World Journal of Advanced Research and Reviews

eISSN: 2581-9615 CODEN (USA): WJARAI

Cross Ref DOI: 10.30574/wjarr

Journal homepage: https://wjarr.com/

(RESEARCH ARTICLE)

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Hybrid experimental and artificial neural network modeling for cold start emissions prediction in PCM-assisted diesel engines

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World Journal of Advanced Research and Reviews, 2025, 28(01), 1094-1103

Publication history: Received on 19 Au 2025; revised on 12 October 2025; accepted on 15 October 2025

Article DOI: https://doi.org/10.30574/wjarr.2025.28.1.3530

Abstract

This study presents a hybrid experimental–computational approach integrating phase change materials (PCMs) and artificial neural network (ANN) modeling to predict cold-start emissions in diesel engines. During cold starts, insufficient fuel vaporization causes incomplete combustion and significantly increases CO, HC, and NO emissions. To mitigate this problem, a PCM-assisted thermal energy storage (TES) system was designed to preheat the intake air, utilizing latent heat stored in the PCM. Experiments were performed on a two-cylinder, water-cooled, direct-injection diesel engine under various PCM initial temperatures (6–60 °C). Measured parameters included PCM temperature, intake air temperature, and exhaust emissions (CO, CO_2, HC, NO). Building upon these data, a multilayer perceptron ANN model was developed with four inputs (initial PCM temperature, time, PCM temperature, and intake air temperature) and four outputs (CO, HC, CO_2, NO). The network architecture comprised six hidden layers and 500 neurons, using sigmoid and tanh activation functions. The model achieved high predictive accuracy with coefficients of determination (R^2) of 0.913, 0.984, 0.959, and 0.926 for CO, CO_2, HC, and NO, respectively, and correspondingly low RMSE values. These results confirm that the ANN successfully captured the nonlinear dependencies between thermal conditions and emission behavior. The proposed hybrid methodology reduces the need for extensive experimental testing while maintaining high prediction reliability. Consequently, this study demonstrates the potential of PCM-assisted intake air heating combined with ANN-based prediction for efficient cold-start management, reduced emissions, and the intelligent thermal optimization of diesel engines.

Keywords: Cold start; Diesel engine; Intake air heating; Phase change material; Artificial neural network; Hybrid modeling

1. Introduction

Cold start is a significant issue for compression-ignition engines and is a cause of both reduced engine performance and increased exhaust emissions. This is because it hinders fuel vaporization, delaying mixture formation and deteriorating combustion quality, which in turn prolongs the cranking duration. Moreover, it leads to increased emissions of carbon monoxide (CO), unburned hydrocarbons (HC), nitrogen oxides (NOx), and particulate matter (PM). Since the emission levels produced during the first start account for a significant proportion, cold start has become a focal point in emission reduction studies [1,2]. To mitigate these effects and enable the engine to quickly reach stable operating conditions, various strategies have been developed. Among these, the use of phase change materials (PCMs) has been proposed to increase the intake air temperature, thereby reducing the initial cranking time and promoting more efficient in-cylinder combustion [3].

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PCMs, which can store latent heat during phase transitions, have emerged as promising solutions for thermal energy storage in internal combustion engines [4,5]. PCMs can store waste heat recovered from the engine coolant or exhaust gases. The stored heat can subsequently be used to preheat the intake air or engine components during cold start [6–8]. This approach has been shown to reduce cold start-related CO and HC emissions by approximately 60–80% [9], improve warm-up times, and enhance engine thermal efficiency [10].

Through thermal energy storage (TES) systems, the intake air temperature of diesel engines can be raised above ambient temperature by utilizing exhaust gas energy [11]. Ugurlu [12], designed a PCM-assisted heat energy storage system and modified it onto the engine coolant line. This system significantly improved cold start performance within 12 hours after engine shutdown. Similarly, Gumus [13], employed PCM to preheat a catalytic converter in internal combustion engines to reduce cold start emissions, resulting in decreases of CO and HC emissions by 64% and 15%, respectively. Furthermore, Gumus and Ugurlu [14], applied PCM to improve cold start performance in an liquefied petroleum gas (LPG) fueled engine. Their TES system achieved reductions in HC and CO emissions of 17.32% and 28.71%, respectively. In another study, Gürbüz et al. [15] designed a latent heat storage system supported by PCM to store exhaust waste heat from a spark ignition engine.

By utilizing waste heat from the engine coolant circuit, the latent heat stored in PCMs can be employed to raise the temperature of the fresh intake air, thereby improving both engine performance and exhaust emissions throughout the warm-up period. In this context, Kaltakkıran and Ceviz [16], designed a TES system to increase the intake air temperature of a conventional direct injection engine under cold start conditions and evaluated the system efficiency using energy–exergy analysis. Experiments conducted at a constant ambient temperature demonstrated that the PCM-TES system reduced the cranking time compared to the conventional system and decreased CO and HC emissions by 68.2%, 27.5%, and 44%, respectively. These results indicate that PCM-integrated TES systems can effectively enhance cold start performance and emission characteristics of diesel engines.

In experimental studies on internal combustion engines, the wide variety of operating parameters, performance metrics, and emission characteristics often makes the experimental process challenging, time-consuming, and costly. To overcome these difficulties, optimization and data-driven modeling techniques, particularly artificial neural network (ANN), have been increasingly used in recent years to predict engine performance and emissions. These methods offer advantages over conventional mapping approaches by accurately estimating engine parameters with limited test data [17]. Accordingly, experimental designs combined with ANN-based studies for diesel engines have enabled precise prediction of performance and emissions while reducing experimental effort. This approach also facilitates the improvement of engine efficiency and the identification of optimal injection strategies for low emissions [18].

Considering the environmental impacts of internal combustion engines, artificial intelligence (AI)-based strategies have been proposed to optimize engine performance and emissions. In this context, data from a single-cylinder engine operating with different compression ratios and ethanol/water blends were used, and torque and emission values were predicted using a random forest algorithm [19]. Moreover, numerous studies have employed AI to predict and optimize the complex characteristics of various engine types with different fuels [20], to forecast the behavior of engine cooling systems under both steady and transient conditions using various nanofluids [21], and to model pollutant emissions from a single-cylinder spark-ignition research engine under different operating conditions [22].

The novelty of the present study lies in integrating the thermal management approach described above with an ANN-based emission prediction model. Traditional analytical or semi-empirical models often struggle to capture the complex multivariable relationships among PCM initial temperature, ambient temperature, heat transfer, intake air temperature profile, engine speed and load, and instantaneous emission rates. In recent years, artificial neural networks have emerged as a particularly suitable method for learning such complex mappings. In engine research, ANN models are increasingly used to predict emissions and performance parameters when provided with multiple interacting input variables, such as intake air temperature, PCM temperature, engine load, and speed [23,24]. Their ability to generalize from experimental data and provide rapid predictions makes them highly attractive for real-time control and optimization schemes.

The effects of different PCM initial temperatures and intake air temperatures on engine performance and exhaust emission characteristics have been previously investigated experimentally [16]. In this follow-up study, an ANN model was developed to predict exhaust emissions using experimental data. The input parameters of the model include the initial temperature of the PCM used for energy storage with engine coolant, time, the temperature of the fresh intake air supplied to the engine intake manifold, and the instantaneous PCM temperature, while CO, CO_2, HC, and NO emissions were defined as output parameters. In the model, implemented as a multilayer perceptron (MLP), the determination coefficient (R^2) and RMSE values were examined by varying the number of neurons in the input and hidden layers as well as the activation functions. This approach enables accurate prediction of emission characteristics under PCM-assisted different intake air heating strategies, supports intelligent control of intake heating systems, and provides insights for system optimization. Considering the limited number of studies in the literature on PCM-assisted intake air heating in internal combustion engines and the wide variety of engine operating conditions, the ability to predict the effects of varying intake air temperatures on engine performance and emissions highlights the significance of the present study.

2. Methodology

2.1. Experimental layout

All experiments were conducted using a water-cooled, four-stroke, direct-injection diesel engine (Super Star 7728) mounted on a hydraulic dynamometer test bench. The detailed technical specifications of the engine are presented in Table 1.

Table 1 The engine specifications [16]

Descriptions	Value
Engine	SuperStar / 7728
Cylinder type / Stroke	In line – 2 / 4 stroke
Engine cooling system	Water-cooled
Stroke, (mm)	100
Cylinder diameter, (mm)	98
Cylinder volume, (cm^3)	1540
Compression ratio	17:1
Injection mode	Direct injection
Max. power (at 2750 rpm)	28 HP
Fuel type	Diesel

In the experiments, the temperatures of the ambient air entering the PCM-integrated heat exchanger, the fresh intake air exiting the heat exchanger and entering the engine, and the internal temperature of the PCM within the heat exchanger were measured using type-K thermocouples with an uncertainty of ±0.5 °C. The experiments were performed at the engine's idle speed under five different conditions, corresponding to PCM surface temperatures of 6, 20, 30, 40, 50, and 60 °C, with the PCM placed inside the thermal energy storage system. Exhaust gas emissions were measured using a Bosch BEA 250 emission analyzer, which is suitable for both gasoline and diesel engines. Carbon monoxide (CO), unburned hydrocarbons (HC), carbon dioxide (CO_2), and nitrogen oxides (NO) emissions were recorded for all experimental conditions. The units of measured emission components are volumetric percent (Volume %) for CO and CO_2, and parts per million (PPM) for HC and NO. All temperature and emission measurements were acquired and processed using the LabVIEW software.

2.2. Artificial Neural Network (ANN) Model

The developed Artificial Neural Network (ANN) model employed in this study is depicted in Figure 1. The schematic illustrates a multilayer neural network comprising one input layer, six hidden layers, and one output layer, with each layer containing a specific number of neurons. This architecture allows the network to capture complex nonlinear relationships between the input variables and the target emission outputs.

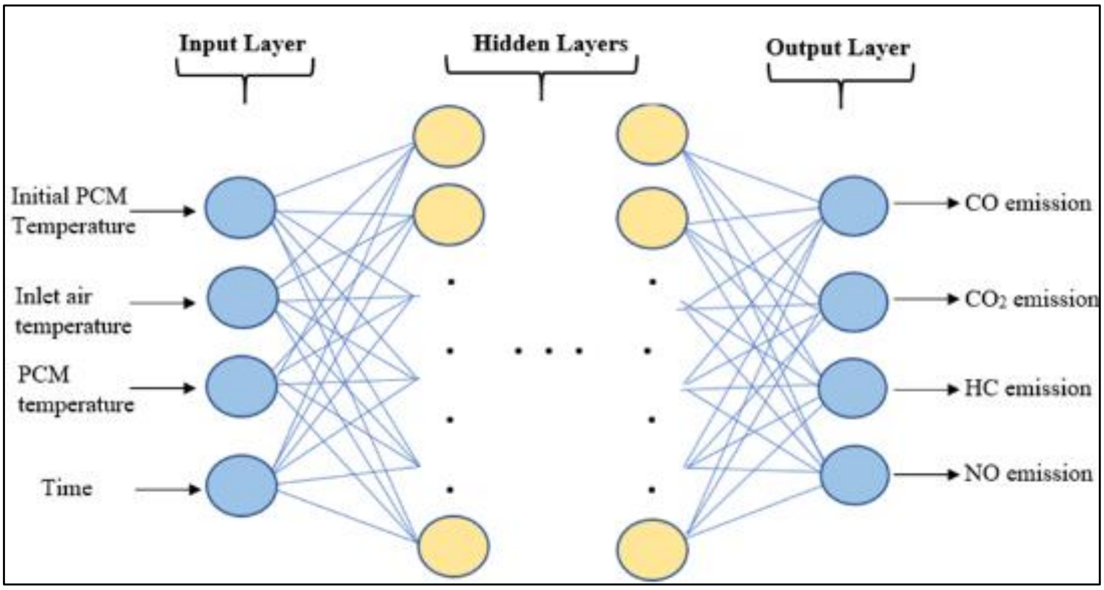

Figure 1 Structure of the proposed Artificial Neural Network (ANN) model

In this study, the prediction performance of the model was assessed using statistical metrics, including Root Mean Square Error (RMSE) and Coefficient of Determination (R^2). The following Eqs. (1) and (2) define these statistical evaluation metrics.

$$RMSE = \left[\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2\right]^{1/2} \quad (1)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \quad (2)$$

where y_i and $\hat{y}_i$ represent the *i*th measured and predicted values, respectively. $\bar{y}_i$ denotes the average of the measured values, and n represents the total number of data points.

3. Result and Discussion

In a previous experimental study, a PCM-assisted heat exchanger system was integrated into the intake air system of an internal combustion diesel engine to utilize the latent heat storage capability of the PCM and provide high-temperature intake air support during cold start conditions [16]. In this way, the effects of different PCM temperatures and intake air temperatures on engine performance and exhaust emission characteristics were investigated. In the present study, which is a continuation of the previous experimental work, an artificial neural network (ANN) model was developed to predict exhaust emission values using the data obtained from the experiments.

In the modeling phase, a multilayer perceptron model was constructed, where the initial temperature of the PCM, time, engine intake air temperature, and instantaneous PCM temperature were considered as input parameters, while CO, CO_2, HC, and NO emissions were defined as output parameters. In this developed model, the number of neurons in the input and hidden layers as well as the activation functions were varied to observe the coefficient of determination (R^2) and root mean square error (RMSE) values. By adjusting the learning rate and performing several trials, the most suitable model configuration was determined. A total of 444 experimental data points were used to train and validate the model. Among these, 80% were randomly selected for training, while the remaining 20% were used for testing. The structural and training parameters of the developed ANN model are summarized in Table 2.

Table 2 Selected model parameters

Descriptions		**Value**
Number of Hidden Layer		6
Learning Rate		0.001
Training Iterations (Epoch)		500
Number of Neurons	Input Layer	4
	Hidden Layer	500
	Output Layer	4
Activation Function	Input Layer	Sigmoid
	Hidden Layer	Tanh
	Output Layer	Sigmoid

As shown in Table 2, the model consists of six hidden layers positioned between the input and output layers, comprising a total of 500 neurons. To balance the data flow and ensure that the outputs remain within an appropriate range, a sigmoid activation function was employed in the input and output layers, while the tanh activation function was utilized in the hidden layers to better capture nonlinear relationships. Furthermore, the model was trained with a learning rate of 0.001 over 500 epochs to achieve an optimal balance between prediction accuracy and computational efficiency.

During training, the network learns from the training dataset by comparing the predicted outputs (generated based on the network's weight coefficients) with the corresponding actual values, and an error value is computed for each iteration. This error is minimized through successive weight updates throughout the training process. The variation of the mean absolute error (MAE) between the measured and predicted values during the weight update process in the training phase of the artificial neural network model is illustrated in Figure 2.

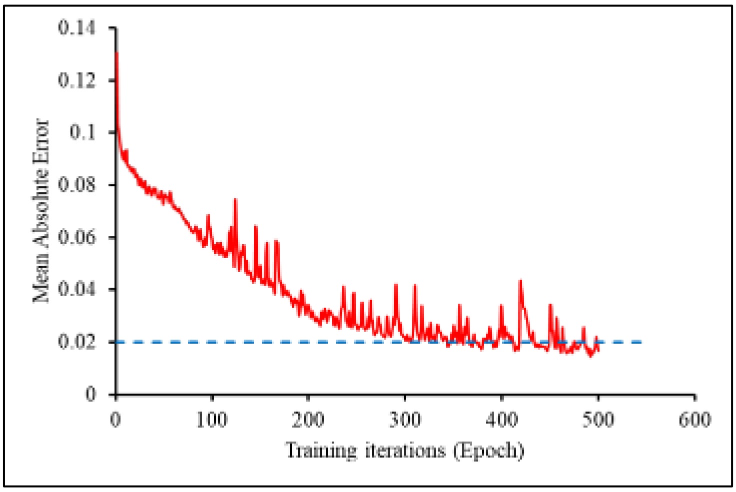

Figure 2 Mean absolute error between the measured and predicted values for the training dataset

As illustrated in Figure 2, the error between the actual and predicted values of the training data is relatively high at the beginning of the training process. Examination of Figure 2 reveals that during the first 0–50 epochs, the error rate remains considerably high (approximately 0.13). Subsequently, a rapid decrease is observed, indicating that the model quickly begins to learn. Between 50 and 300 epochs, the error rate continues to decline with minor fluctuations. In the later stage of training (epochs =300-500), the error stabilizes at around 0.02, suggesting convergence of the network. Overall, although slight oscillations are present in the graph, these fluctuations reflect fine-tuning of the weights rather than instability, implying that the system has effectively converged. This indicates that a successful training process has been achieved.

During the modeling process, 80% of the dataset was used for training the network, while the remaining 20%, which had not been previously introduced to the model, was used for testing. The predicted outputs obtained from the trained network were compared with the corresponding experimental results for all output parameters. The actual emission results from engine experiments and the predicted values obtained from the artificial neural network model are presented in Figures 3–6 for CO, CO_2, HC, and NO emissions, respectively.

As shown in the parity plot for CO emissions in Figure 3, a strong correlation exists between the measured and ANN-predicted values, demonstrating that the model successfully captures the general trend of CO emissions. However, a slight underestimation tendency is observed at higher CO concentration levels, which can be attributed to the limited number of high-concentration samples within the training dataset. To minimize this effect and improve the model's accuracy, incorporating a more diverse dataset that includes a wider range of CO concentration values is recommended.

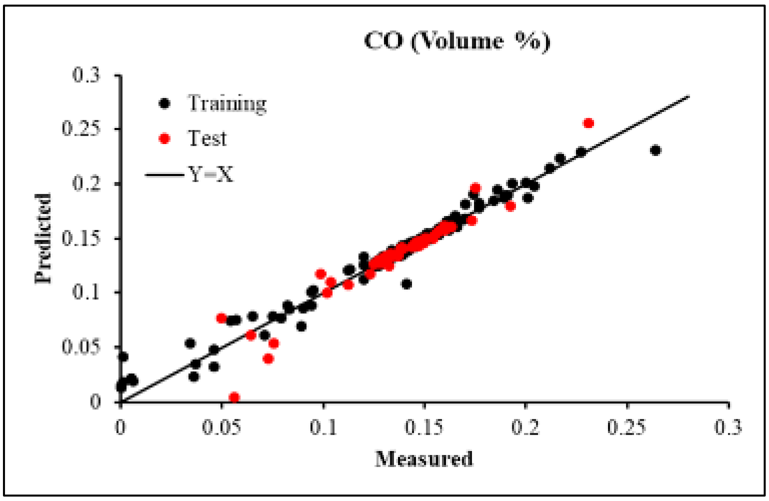

Figure 3 Parity plot between test and training values for CO emission

As shown in Figure 4, the model exhibited excellent performance in predicting CO_2 emissions. The parity plot demonstrates that the data points are tightly clustered around the Y = X reference line, indicating that the deviation between the measured and predicted values is minimal. These findings further confirm that the model effectively captures the dynamics of CO_2 emissions and provides reliable predictive accuracy.

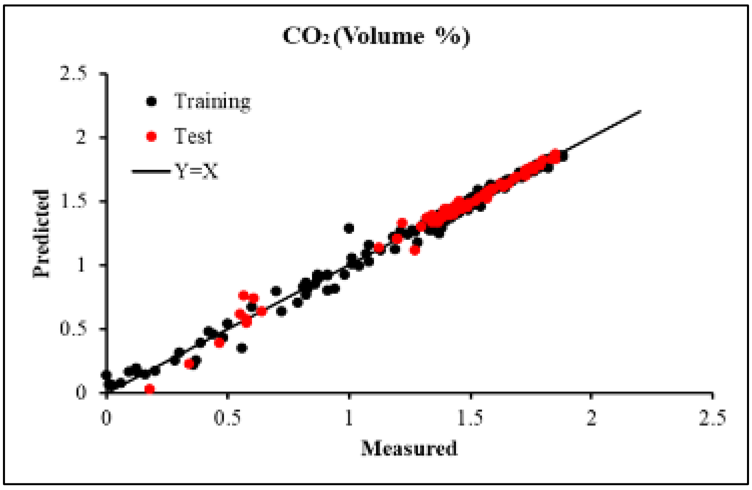

Figure 4 Parity plot between test and training values for CO_2 emission

As illustrated in Figure 5, the parity plot for HC emissions demonstrates a good level of agreement between the measured and predicted values. However, a closer examination of the graph reveals a few individual prediction errors that the model could not fully capture. These deviations may be attributed to the influence of numerous uncontrollable factors that inherently affect HC emissions.

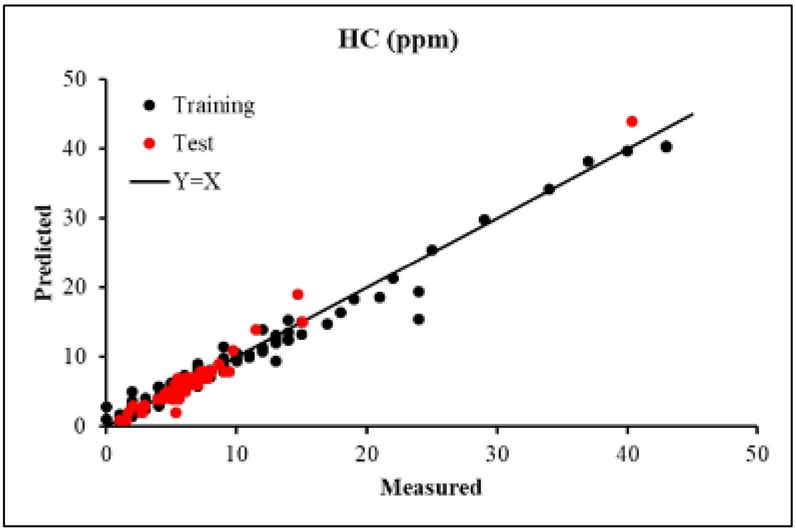

Figure 5 Parity plot between test and training values for HC emission

As shown in Figure 6, the model accurately reflects the overall trend and short-term fluctuations of NO emissions. However, some transient peaks are slightly underestimated, which likely indicates that the model was unable to fully capture the rapid variations in NO concentration levels. Therefore, to improve prediction accuracy, it may be advisable to incorporate additional temporal features or employ more dynamic modeling approaches capable of better representing such transient behaviors.

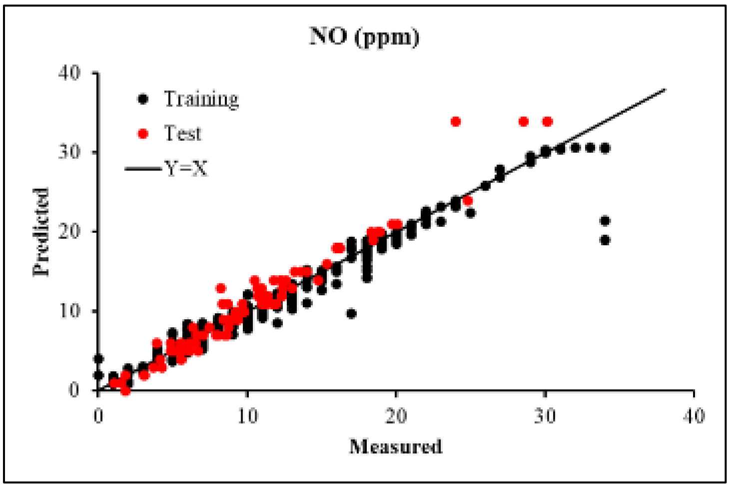

Figure 6 Parity plot between test and training values for NO emission

Table 3 Performance metrics of the predictive model for different emission components

Emission	Performance Metrics	
	R^2	RMSE
CO	0.913	0.009
CO_2	0.984	0.043
HC	0.959	0.961
NO	0.926	1.807

A detailed examination of the emission graphs presented in Figures 3–6 clearly indicates that the predicted values obtained from the model are in strong agreement with the corresponding experimental results across all output parameters. Moreover, to quantitatively assess the discrepancies between the predicted and measured values, the coefficient of determination (R^2) and the root mean square error (RMSE) metrics were employed. The calculated error function values for all output parameters are summarized in Table 3.

The coefficient of determination (R^2) and root mean square error (RMSE) values presented in Table 3 indicates that the discrepancy between the test and predicted data is generally low. Considering the R^2 and RMSE metrics, the performance of the artificial neural network (ANN) model appears highly satisfactory. The coefficients of determination obtained for CO, CO_2, HC, and NO emissions are 0.913, 0.984, 0.959, and 0.926, respectively, indicating that the model can explain over 90% of the variability in the experimental data. Similarly, the RMSE values support the predictive performance of the model. Specifically, the RMSE values for CO (0.009) and CO_2 (0.043) are very low, demonstrating that the model provides highly reliable predictions for these two components. In contrast, the RMSE values for HC (0.961) and NO (1.807) are relatively higher, which may be attributed to the more complex or nonlinear behavior of these emissions in the dataset.

Overall, the developed ANN model exhibits strong generalization capability, achieving highly accurate predictions for CO and CO_2 emissions, while providing acceptable accuracy for HC and NO. When considered together, these error metrics indicate that the model, developed based on instantaneous PCM temperature, intake manifold air temperature, initial PCM temperature, and time, is highly effective in predicting CO, CO_2, HC, and NO emissions. Consequently, the emission characteristics produced in the engine can be determined for varying PCM and intake air temperatures over time within a specific operating range.

4. Conclusion

In this study, the effects of increasing intake air temperature with the assistance of phase change material (PCM) under cold start conditions on exhaust emissions in an internal combustion diesel engine were investigated using artificial neural network (ANN) modeling. One of the main objectives of the study was to apply a neural network model, which has proven successful in modeling complex systems, to predict exhaust emissions from internal combustion engines.

During the development of the ANN model, four input parameters were considered: the initial temperature of the PCM, engine intake air temperature, time, and instantaneous PCM internal temperature. The output parameters comprised four emission components: CO, CO_2, HC, and NO. While designing the network, parameters affecting model accuracy and performance, including the number of layers, number of neurons, activation functions, and learning rate, were systematically adjusted, leading to the adoption of a multilayer perceptron structure. Eighty percent of the experimental dataset was used for training the model, while the remaining 20% was reserved for testing. The network was evaluated using different error metrics, demonstrating successful prediction of CO, CO_2, HC, and NO emissions.

The developed ANN model exhibited overall satisfactory performance in emission prediction. Specifically, CO and CO_2 emissions were predicted with high accuracy ($R^2 > 0.9$, low RMSE values), while acceptable accuracy was achieved for HC and NO. These results indicate that the ANN approach is an effective and reliable method for predicting engine emissions. The particularly high agreement observed for CO and CO_2 emissions suggests that this methodology could be applied to similar predictive tasks in different contexts.

In conclusion, this modeling study, based on experimental data, provides significant insights into the effects of varying PCM and intake air temperatures on post-combustion exhaust emission characteristics without the need for extensive experimental campaigns. Consequently, a properly developed model can predict emissions using a limited dataset, offering substantial savings in both fuel and time for intensive engine testing. Furthermore, the current study can be extended by incorporating different experimental conditions and alternative predictive modeling approaches.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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