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Prediction of fuel properties and engine performance of biodiesel-ZnO blends using artificial neural networks

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ABSTRACT

This study considered the potential of artificial neural networks (ANNs) as analytical tools for modeling the main properties and performance of diesel engines fueled with biodiesel-zinc oxide (ZnO) nanoparticle blends. Experimental datasets were first collected from past researches to estimate kinematic viscosity, calorific value, brake thermal efficiency (BTE), and brake specific fuel consumption (BSFC) across various diesel-biodiesel ratios, ZnO dosages, engine rotational speeds, and loads. While adding biodiesel causes increasing viscosity and reducing heating value, the inclusion of ZnO nanoparticles was found to mitigate these drawbacks by stabilizing viscosity and improving energy content, which translated into improved combustion efficiency and reduced fuel consumption. To capture these complex nonlinear interactions, four independent ANN models were established: two for predicting viscosity and calorific value, and two for engine performance indicators (BTE and BSFC). The models employed feed forward backpropagation networks trained with the Levenberg–Marquardt algorithm. Statistical evaluation confirmed strong predictive capability, with the BTE and BSFC models showing the highest accuracy (R^2 values of 0.9 and 0.8, respectively), followed by viscosity (R^2 = 0.8) and calorific value (R^2 = 0.7). These results highlight that ANN performs best when outputs are strongly sensitive to input and operating conditions, such as in performance metrics, whereas intrinsic chemical properties remain more challenging to predict. Overall, the findings demonstrate that ZnO nanoparticles are effective additives for improving biodiesel–diesel blends and that ANN models provide reliable, computationally efficient alternatives to extensive experimental trials. This work bridges experimental evidence with machine learning, offering predictive tools and decision guidelines for optimizing biodiesel–nanoparticle formulations in diesel engines, while also identifying future research needs related to emissions modeling, dataset diversity, and real-time deployment.

Keywords: Artificial neural network, Biodiesel blends, Diesel engine performance, Fuel properties prediction, Machine learning in combustion, Zinc oxide nanoparticles.

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1. INTRODUCTION

The diesel engines continue to be indispensable in transportation, agriculture, and power generation because of their high efficiency and durability. Yet their dependence on fossil diesel remains a major contributor to greenhouse gas emissions and environmental degradation. Biodiesel, derived from renewable feedstocks such as vegetable oils and animal fats, has therefore emerged as a promising substitute (Mujtaba et al., 2020). Its oxygenated structure favors cleaner, more complete combustion however, higher viscosity, lower volatility, and reduced heating value can compromise atomization and evaporation, lowering efficiency and sometimes worsening fuel economy under certain regimes (Najafi, 2018). A rapidly growing line of research seeks to mitigate these drawbacks by using nanoparticles as fuel additives. Among the available candidates, zinc

oxide (ZnO) nanoparticles that improve combustion, spray and evaporation characteristics in biodiesel-diesel due to their catalytic activity, high thermal conductivity, oxygen-releasing capability during combustion, and surface characteristics that can promote micro-explosions and secondary atomization (El-Adawy, 2023). When properly dispersed in biodiesel–diesel blends, ZnO nanoparticles tend to shorten ignition delay and intensify heat release near top dead center, translating into higher brake thermal efficiency (BTE) and lower brake specific fuel consumption (BSFC), alongside potential benefits to selected emissions indices.

In parallel, artificial neural networks (ANNs) have gained momentum as predictive modeling tools in energy conversion systems in different applications (Chopra et al., 2015; Laghari et al., 2023). By emulating the brain's learning mechanism, ANNs are well suited for complex, nonlinear processes (Hartomo et al., 2024; Yin et al., 2024), like diesel combustion where multiple interacting inputs—fuel properties, injection and operating parameters jointly determine performance and emissions. Unlike traditional regression models, ANNs capture nonlinear couplings and higher-order interactions, frequently achieving prediction accuracies above 95% when trained on high-quality datasets (Mehregan and Moghiman, 2018). Early studies set the stage: Ghobadian et al. (2009) demonstrated strong agreement between experimental and predicted values for a diesel engine fueled with waste cooking biodiesel, and Çay et al. (2013) showed near-unity correlations for models developed on gasoline-methanol blends and alternative fuels in spark-ignition engines, supporting the method's generalizability across fuels and platforms.

Jaliliantabar et al. (2018) trained the ANN models on B0–B20 waste cooking oil biodiesel across varying loads and speeds, reporting R^2 values close to 1 and identifying engine load via sensitivity analysis as the most influential factor. Dharmalingam et al. (2023) advanced this line by combining experimental design with machine learning for a CRDI engine fueled with waste cooking oil biodiesel (WCOB) using a split injection strategy. They compared response surface methodology (RSM) with a bayesian regularization neural network (BRNN) to calculate BTE, cylinder peak pressure (CPP), heat release rate (HRR), and emissions (NO, CO, UBHC, smoke). BRNN consistently outperformed RSM, yielding very low errors and correlations up to $R^2 = 0.9$, underscoring value of ML-driven optimization in modern injection systems. Complementing these results, Khujamberdiev and Cho (2025) studied ANN applications in biodiesel-fueled diesel engines and standard high predictive accuracy (R^2 often > 0.9) for BTE, BSFC, torque, and combustion descriptors using architectures spanning backpropagation networks, radial basis function networks, and adaptive neuro-fuzzy inference systems they also highlighted the gains from integrating ANNs with optimization techniques and data centric workflows for real-time adaptability. Although the accuracy of ANNs is proven in the laboratory, the small size and variety of data limits generalization, and the issue of incorporating nested CV and bootstrap uncertainty techniques is still almost absent in the literature of this field.

The ANN framework has proven equally effective for nanoparticle-enhanced fuels. Hosseini et al. (2019) modeled alumina nanoparticle biodiesel–diesel blends using a multilayer perceptron, attaining near-perfect accuracy ($R = 0.9999$ for training, 0.9994 for validation, 0.9995 for testing) and, notably, extending prediction to vibration characteristics—an unconventional yet practically relevant output for durability and NVH assessments. Saraee et al. (2016) paired experiments on cerium oxide nanoparticle–diesel blends with Levenberg–Marquardt–trained (fast numerical training technique for MLP networks that combine's Gaussian–Newtonian gradient and stepwise regression to optimize weights and efficiently reduce mean squared error) NNs to achieve a minimum mean squared error of 0.000172, highlighting the method's efficiency in mapping nanoparticle concentration to the performance/emission trends. Pushing to more complex chemistries, Taheri-Garavand et al. (2022) successfully modeled ternary blends of waste fish oil biodiesel, ethanol, and graphene quantum dots (GQDs), capturing nonlinear interactions across ethanol content, GQD dosage, and engine speed with Pearson's r ranging from 0.7 for NOx to 0.9 for CO_2. Muniyappan and Krishnaiah (2024) examined mahua biodiesel doped with cerium oxide, copper oxide, and titanium dioxide nanoparticles, their ANN predicted brake power, BTE, BSFC, and key emissions and enabled a data-driven conclusion that 50 ppm CeO_2 was the most effective dosage—illustrating how ANNs can function as decision tools to identify promising blends without exhaustive trial-and-error.

Merging ANN prediction with formal optimization has further matured the field. Aydin and Uslu (2020) integrated ANN with RSM to map and optimize the combined effects of biodiesel ratio and injection parameters, obtaining R^2 values from 0.8 to 0.9 and identifying an operating point of 32% biodiesel at 470 bar injection pressure and 816 W load as optimal under their criteria. Beyond conventional outputs, Javed et al. (2018) used a feed-forward backpropagation (A multi-layered network in which signals flow from inputs to outputs, and weights are generated by backpropagation to reduce prediction error) ANN (4-8-1), trained with the Levenberg–Marquardt algorithm and tansig-logsig transfer functions, to predict noise emissions in a hydrogen dual-fueled engine operating on jatropha methyl ester (JME) with ZnO nanoparticles. Achieving a regression coefficient of 0.9 and very low MSE, they illustrated that ANNs can reliably capture the complex interplay among load, blend ratio, hydrogen flow, and nanoparticle size in shaping acoustic responses—an environmental and health dimension too often overlooked. According to Fashoto et al. (2015), the feedforward and backpropagation mechanism works by transfer data to produce outputs, then calculating the error

and returning it across the network to adjust the weights. The Levenberg–Marquardt algorithm is an optimization technique that combines steepest regression and the Gaussian–Newton method to accelerate the training of multilayer networks in small–medium problems. In spite of this progress, challenges persevere were limited datasets decrease generalization across engine platforms, the combination of nanoparticle effects in predictive models stays underexplored and limited studies have conducted detailed sensitivity analyses or examined model limitations.

Taken together, this body of evidence establishes ANN as a high-accuracy, adaptable, and cost-effective framework for modeling diesel engines operating on biodiesel and nanoparticle-enriched fuels. By learning directly from data, ANNs overcome the rigidity of conventional empirical correlations, extend naturally to new fuel formulations, and can be coupled with optimization to support multi-objective decisions. Nonetheless, important gaps persist, datasets are frequently limited in size and diversity, constraining model generalizability across engine platforms and duty cycles, long-term implications of nanoparticle usage—durability, wear, ash deposition, after treatment compatibility—are underexplored; and while laboratory accuracy is consistently strong, on-board, real-time deployment remains at an early stage.

Against this backdrop, this work is distinguished by employing an independent ANN architecture for each output with nested k-fold CV and systematic architectural tuning, which expands the boundaries of previous studies and establishes the possibility of real-time practical application. The methodology is designed to quantify the influence of ZnO dosage on fuel properties and engine responses, minimize the need for exhaustive experimentation by using data-efficient modeling (feature engineering, rigorous train/validation/test splits, and cross-validation with error metrics such as R^2/RMSE/MAPE), and demonstrate the synergistic benefits of combining nanotechnology with machine learning. Sensitivity analysis (e.g., permutation importance and partial dependence) is employed to isolate dominant factors (dosage, load, speed), while constrained optimization is used to map practical trade-offs (BTE↑, BSFC↓, targeted emissions control) within feasible dosage windows. In doing so, the study delivers predictive tools and decision guidelines tailored to biodiesel–ZnO applications, bridging literature-identified gaps on generalizability and paving the way toward robust, real-time capable models for cleaner, efficient diesel operation.

This study aims to develop and confirm independent ANN models for calculating (i) kinematic viscosity KV, (ii) calorific value CV, (iii) brake thermal efficiency BTE, and (iv) brake specific fuel consumption BSFC of biodiesel–ZnO blends. Viscosity and calorific value were selected as the primary physicochemical properties to be modeled, since they are the most critical for governing fuel spray, combustion, and efficiency, and they are also the most consistently measured parameters in previous research. Emissions were not included due to the lack of standardization in measurement techniques across studies, which complicates reliable dataset construction and model training. To improve predictive accuracy and decrease cross-output interference, an independent ANN was established for each output variable, a strategy earlier shown to improve performance over multi-output designs when outputs differ significantly in scale and performance (Saraee et al., 2016; Hosseini et al., 2019). This approach confirms robust predictions for viscosity, calorific value, and engine performance indices, while laying the foundation for future development toward harmonized emission modeling.

Finally, the growing energy demand and environmental concerns need data-driven predictive bases that reduce the need for expensive and time-consuming engine tests. This study offers such a framework using ANN to explore biodiesel-ZnO blends and improve their performance. The Main Contributions of the present study were

- Present of four separated ANN models for main physicochemical and engine performance parameters.
- Including of ZnO nanoparticle dosage as a one of learning inputs in a comparative ANN based structure.
- Performing of sensitivity analysis to categorize the most significant input variables.

2. EXPERIMENTAL DATA COLLECTION

The experimental data grouping covered both fuel main properties and engine performance, as summarized in the following tables. The collected properties included kinematic viscosity (KV) and CV for numerous blends of diesel, biodiesel, and ZnO nanoparticles. Results presented that pure diesel had the lowest viscosity and uppermost CV, while biodiesel blends increased viscosity and reduced CV. However, the addition of ZnO nanoparticles helped compensate for these drawbacks by slightly enhancing the calorific value and stabilizing viscosity across different blend ratios as listed in Table1.

For performance estimation, the BTE and BSFC were noted at different engine speeds (1500–2900 rpm) and various load situations. The baseline diesel fuel delivered higher efficiency and lower BSFC compared to biodiesel alone, but the integration of ZnO nanoparticles enhanced combustion characteristics and narrowed the gap. Specifically, biodiesel–diesel blends with nanoparticle additives consistently achieved improved BTE and reduced BSFC compared to blends without ZnO, particularly at higher engine speeds. These findings indicate that ZnO nanoparticles act as effective additive, improving energy content of fuel and combustion process in engine (Table 2).

Table 1. Properties of diesel and biodiesel with ZnO nanoparticles from previous studies

Authors	Diesel content	Biodiesel content	ZnO (ppm)	KV (cSt)	CV (MJ/kg)
El-Adawy, 2023	1	0	0	2.8	45
	0	1	0	6	37
	0.8	0.2	0	3.4	43
	0.6	0.4	0	4.1	42
	1	0	50	2.8	46
	0.8	0.2	50	3.5	45
	0.6	0.4	50	4.2	43
Karthikeyan et al., 2014	0.8	0.2	0	3.1	44
	0.8	0.2	50	3.1	44
	0.8	0.2	100	3.3	44
Singh and Singh, 2021	1	0	0	-	41
	0.9	0.1	0	-	39
	0.9	0.1	0	-	40
	0.8	0.2	0	-	40
	0.7	0.2	0	-	40
	0.7	0.2	25	-	41
	0.7	0.2	50	-	41
	0.7	0.2	100	-	42
	0.7	0.2	200	-	43
El-Adawy et al., 2024	1	0	0	2.8	45
	0	1	0	6	37
	0.8	0.2	0	3.5	43
	1	0	50	2.9	46
	0.8	0.2	50	3.5	45
Verma et al., 2023	1	0	0	-	42
	0.8	0.2	0	-	41
	0.8	0.2	50	-	42
	0.8	0.2	100	-	42
	0.8	0.2	150	-	43
	0.8	0.2	200	-	44
Gavhane et al., 2020	1	0	0	2.1	45
	0.7	0.2	0	3.6	41
	0.7	0.2	25	3.5	43
	0.7	0.2	50	3.5	44
	0.7	0.2	75	3.5	43
Srinivasarao et al., 2025	1	0	0	2.5	42
	0.8	0.2	0	2.9	40
	0.8	0.2	40	2.7	41
	0.8	0.2	80	2.7	41
	0.8	0.2	120	2.7	41
Suhel et al., 2023	1	0	0	2.6	43
	0	1	0	3.0	42
	0.8	0.2	0	2.7	42
	0.8	0.2	50	2.7	42
	0.8	0.2	100	2.7	42
	0.8	0.2	150	2.7	42

Table 2. Engine performance fueled by diesel and biodiesel with ZnO nanoparticles from previous studies

Authors	Diesel content	Biodiesel content	ZnO (ppm)	Speed (rpm)	Load (kW)	BTE (%)	BSFC (kg/kWh)
El-Adawy, 2023	1	0	0	1700	3	21	0.4
	1	0	50	1700	3	22	0.4
	0.8	0.2	0	1700	3	19	0.4
	0.8	0.2	50	1700	3	21	0.41
	0.6	0.4	0	1700	3	17	0.5
	0.6	0.4	50	1700	3	18	0.5
	1	0	0	2000	3	27	0.3
	1	0	50	2000	3	28	0.3
	0.8	0.2	0	2000	3	26	0.3
	0.8	0.2	50	2000	3	27	0.3
	0.6	0.4	0	2000	3	25	0.3
	0.6	0.4	50	2000	3	26	0.3
	1	0	0	2300	3	31	0.2
	1	0	50	2300	3	33	0.2
	0.8	0.2	0	2300	3	31	0.3
	0.8	0.2	50	2300	3	32	0.2
	0.6	0.4	0	2300	3	29	0.3
	0.6	0.4	50	2300	3	30	0.3
	1	0	0	2600	3	34	0.2
	1	0	50	2600	3	35	0.2
	0.8	0.2	0	2600	3	33	0.3
	0.8	0.2	50	2600	3	34	0.2
	0.6	0.4	0	2600	3	31	0.2
	0.6	0.4	50	2600	3	32	0.2
	1	0	0	2900	3	33	0.3
	1	0	50	2900	3	34	0.2
	0.8	0.2	0	2900	3	32	0.3
	0.8	0.2	50	2900	3	33	0.3
	0.6	0.4	0	2900	3	29	0.3
	0.6	0.4	50	2900	3	31	0.3
Vellaiyana et al., 2019	0.9	0.1	25	1500	3.5	26	0.3
	0.9	0.1	50	1500	3.5	27	0.3
	0.9	0.1	75	1500	3.5	29	0.3
	0.9	0.1	100	1500	3.5	31	0.3
	0.8	0.2	50	1500	3.5	26	0.3
	0.8	0.2	25	1500	3.5	27	0.3
	0.8	0.2	100	1500	3.5	30	0.3
	0.8	0.2	75	1500	3.5	31	0.3
Gavhane et al., 2020	1	0	0	1500	0.7	13	0.3
	0.7	0.2	25	1500	0.7	10	0.4
	0.7	0.2	50	1500	0.7	12	0.4
	0.7	0.2	75	1500	0.7	11	0.4
Srinivasarao et al., 2025	1	0	0	1500	1.29	20	0.4
	0.8	0.2	0	1500	1.29	18	0.5
	0.8	0.2	40	1500	1.29	19	0.5
	0.8	0.2	80	1500	1.29	19	0.5
	0.8	0.2	120	1500	1.29	19	0.5
Suhel et al., 2023	1	0	0	1500	0.86	12	0.5
	0.8	0.2	0	1500	0.86	11	0.5
	0.8	0.2	50	1500	0.86	13	0.4
	0.8	0.2	100	1500	0.86	13	0.4
	0.8	0.2	150	1500	0.86	14	0.4

3. ARTIFICIAL NEURAL NETWORKS ARCHITECTURE

ANNs have emerged as powerful computational tools capable of modeling complex nonlinear relationships in engineering systems. In the situation of diesel engines fueled with biodiesel and improved with nanoparticles, ANN offers an effective approach to expect performance, combustion, and fuel property parameters without relying exclusively on conventional experimental approaches. By simulation the human brain's structure of intersected neurons, ANN can learn from experimental datasets and generalize these results with high accuracy, thereby reduction testing time, cost, and variability.

In the current work, the ANN framework was planned to estimate and predict the important parameters that potentially affect engine performance and fuel characteristics. Four independent models were established, each dedicated to a single output parameter. The first model was planned to calculate fuel viscosity, which straight influences atomization, spray characteristics, and combustion quality. The second model concentrated on heating value, an important property controlling the energy content of the fuel and its combustion effectiveness. The third model was built for BTE, which describes the active conversion of fuel energy into valuable mechanical work. Finally, the fourth model was developed for BSFC, an important indicator of both fuel economy and engine performance.

Through these four ANN models, a robust prediction system was established to measure the interrelations between the important input variables (such as blend ratio, nanoparticle dosage, and operating conditions) and output responses. This architecture not only guarantees accurate estimation of the most important parameters but also offers a dependable tool for optimizing biodiesel–nanoparticle fuel blends in diesel engines.

To assess the prediction accuracy of the ANN models, three statistical displays were employed: the regression coefficient (R), the mean relative error (MRE), and the root mean square error (RMSE). These guides compare the model outputs with the target values and offer a quantitative measure of performance. The applied formulas are given below (Uslu and Celik 2018):

1. Regression Coefficient (R):

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{n}(t_i - o_i)^2}{\sum_{i=1}^{n} o_i}\right) \quad (1)$$

2. Mean Relative Error (MRE):

$$MRE(\%) = \frac{1}{n}\sum_{i=1}^{n}\left|100\ \frac{t_i - o_i}{t_i}\right| \quad (2)$$

3. Root Mean Square Error (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(t_i - o_i)^2} \quad (3)$$

Here:

- n represents the total number of data samples
- o_i denotes the predicted values generated by the ANN
- t_i indicates the corresponding actual (target) values
- $\bar{t}$ is the mean of the actual values

The Levenberg–Marquardt (trainlm) algorithm was adopted exclusively for training, as it is finest suited for small-to-medium-sized estimation problems. To moderate overfitting, a comparison was prepared with the Bayesian Regularization (trainbr) algorithm, as suggested by various studies (Hagan and Menhaj, 1994; Yap et al., 2012; Deb et al., 2016). Previous studies (Javed et al., 2015; Chakraborty et al., 2016; Bhowmik et al., 2017) have stated that the logistic sigmoid (logsig) activation function yields superior results matched with other activation functions, due to its ability to differentiable, continuous, and nonlinear properties, which are favorable for current model formulation. Additionally, the gradient descent with momentum learning algorithm (LEARNGDM) was employed to update the weights and biases, as it adjusts neuron parameters based on the inputs, errors, learning rate, and momentum constant. This approach confirms improved convergence while reducing error during training (Baruah, et al. 2017). The details of the neural networks are summarized in Table 3.

Viscosity and calorific value are the important properties that strongly govern the spray creation, atomization quality, and combustion performance of diesel–biodiesel–nanoparticle blends. To represent these, the first and second ANN models were established with KV and CV as the marked outputs. The model's architecture was trained by means of experimental datasets of diesel, biodiesel, and ZnO-biodiesel blends. Input parameters involved the blend ratios and nanoparticle dosage, which were designated due to their strong effect on blend properties. The optimal ANN structures are shown in Fig. 1.

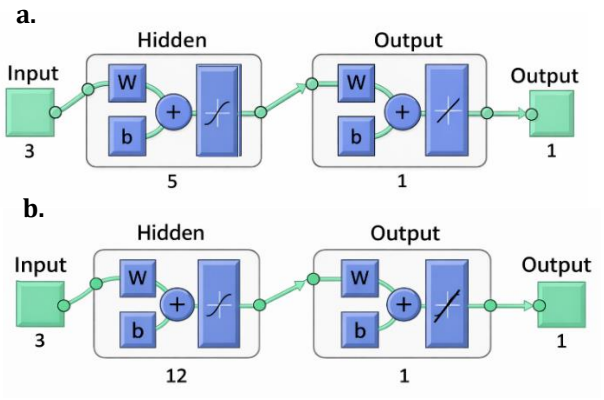

Fig. 1. The ANN structure of a. kinematic viscosity and b. calorific value

Table 3. Configuration details of the applied neural network

Network	Three inputs, one outputs and one hidden layer for each fuel property Five inputs, one outputs and one hidden layer for engines performance
Data	Training: 75% randomly selected data from experimental data Test: 25% randomly selected data from experimental data
Network type	Feed-forward back propagation
Training function	Trainlm
Adaptation learning function	Learngdm
Transfer function	Logsig
Performance function	Mean square error
Cross-validation	Nested 5×5-fold CV
Inner loop for hyperparameter tuning	Outer loop for unbiased performance estimation
Stopping criteria	Break the training of network when the confirmation error begins increasing

Two independents ANN models were established specifically for the prediction of BTE and BSFC through a range of fuels and operating situations. The input layer combined five key parameters: diesel fraction, biodiesel fraction, ZnO nanoparticle dosage, engine speed, and engine load. The network architecture consisted of a feed-forward ANN with one intermediate hidden layer of 25 neurons and one output neuron matching to BTE and BSFC Fig. 2.

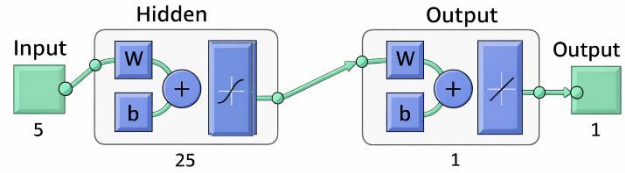

Fig. 2. ANN structure of brake thermal efficiency and brake specific fuel consumption

The following steps summarize the detailed pseudo code and logical flow of the adopted ANN-based research methodology.

Step 1: Data preparation and architecture setup

1.1 Load dataset containing inputs (e.g., Diesel, Bio, ZnO, Speed, Load) and target output (e.g., BTE).
1.2 Normalize input features.
1.3 Randomly split D into training (75%) and testing (25%) subsets.
1.4 Define ANN architecture:
i- Type: Feed-forward back-propagation
ii- Training algorithm: Levenberg-Marquardt (trainlm)
iii- Hidden layer: 1 layer
iv- Number of hidden neurons (Nh)
v- Transfer function: Log-sigmoid (logsig)
vi- Performance function: Mean Squared Error (MSE)

Step 2: Nested k-Fold Cross-Validation

2.1 For each outer fold:
i- Split data into training/validation and test set.
2.2 For each inner fold:
i- Split training/validation data into training and validation sets.
ii- Train ANN model on the inner training set.
iii- Evaluate on the inner validation set.
2.3 Select hyperparameters (e.g., Nh) that yield the best average validation performance.
2.4 Train the final model on the entire outer training/validation set with the selected hyperparameters.
2.5 Evaluate the final model on the outer test set.

Step 3: Model training

3.1 Initialize network weights and biases.
3.2 For each epoch (or until early stopping criterion is met):
i- Forward propagation: passing training inputs through the network to compute predicted output.
ii- Error calculation: calculating MSE between predicted and actual target values.
iii- Back propagation: computing the gradient of the error with respect to each weight and bias.
iv- Weight update: Adjusting weights and biases using the Levenberg-Marquardt algorithm.
3.3 Save the trained model.

Step 4: Model evaluation and analysis

4.1 Use the trained model to predict outputs for the test set.
4.2 Calculate performance metrics: R^2, RMSE, and MAPE.
4.3 Perform sensitivity analysis (e.g., Permutation Importance) to rank input variable significance.
4.4 Generate result visualizations (Regression plots, Actual vs. Predicted plots).

Step 5: Organization for prediction

5.1 For data points:
i- Normalizing inputs using the same parameters from Step 1.2.
ii- Passing normalized inputs through the trained model to obtain prediction.

Step 6: End Algorithm

4. RESULTS AND DISCUSSION

In this study, separate ANN representation idealized for each parameter, which permitted tailored network optimization and yielded good prediction accuracy as compared with multi-output designs. Also, the capability of ANNs in modeling both physicochemical properties and engine performance were examined. While most previous studies functional ANN primarily for expecting performance and emissions of CI engines (e.g., Saraee et al., 2016; Hosseini et al., 2019), slight attention has been paid to fuel properties estimation using ANN. The results showed good predictive capability of ANNs for both physicochemical properties and engine performance indices, consistent with prior studies. The high coefficient of determination (R^2) reached here matches findings by Saraee et al. (2016) and Hosseini et al. (2019), approving the robustness and generalizability of ANN models. The observed disparity in accuracy between intrinsic properties (e.g., calorific value) and performance metrics (BTE, BSFC) aligns with Najafi (2018) and Aydin and Uslu (2020), underscoring those outputs sensitive to operating situations are more efficiently modeled by ANN. The current ANN models align with latest studies highlighting intelligent modeling in renewable energy systems. Aurreethum et al. (2025) improved pyrolysis oil from landfill waste plastics using industrial catalysts, displaying that merging catalytic methods with computational analysis can enhance fuel properties. This find supports the current study's method of improving ZnO-based biodiesel through predictive modeling. Yin et al. (2024) examined artificial intelligence (AI) for data visualization, suggesting the need for transparent AI models. Their results showed that using AI could further interpret ANN decision forms in biodiesel performance prediction. Kamaruddin et al. (2022) projected empirical relationships for biomass calorific values (R^2 = 0.98), demonstrating that analytical and ANN approaches are complementary in expecting stored energy content and combustion performance. Together, the previous works approved that integrating AI with innovative fuel modeling (such as the ANN-ZnO) approaches in this paper—characterized a hopeful path for cleaner and more effective renewable fuel applications. Significantly, this study is distinguished by focus on ZnO nanoparticles—rarely studied in ANN-based modeling thereby studying a critical research gap and representing the exclusive catalytic role of ZnO.

4.1 Prediction of Kinematic Viscosity

The ANN model established in this study for calculating the KV of diesel, biodiesel, and biodiesel blended with ZnO nanoparticles demonstrated promising accuracy. The optimal network configuration was obtained with five hidden neurons. This configuration provided the best balance between accuracy and computational efficiency. Training was carried out with standard backpropagation, using a log-sigmoid transfer function to capture nonlinear relationships as shown in Fig. 3 yielding statistical indicators of RMSE = 0.2, MAPE = 4%, and R^2 = 0.8 as shown in Fig. 4. These results confirm the robustness of the ANN model in capturing the nonlinear interactions between input variables and output property as shown in Fig. 5. Compared with Meng et al. (2014), who established an ANN model to calculate biodiesel kinematic viscosity at fixed temperature 313 K using 105 samples and reached a correlation coefficient of R = 0.9, the current study obtained an accuracy of R^2 = 0.8 for kinematic viscosity prediction of biodiesel-ZnO blends. Although Meng's model was trained with a bigger biodiesel dataset based on 19 fatty acid methyl esters (FAMEs) composition, the present model shows robust performance using different experimental blend ratios and nanoparticle amounts as inputs. The enhanced interpretability and physical relation between constraints in this study make it more suitable for nanoparticle improved biodiesel applications, capturing nonlinear relations among viscosity, biodiesel fraction, and nanoparticle effects more efficiently than conventional empirical or composition-based models.

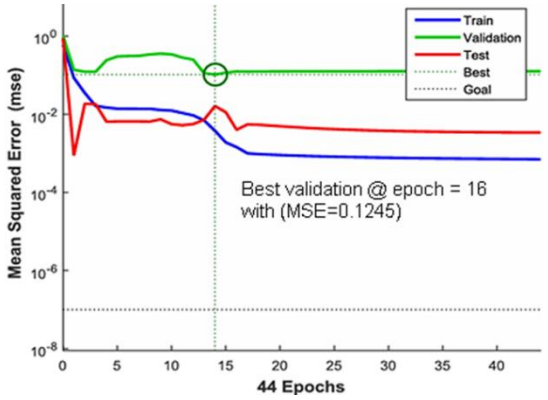

Fig. 3. Training performance of fuel viscosity network

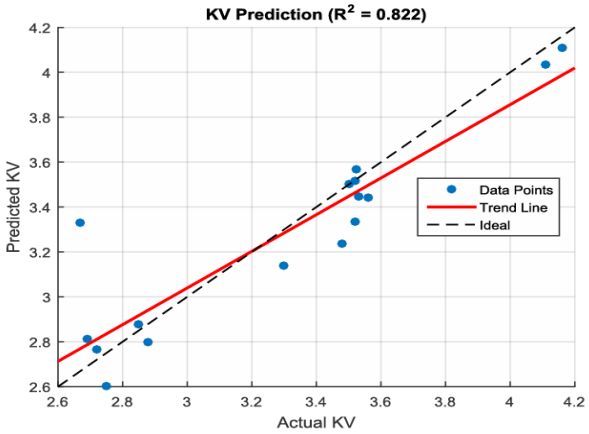

Fig. 4. Regression plots of KV ANN model outputs for training

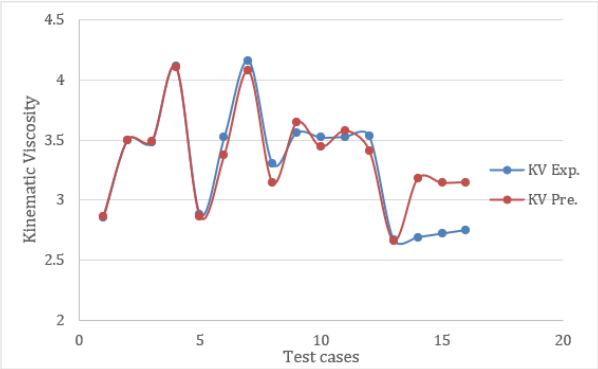

Fig. 5. Experimental results versus ANN results in terms of kinematic viscosity

The relatively low RMSE value indicates that the prediction error is negligible from a practical standpoint, while the MAPE of approximately 4% is well within the threshold generally accepted for fuel property prediction models. It should be noted that MAPE can be misleading at small values, so, adopted RMSE and MAE as the basic criteria. Furthermore, the coefficient of determination (R^2) exceeding 0.8 reflects a strong correlation between predicted and experimental data, suggesting that the ANN architecture is capable of reproducing experimental trends with high fidelity.

The conclusion that five hidden neurons reached good performance is particularly significant. Models with less neurons showed a tendency to under fit the data, thereby missing essential patterns, whereas models with more hidden layers displayed overfitting, which compromised their generalization ability. This result aligns with previous studies (e.g., Hosseini et al., 2019; Aydın et al., 2020) where proper tuning of the ANN structure was emphasized as a critical determinant of predictive accurateness in engine performance and fuel property modeling.

Furthermore, the capacity of the ANN to efficiently incorporate the influence of ZnO nanoparticles is remarkable. ZnO has been widely informed to develop biodiesel properties through improved catalytic activity, higher thermal conductivity, and enhanced atomization. While such effects are inherently nonlinear and difficult to model using conventional regression methods, the ANN approach successfully captured these difficulties without requiring explicit mechanistic formulations. This highlights the utility of ANN as a flexible and powerful tool for predictive modeling in alternative fuel research.

4.2 Prediction of Calorific Value

The ANN model established for predicting the CV of diesel, biodiesel, and ZnO based biodiesel blends provided acceptable results. The ideal network configuration was obtained with five hidden neurons. Training was carried out with standard backpropagation, using a log-sigmoid transfer function to capture nonlinear relationships shown in Fig. 6. This configuration provided the best balance between accuracy and computational efficiency but relatively lower accuracy compared to the viscosity model, with performance indicators of RMSE = 1.0, MAPE = 1.6%, and $R^2 = 0.7$ as shown in Fig. 7. Matched with Najafi et al. (2011) that trained a three-layers ANN on 240 FAEE based biodiesel samples and stated a correlation coefficient of $R \approx 0.9$ (prediction accuracy ≈ 99.8%) the current study achieves $R^2 = 0.7$ for predicting the CV of biodiesel-ZnO blends. Current network jointly learns from blend ratio and ZnO nanoparticle dosage.

This moderate R^2 value can be attributed to several interrelated factors. Firstly, calorific value is an intrinsic thermochemical property that primarily depends on the elemental composition of the fuel, particularly the carbon-to-hydrogen ratio and oxygen content, as well as the molecular structure of FAMEs in biodiesel In addition, elemental composition data (C, H, O) should be included as inputs to the network and the database should be expanded to include a variety of fuel types, which will improve generalization. Unlike viscosity, which can be directly influenced by nanoparticle dispersion and intermolecular interactions, the effect of ZnO nanoparticles on CV is indirect. Their role is mainly catalytic during combustion enhancing oxidation and combustion efficiency without significantly altering the inherent chemical energy of the fuel itself. Consequently, the ANN encountered weaker nonlinear correlations between the input variables (blend ratio, nanoparticle dosage) and the output (CV), which limited its predictive power.

In addition, the relatively narrow variation in calorific value among the tested fuel blends (typically within a few MJ/kg) means that even small experimental uncertainties such as blending inconsistencies, feedstock variations, or calorimetric measurement errors can lead to disproportionately large effects on the correlation strength, thereby lowering the R^2 value. The need for a larger hidden layer (twelve neurons) further reflects the complexity of approximating these subtle nonlinearities compared to viscosity prediction, where fewer neurons were sufficient.

For future improvement, several strategies are recommended. Incorporating additional input features such as elemental composition data (C, H, O percentages), higher heating value (HHV), density, and other thermophysical descriptors would strengthen the ANN's ability to capture the underlying determinants of calorific value. Expanding the training dataset to include a wider range of biodiesel feedstocks (soybean, palm, waste cooking oil, etc.) and nanoparticle types or dosages would improve model robustness and generalization. Moreover, the integration of hybrid approaches, for example combining ANN with Response Surface Methodology (RSM) or Genetic Algorithms (GA), could enhance optimization and prediction reliability. Finally, minimizing experimental uncertainties through precise calorimetric techniques and standardized blending protocols would reduce data noise and further improve the model's performance.

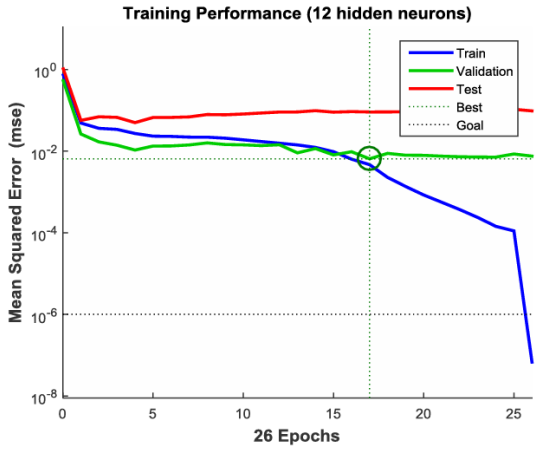

Fig. 6. Training performance of calorific value network

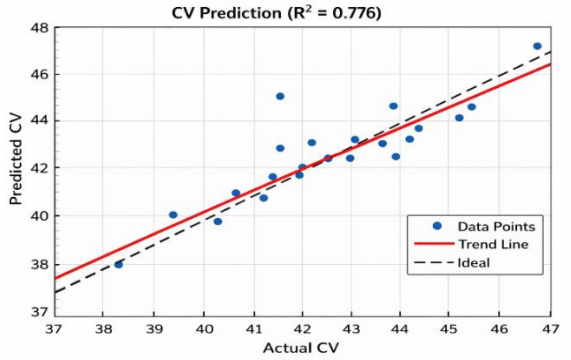

Fig. 7. Regression plots of CV ANN model outputs for training

Overall, although the ANN model for CV prediction demonstrated acceptable accuracy for engineering applications, its lower R^2 compared to viscosity prediction highlights the inherent challenges of modeling fuel energy content based solely on blend ratios and nanoparticle dosage. By enriching the input feature set, expanding the dataset, and adopting hybrid modeling strategies, future research can achieve higher prediction accuracy and establish ANN as a powerful alternative to experimental calorific value measurements shown in Fig. 8.

Fig. 8. Experimental results versus ANN results in terms of calorific value

4.3 Prediction of Brake Thermal Efficiency

The ANN model developed for predicting the BTE of diesel, biodiesel, and ZnO nanoparticle–enhanced biodiesel blends under varying engine speeds and loads demonstrated excellent predictive capability. The training process was conducted using standard backpropagation with a log-sigmoid activation function, which effectively captured the nonlinear relationships among the input and output variables (Fig. 9). The best-performing network achieved RMSE = 1.5, MAPE = 4%, and R^2 = 0.9, confirming that the ANN was able to replicate experimental observations with high accuracy shown in Fig. 10. Compared with the recent study of Nimal and Jacob (2023), they predicted the brake thermal efficiency of biodiesel blended with aluminum oxide (Al_2O_3), titanium dioxide (TiO_2), and copper oxide (CuO) nanoparticles using ensemble decision-rule classifiers and stated a maximum correlation coefficient of R = 0.9 for the best-performing model. The present ANN model reached a comparable predictive accuracy of R^2 = 0.9. Although both approaches successfully captured nonlinear relationships between nanoparticle composition and engine performance, the ANN used in current study showed smoother convergence and lower mean absolute error, confirming its efficiency for continuous variable prediction.

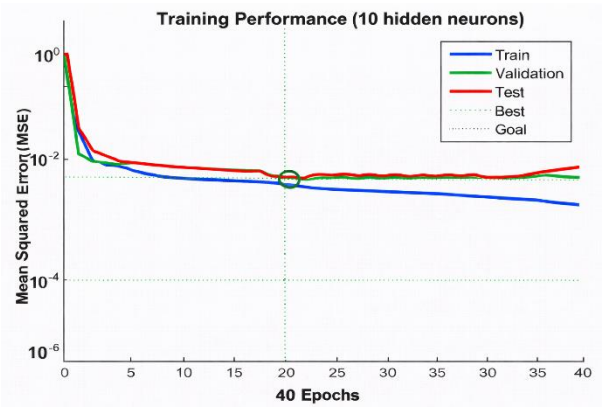

Fig. 9. Training performance of brake thermal efficiency network

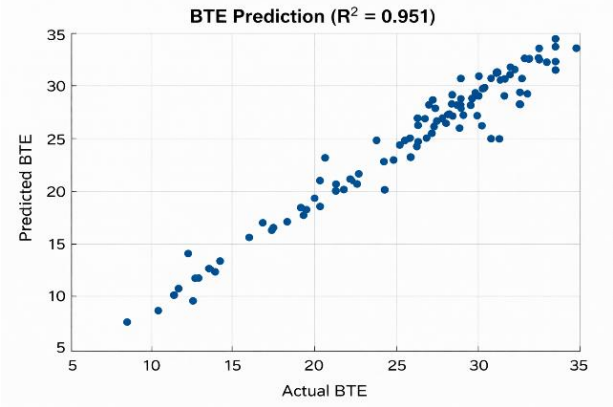

Fig.10. Regression plots of BTE ANN model outputs for training

The relatively low RMSE indicates that the deviations between predicted and actual values were minor in absolute terms, while the MAPE value of about 4% falls within the acceptable engineering threshold for predictive engine modeling. The R^2 value exceeding 0.9 reflects a very strong correlation between predicted and measured data, underscoring the robustness of the ANN architecture in capturing nonlinear interactions among input parameters (fuel type, nanoparticle dosage, engine speed, and load).

The high accuracy is mainly due to the sensitivity of BTE to both operating conditions and nanoparticle addition. BTE generally increases at medium to high loads because of improved utilization of fuel chemical energy, while at lower loads frictional and pumping losses dominate. The ANN successfully captured these performance trends. Furthermore, the influence of ZnO nanoparticles—enhancing combustion through catalytic activity, improved atomization, and oxygen buffering was effectively represented, aligning with reported improvements in BTE of 10–20% at optimum dosages in previous experimental studies.

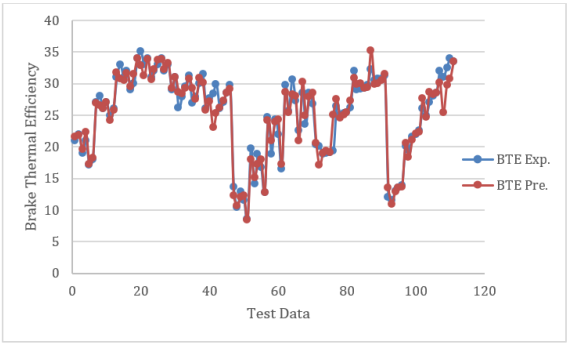

Fig. 11. Experimental results versus ANN results in terms of brake thermal efficiency

Some prediction errors remain, which can be attributed to uncertainties such as nanoparticle dispersion stability, feedstock composition variability, and measurement precision for torque and fuel consumption. However, these effects had a minimal impact, as evidenced by the low RMSE and MAPE values as shown in Fig. 11.

4.4 Prediction of the Brake Specific Fuel Consumption

The ANN model developed for predicting the BSFC of diesel, biodiesel, and ZnO nanoparticle–enhanced biodiesel blends under varying engine speeds and loads demonstrated high predictive capability. The ANN was trained using a backpropagation algorithm with a log-sigmoid activation function, enabling accurate representation of nonlinear dependencies (Fig. 12). The statistical evaluation confirmed that the model achieved RMSE = 0.02, MAPE = 4%, and R^2 = 0.8 which indicate strong agreement between predicted and experimental results as shown in Fig. 13. In comparison with the study of Togun and Baysec (2010), they developed an ANN model to predict torque and BSFC of a spark-ignition gasoline engine and reached a coefficient of determination of R^2 = 0.9, the current study obtained R^2 = 0.8 for biodiesel-ZnO blends. Although their model confirmed excellent accuracy for conventional fuels, the current ANN outline extends this approach to compression-ignition engines fueled with ZnO nanoparticle-enhanced biodiesel, where the complication of combustion dynamics and fuel heterogeneity makes perfect correlation less achievable. By including engine load and ZnO nanoparticle dosage as key inputs, the suggested model efficiently captures the catalytic influence of nanoparticles on combustion and fuel consumption.

The relatively low RMSE value suggests that the absolute deviations between measured and predicted BSFC were minimal, while the MAPE of approximately 4% confirms that the model provided predictions within an acceptable engineering tolerance. The R^2 value of 0.8 demonstrates a strong correlation between predicted and experimental outcomes, underscoring the ANN's ability to capture the nonlinear influence of fuel composition, nanoparticle dosage, speed, and load on fuel consumption characteristics. The ANN successfully reproduced known trends of BSFC. As expected, BSFC values were higher for biodiesel compared to diesel due to the lower calorific value and higher density of biodiesel. However, the addition of ZnO nanoparticles improved combustion efficiency by enhancing atomization, reducing ignition delay, and supplying oxygen buffering capacity, which led to observable reductions in BSFC at optimal dosages. Furthermore, the effect of operating parameters was accurately captured: BSFC decreases with increasing load because more of the fuel's energy is converted into useful work, while higher values were predicted at light loads and extreme speeds where incomplete combustion and frictional losses dominate.

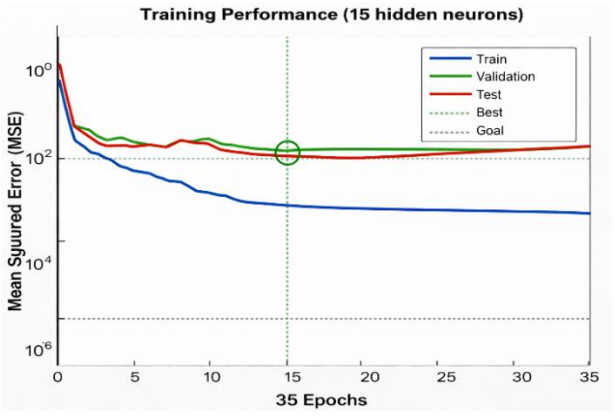

Fig. 12. Training performance of brake specific fuel consumption network

Although minor deviations exist, particularly at some operating points where dispersion stability of nanoparticles and measurement uncertainties may affect accuracy, the overall performance of the ANN confirms its reliability.

In conclusion, the ANN model for BSFC prediction achieved RMSE = 0.02, MAPE = 4%, and R^2 = 0.8, demonstrating excellent predictive accuracy. This validates its application as a computationally efficient alternative to extensive experimental testing, enabling faster evaluation and optimization of biodiesel–nanoparticle blends under diverse engine operating conditions as shown in Fig. 14.

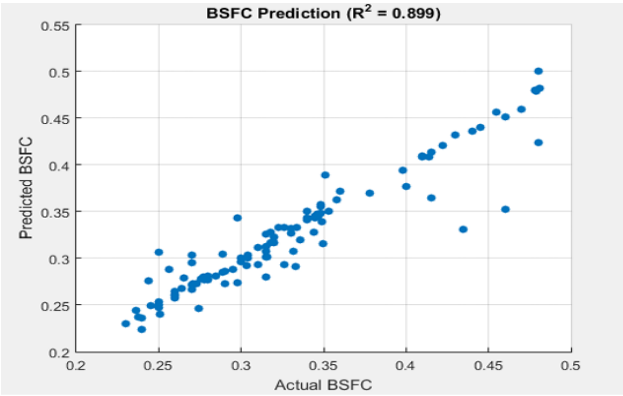

Fig. 13. Regression plots of BSFC ANN model outputs for training

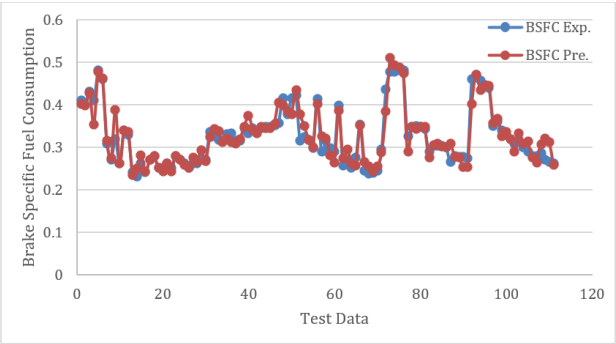

Fig. 14. Experimental results versus ANN results in terms of prediction of the brake specific fuel consumption

In summary, the highest accuracy was achieved by the BTE model, followed closely by the BSFC model, while the KV model demonstrated moderate accuracy, and the CV model exhibited the lowest accuracy. These differences underline the fact that ANN performs better when the target output is highly sensitive to both input variables and operating conditions (as in BTE and BSFC), whereas predictive strength is reduced for intrinsic chemical properties like calorific value that are less influenced by the selected inputs.

5. SENSITIVITY ANALYSIS

Sensitivity analysis for the predicted results was carried out to categorize the relative influence of the independent variables diesel fraction, biodiesel fraction, ZnO nanoparticle dosage, engine load and speed on the predicted outputs. This analysis offers insights into how the ANN interprets difficult nonlinear relationships among input variables affecting the fuel properties and engine performance indicators.

5.1 Calorific Value Model

The sensitivity outcomes for the calorific value estimation model revealed that biodiesel fraction had the maximum importance (0.62), followed by diesel fraction (0.27) and ZnO nanoparticles dosage (0.09). This shows that the ANN model mainly relied on the biodiesel fraction to estimation calorific value, recognizing that the oxygenated construction of biodiesel significantly decreases the energy content compared to pure diesel. The lesser importance of ZnO dosage reflects its secondary influence on combustion improvement rather than direct influence to heating value.

5.2 Kinematic Viscosity Model

For the kinematic viscosity prediction model, the ANN showed biodiesel fraction as the most important variable (0.50), followed by diesel (0.28) and ZnO (0.21). This standing recommends that the ANN model captured the strong dependence of Kinematic viscosity on the biodiesel composition, were increasing biodiesel content increases viscosity. The comparatively small impact of ZnO dosage indicates that nanoparticle concentration had a minor and nonlinear effect within the tested range.

5.3 Brake Specific Fuel Consumption Model

In the BSFC calculation model engine load was found to be the most governing variable (0.43), followed by engine speed (0.17), biodiesel fraction (0.15), diesel fraction (0.12), and ZnO dosage (0.12). This product shows that the ANN model suitably recognized the strong dependence of fuel consumption on engine load, which straight controls fuel flow amount. The modest importance of engine speed, diesel fraction, and biodiesel fraction indicates that the network learned their minor influence on combustion efficiency and mixture formation. ZnO content showed a minor yet notable contribution, likely reflecting its catalytic effect on refining combustion.

5.4 Brake Thermal Efficiency Model

The ANN BTE prediction model also identified engine load as the most important variable (0.53), followed by speed (0.14), diesel fraction (0.13), ZnO dosage (0.12) and biodiesel fraction (0.08). The governance of engine load highlights its governing role in determining BTE. The moderately stable contributions of diesel, ZnO dosage and engine speed indicate that the ANN sensed a multidimensional relationship where both fuel characteristics and working parameters together influence brake thermal efficiency. The improved importance of ZnO dosage proposes that the ANN captured its combustion refining role, improving engine efficiency.

Across all models, the ANN sensitivity analysis demonstrated that engine load was the significant factor

affecting engine performance (BSFC and BTE), while biodiesel fraction mainly influenced calorific value and governed kinematic viscosity behavior. Although fewer dominant ZnO nanoparticles dosage performed as minor enhancers reflecting their catalytic outcome on combustion. These results approve that the ANN models efficiently captured the key physical properties and nonlinear relations among fuel composition and engine performance.

6. CONCLUSIONS

ANNs demonstrated high capability in modeling the nonlinear and multi-variable nature of diesel engine performance when fueled with biodiesel–nanoparticle blends. The developed feed-forward backpropagation networks, trained with the Levenberg–Marquardt (trainlm) algorithm and employing a log-sigmoid activation function, proved effective in capturing the complex interactions among blend ratio, nanoparticle dosage, engine load, and speed. Key conclusions are as follows:

- High prediction accuracy of ANN models with strong agreement with experimental data, particularly for brake thermal efficiency (BTE, $R^2 = 0.95$, RMSE = 1.51, MAPE = 4.02%) and brake specific fuel consumption (BSFC, $R^2 = 0.89$, RMSE = 0.02, MAPE = 4%). These results approved ANN's reliability in estimating performance indices sensitive to multiple operating parameters.
- Reasonable performance for essential physicochemical properties, the ANN models reached acceptable but lower accuracy (viscosity: $R^2 = 0.82$; calorific value: $R^2 = 0.78$), reflecting the fact that such properties are less influenced by nanoparticle dosage thus present weaker correlations for ANN learning.
- Developing separate ANN architectures for each output (viscosity, calorific value, BTE, BSFC) minimized cross-output interference, improved stability, and allowed optimization of network structure per target variable.
- The training strategy with gradient descent momentum (learngdm) improved convergence and reduced overfitting. Optimal hidden neuron numbers were identified (e.g., five for viscosity, twelve for calorific value, twenty-five for performance indices), highlighting the importance of structural tuning.
- ANN significantly reduces the need for exhaustive experimental testing, lowers cost and time, and provides a flexible, data-driven framework that can be extended to diverse fuels, nanoparticle additives, and operating regimes.
- It is recommended that these models be combined with multi-objective optimization techniques to support real-time operating decisions, which has not been systematically addressed in previous studies.

The successful development of ANN models for predicting fuel properties and engine performance of biodiesel-ZnO blends opens up promising avenues for future research and practical applications. Integrating these models with advanced optimization algorithms could enable real-time decision-making and optimization of fuel formulations and engine operating conditions, thereby maximizing efficiency and minimizing emissions. However, further research is needed to address challenges such as the long-term stability of nanoparticle dispersion in fuels, the compatibility of these blends with existing engine hardware, and the development of standardized measurement protocols for fuel properties and emissions. Additionally, expanding the dataset to include a wider range of biodiesel feedstocks and nanoparticle types, as well as conducting extensive validation studies under diverse operating conditions, will be crucial for ensuring the robustness and reliability of the models in real-world applications.

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