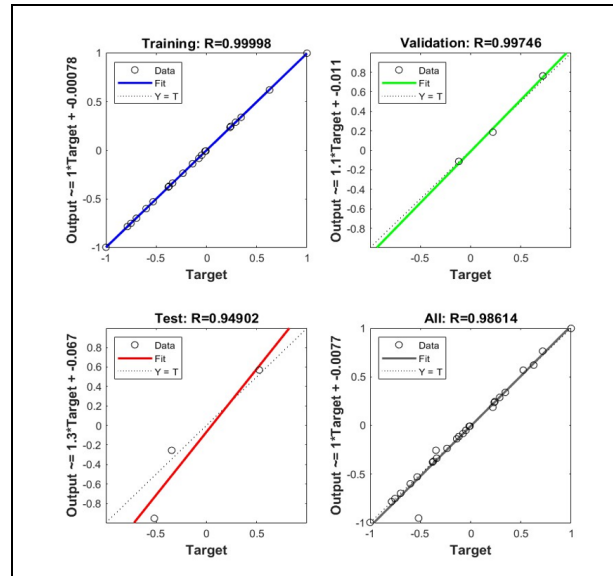


Fig. 7: Regression plots showing the correlation between experimental and ANN-predicted biodiesel yield

The slight discrepancy between anticipated and real values shows that ANN model effectively captures intricate nonlinear interactions that regulate the transesterification process. The results unequivocally indicate that the ANN model offers enhanced predictive accuracy relative to conventional statistical models.

3.5.2 Comparative Analysis of AI Models

A comparison analysis was conducted to validate the superiority of the ANN model against the Radial Basis Function (RBF) and Random Forest (RF) models.

Table 6. Performance comparison of AI models

Model	R ²	RMSE	MAE
BP-ANN	0.99937	0.17836	0.08264
RBF	0.99344	0.57446	0.43659
RF	0.86262	2.62818	2.12914

Table 6 indicates that the BP-ANN model attained the maximum R² and the lowest error values, hence affirming its superiority relative to the RBF and RF models. Figure 8 displays the regression plots of various models.

A comprehensive comparison of actual, ANOVA-predicted, and ANN-predicted biodiesel yields is provided in Table 7. The ANN-predicted values demonstrate greater concordance with the experimental data under all operating circumstances than the ANOVA predictions. The discrepancy between ANN forecasts and experimental values is negligible, signifying elevated robust generalization capacity and predictive accuracy of ANN model. Conversely, the ANOVA-based regression model demonstrates significantly greater deviations,

especially in regions of higher yield, owing to its constrained capacity to encapsulate intricate nonlinear interactions among process variables. This comparison unequivocally illustrates the superiority of the ANN model compared to the traditional ANOVA method in precisely forecasting biodiesel yield. Consequently, the ANN model is deemed more dependable for future optimization and process analysis.

Table 7. Comparison of experimental, ANOVA-predicted, and ANN-predicted biodiesel yield under different process conditions

US time (min)	ZnO (wt%)	Molar ratio	Experimental (%)	ANOVA Predicted (%)	ANN Predicted (%)
30	0.5	6	65.8	63.8	65.9
30	0.5	9	70.2	70.3	74.3
30	0.5	12	74.9	76.1	78.
30	1	6	71.6	71.9	71.7
30	1	9	78.3	78.4	79.1
30	1	12	83.7	84.2	83.9
30	1.5	6	68.9	68.4	68.8
30	1.5	9	75.4	74.9	75.2
30	1.5	12	80.1	80.7	80.5
35	0.5	6	69.4	68.3	69.2
35	0.5	9	74.8	74.8	75.0
35	0.5	12	80.2	80.6	80.2
35	1	6	75.3	76.4	75.7
35	1	9	83.5	82.9	82.7
35	1	12	89.4	88.7	88.5
35	1.5	6	72.6	72.9	72.2
35	1.5	9	79.2	79.5	79.2
35	1.5	12	85.3	85.2	84.2
40	0.5	6	72.8	72.7	72.7
40	0.5	9	78.6	79.3	78.6
40	0.5	12	84.5	85.0	84.5
40	1	6	79.6	80.8	80.2
40	1	9	87.9	87.4	87.6
40	1	12	94.8	93.1	94.9
40	1.5	6	76.9	77.4	77.0
40	1.5	9	83.8	83.9	83.8
40	1.5	12	90.7	89.7	90.4

The RBF model exhibits a robust correlation between predicted and experimental results, evidenced by an R^2 value of 0.99344. The data points are proximate to the optimal regression line. Yet, minor deviations are evident, particularly at elevated yield levels. This suggests that while the RBF model may identify nonlinear correlations, its predictive accuracy is somewhat inferior to that of the ANN model.

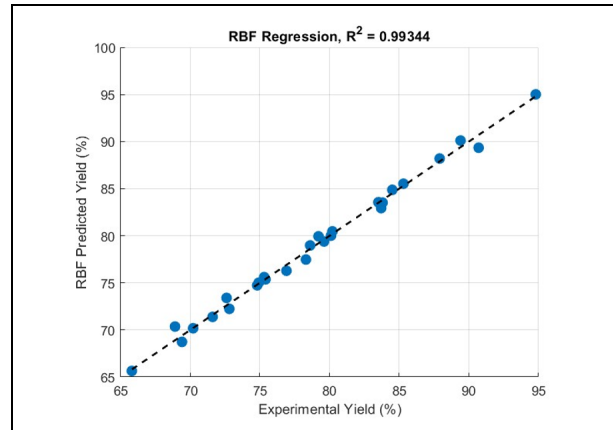


Fig. 8: Experimental vs RBF predicted yield

Conversely, the RF model demonstrates a relatively smaller association, evidenced by an R^2 value of 0.86262. The regression diagram exhibits significant dispersion of data points around the reference line, signifying an elevated prediction error. This result might be ascribed to the RF model's incapacity to adequately capture the nonlinear interactions and continuous characteristics of the process variables. The RF model's underfitting characteristic leads to diminished prediction performance relative to the ANN and RBF models.

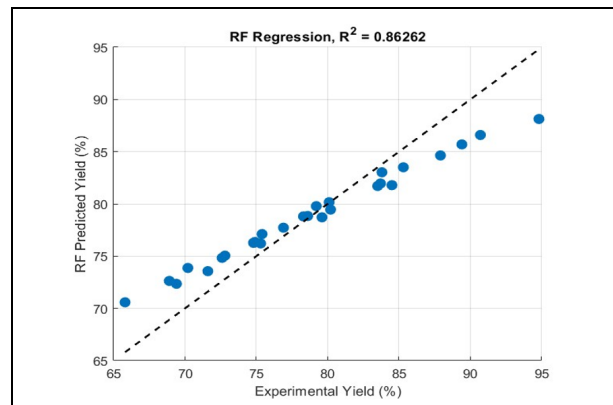


Fig. 9: Experimental vs RF-predicted yield

The comparative analysis demonstrates that the BP-ANN model surpasses both the RBF and RF models for predictive accuracy, consistency, and reliability. Consequently, the BP-ANN model was deemed the most appropriate for subsequent optimization investigations.

3.5.3 Optimization Using BP-ANN-GA

A genetic algorithm was combined with the BP-ANN model to find optimal process parameters to maximize biodiesel yield. The optimum results have shown that the maximum biodiesel production is achieved at an ultrasonic time of 40 minutes, a ZnO catalyst mass of 1.2317 wt%, and molar ratio of 12. The predicted yield of biodiesel at optimized conditions is 96.042%, and this means that the maximum yield can be

achieved within the considered range of parameters. This result highlights the significance of the synergistic role of process factors on overall response efficiency. The optimization results suggest that longer ultrasonication increases cavitation, thereby increasing the mass transfer and reaction kinetics. Optimum ZnO catalyst loading ensures that the active sites are sufficient with no agglomeration and the appropriate molar ratio is used to bias the reaction towards product formation. The optimization process confirms the presence of a well-defined operational window, in which the interaction of process parameters results in optimum conversion to biodiesel. Going beyond this optimal range can lead to diminishing returns, or even adverse impacts of further increase in parameters.

3.5.4 Experimental Validation of Optimized Conditions

Experimental validation was performed under the optimal circumstances derived from the BP-ANN-GA model to ascertain the credibility of the optimization outcomes. Experimental biodiesel yield achieved was 94.5%, closely aligning with projected value of 96.042%. In a previous study, ANN enabled accurate prediction of engine combustion, performance and emission parameters for GO and ZnO nanoparticle-blended B20 fuel. The ANN model demonstrated high reliability with R^2 values ranging from 0.93 to 0.99, effectively capturing nonlinear relationships and supporting optimization of operating conditions (Pala *et al.* 2025).

The difference between the expected and experimental values was established to be 1.605%, a very small percentage. The small error indicates high precision of the developed model and confirms ability of the ANN-GA methodology to reliably predict optimal conditions of the processes. The value of error (<5%) shows outstanding correspondence of the anticipated and experimental results. The high agreement between projected and experimental results shows that the model well represents the basic behaviour of the process and can be used to optimize processes and scale-up processes. The small error margin also supports the effectiveness of the hybrid ANN-GA approach in the control of complex nonlinear systems.

4. CONCLUSION

This study demonstrates the production of biodiesel from mahua oil (*Madhuca longifolia*), a non-edible and low-cost feedstock, using a two-step ultrasonic-assisted esterification–transesterification process catalysed by green-synthesized ZnO nanoparticles. The ZnO nanocatalyst, prepared using *Moringa oleifera* leaf extract, was characterized by XRD, FTIR, particle size analysis, SEM, and EDX, confirming its crystalline nature, nanoscale size distribution, and suitable morphology and composition for catalytic applications. Taguchi design and ANOVA identified the

molar ratio as the most influential parameter affecting biodiesel yield, followed by ultrasonication time and catalyst loading. Although the regression model exhibited strong predictability ($R^2 = 98.76\%$), it showed limitations in capturing nonlinear interactions. To overcome this, artificial intelligence-based modelling was employed, where the BP-ANN model achieved superior predictive performance ($R^2 = 0.999$) with lower errors compared to RBF and RF models. Further optimization using a hybrid BP-ANN-GA approach determined the optimal conditions as 40 min ultrasonication time, 1.2317 wt% ZnO loading, and a molar ratio of 12, yielding a predicted biodiesel output of 96.042%, closely matching the experimental yield of 94.5% with minimal error (1.605%). Ultrasonication significantly enhanced reaction kinetics through improved cavitation and mass transfer, enabling high conversion with lower catalyst usage. Overall, the integration of green nanocatalysis, ultrasonic processing, and advanced optimization techniques provides a sustainable and efficient strategy for large-scale biodiesel production from non-edible feedstocks.

FUNDING

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

COPYRIGHT

This article is an open-access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).



REFERENCES

- Ahmad, A., Yadav, A. K. and Singh, A., Biodiesel production from mahua oil: characterisation, optimisation, and modelling with a hybrid statistical approach, *Int. J. Amb. Energy*, 44(1), 2618–2627(2023).
<https://doi.org/10.1080/01430750.2023.2262468>
- Baskar, G., Gurugulladevi, A., Nishanthini, T., Aiswarya, R. and Tamilarasan, K., Optimization and kinetics of biodiesel production from Mahua oil using manganese doped zinc oxide nanocatalyst, *Renewable Energy*, 103, 641–646(2017).
<https://doi.org/10.1016/j.renene.2016.10.077>

- Chong, N. S., Nwobodo, I., Strait, M., Cook, D., Abdulramoni, S. and Ooi, B. G., Preparation and Characterization of Shell-Based CaO Catalysts for Ultrasonication-Assisted Production of Biodiesel to Reduce Toxicants in Diesel Generator Emissions, *Energies*, 16(14), 5408(2023). <https://doi.org/10.3390/en16145408>
- Darvishvand, H. P., Shabani, N., Farzaneh, F. and Azarkamanzad, Z., The Effect of Different Morphologies of ZnO and Cr Doped ZnO NPs as Heterogeneous Catalyst for Biodiesel Production from Soybean Oil, *Catal. Lett.*, 154(9), 5075–5085(2024). <https://doi.org/10.1007/s10562-024-04710-1>
- Dhingra, S., Bhushan, G. and Dubey, K. K., Comparative performance analysis of jatropha, karanja, mahua, and polanga based biodiesel engine using hybrid genetic algorithm, *J. Renew. Sustain. Energy*, 8(1), 013103 (2016). <https://doi.org/10.1063/1.4939513>
- Foroutan, R., Peighambaroust, S. J., Mohammadi, R., Peighambaroust, S. H. and Ramavandi, B., Application of walnut shell ash/ZnO/K₂CO₃ as a new composite catalyst for biodiesel generation from *Moringa oleifera* oil, *Fuel*, 311, 122624(2022). <https://doi.org/10.1016/j.fuel.2021.122624>
- Gugulothu, S. K., Barmavatu, P. and Mulugundam, S. S., Advanced Machine Learning and Response Surface Methodology-Based Optimization of Diesel Engine Performance and Emissions Using 2-Ethylhexyl Nitrate in Mahua Methyl Ester Biodiesel Blends, *J. Energy Res. Technol. Part A: Sustainable Renew. Energy*, 1(5), 052304(2025a). <https://doi.org/10.1115/1.4068940>
- Gugulothu, S. K., Barmavatu, P. and Siva Surya, M., Sustainable evaluation of 2-ethylhexyl nitrate in mahua biodiesel blends: Performance, emissions, thermal stability via RSM & ML, *Case Stud. Therm. Eng.*, 72, 106381(2025b). <https://doi.org/10.1016/j.csite.2025.106381>
- Gupta, A., Chaudhary, R. and Sharma, S., Potential applications of mahua (*Madhuca indica*) biomass, *Waste Biomass Valoriz.*, 3(2), 175–189(2012). <https://doi.org/10.1007/s12649-012-9107-9>
- Kavalli, K., Hebbar, G. S., Shubha, J. P., Adil, S. F., Khan, M., Hatshan, M. R., Almutairi, A. M. and Shaik, B., Green Synthesized ZnO Nanoparticles as Biodiesel Blends and their Effect on the Performance and Emission of Greenhouse Gases, *Mol.*, 27(9), 2845 (2022). <https://doi.org/10.3390/molecules27092845>
- Kumar, D., Chhibber, V. K. and Singh, A., Adding ZnO Nanoparticle in Mahua Oil Methyl Ester (MoME) Biodiesel for Eco-Friendly and Better Performance in DI Engine, *Nat. Academy Sci. Lett.*, 45(2), 161–164(2022). <https://doi.org/10.1007/s40009-021-01090-7>
- Lamba, N., Gupta, R., Modak, J. M. and Madras, G., ZnO catalyzed transesterification of *Madhuca indica* oil in supercritical methanol, *Fuel*, 242, 323–333(2019). <https://doi.org/10.1016/j.fuel.2019.01.044>
- Maleki, B. and Esmacili, H., Ultrasound-assisted conversion of waste frying oil into biodiesel using Al-doped ZnO nanocatalyst: Box-Behnken design-based optimization, *Renewable Energy*, 209, 10–26(2023). <https://doi.org/10.1016/j.renene.2023.03.119>
- Maleki, B., Kalanakoppal Venkatesh, Y., Siamak Ashraf Talesh, S., Esmacili, H., Mohan, S. and Balakrishna, G. R., A novel biomass derived activated carbon mediated AC@ZnO/NiO bifunctional nanocatalyst to produce high-quality biodiesel from dairy industry waste oil: CI engine performance and emission, *Chem. Eng. J.*, 467, 143399(2023). <https://doi.org/10.1016/j.cej.2023.143399>
- Marso, T. M. M., Kalpage, C. S. and Udugala-Ganehenegge, M. Y., ZnO/CuO composite catalyst to pre-esterify waste coconut oil for producing biodiesel in high yield. Reaction Kinetics, *Mech. Catal.*, 132(2), 935–966(2021). <https://doi.org/10.1007/s11144-021-01958-1>
- Pala, S. R., Mohan, M. V. K. and Vanthala, V. S. P., Optimizing performance, combustion and emission characteristics of mahua biodiesel included GO and ZnO nanoparticles: an ANN-RSM approach, *Environ. Sci. Pollut. Res.*, 32(23), 14169–14201(2025). <https://doi.org/10.1007/s11356-025-36530-0>
- Parthiban, J. and Jambulingam, R., Biosynthesis of Lipase-Immobilized Zinc Oxide Nanoparticle and its Role as a Nanocatalyst in the Biodiesel Production of the Lipid obtained from *Anabaena* Cyanobacterial Species Isolated from Saline Water, *Lett. Appl. NanoBioSci.*, 14(3), 126(2025). <https://doi.org/10.33263/LIANBS143.126>
- Pratiwi, S., Hauli, L., Marhadi, R., Mansur, D. and Budiman, A., Investigating the Catalytic Performance of ZnO/Sulfonated Biochar for the Simultaneous Production of Biodiesel from Waste Cooking Oil, *Catal. Surveys Asia*, 30(1), 77–94(2026). <https://doi.org/10.1007/s10563-025-09466-1>
- Rahmawati, Z., Holilah, H., Purnami, S. W., Bahruji, H., Oetami, T. P. and Prasetyoko, D., Statistical Optimisation using Taguchi Method for transesterification of Reutealis Trisperma Oil to Biodiesel on CaO-ZnO Catalysts, *Bulletin Chem. React. Eng. Catal.*, 16(3), 686–695(2021). <https://doi.org/10.9767/BCREC.16.3.10648.686-695>
- Rajavel, P., Arthanarisamy, M. and Ramasamy, S., Hybrid optimization of engine performance and emission using RSM-ANN-GA framework to explore valorization potential of waste cooking oil with green synthesized heterogenous ZnO nanocatalyst, *Fuel*, 395(2025). <https://doi.org/10.1016/j.fuel.2025.135092>

- Rudreshappa, G. E., Sreenivasa, S., Uma, K., Manjunatha, S. and Kumar, A. D. B., Green synthesis of Zinc Oxide nanoparticles, antibacterial studies and investigation as catalyst for the conversion of pumpkin oil into biodiesel, *Res. J. Chem. Environ.*, 28(1), 121–132(2024).
<https://doi.org/10.25303/281rjce1210132>
- Seela, C. R. and Ravi Sankar, B., Investigations on CI engine with nano-sized zinc oxide added Mahua Methyl Ester blends, *Int. J. Amb. Energy*, 41(2), 146–151(2020).
<https://doi.org/10.1080/01430750.2018.1451377>
- Thanikodi, S. and Solairaju, J. A., Green Synthesis and Process Optimization of Zinc Oxide Nanoparticles Using *Pseudomonas fluorescens*: Taguchi–ANN-Based Evaluation of Physico-Chemical Parameters, *Turkish J. Eng.*, 10(1), 204–212(2026).
<https://doi.org/10.31127/tuje.1804146>
- Vardast, N., Haghighi, M. and Zeinalzadeh, H., Catalytic properties/performance evolution during sono-hydrothermal design of nanocrystalline ceria over zinc oxide for biofuel production, *Chem. Eng. J.*, 430, 132764(2022).
<https://doi.org/10.1016/j.cej.2021.132764>
- Yusuf, B. O., Ganiyu, S. A., Peedikakkal, A. M. P. and Oladepo, S. A., ZnO/Cu-BTC metal-organic frameworks as a heterogeneous catalyst for efficient transformation of waste cooking oil into biodiesel, *Biomass Bioenergy*, 204, 108381(2026).
<https://doi.org/10.1016/j.biombioe.2025.108381>
- Yusuff, A. S., Bhonsle, A. K., Trivedi, J., Bangwal, D. P., Singh, L. P. and Atray, N., Synthesis and characterization of coal fly ash supported zinc oxide catalyst for biodiesel production using used cooking oil as feed, *Renewable Energy*, 170, 302–314(2021a).
<https://doi.org/10.1016/j.renene.2021.01.101>
- Yusuff, A. S., Gbadamosi, A. O. and Popoola, L. T., Biodiesel production from transesterified waste cooking oil by zinc-modified anthill catalyst: Parametric optimization and biodiesel properties improvement, *J. Environ. Chem. Eng.*, 9(2), 104955(2021b).
<https://doi.org/10.1016/j.jece.2020.104955>
- Yusuff, A. S., Popoola, L. T., Adeniyi, D. O. and Olutoye, M. A., Coal fly ash supported ZnO catalyzed transesterification of *Jatropha curcas* oil: Optimization by response surface methodology, *Energy Convers. Manage. X*, 16, 100302(2022).
<https://doi.org/10.1016/j.ecmx.2022.100302>
- Zheng, P., Wang, W., Hu, W., Zhang, Q., Zhang, X., Ma, L., Chen, L. and Liu, J., In situ zinc-induced pore engineering: High-performance and inexpensive ZnC₁₀₀₀@SO₃H catalyst derived from zinc citrate for biodiesel production, *Biomass and Bioenergy*, 210, 109057(2026).
<https://doi.org/10.1016/j.biombioe.2026.109057>