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Predictability Evaluation of Artificial Neural Networks and Response Surface Methodology Models for Thermo-physical Properties of Graphene Nanoplatelets–Ethylene Glycol/Water Nanofluids for Heat Transfer Applications

Manikandan Sekar[1*], Dinesh Kumar Venkatesan[2], Saravanakumar Ayannan[3], Sathish Kumar Krishnamoorthy[3]

[1] Department of Mechanical Engineering, National Institute of Technology, 609 609 Karaikal, Puducherry, India
[2] Department of Mechanical Engineering, Shreenivasa Engineering College, 635 301 Dharmapuri, Tamilnadu, India
[3] School of Mechanical Engineering, Bharath Institute of Higher Education and Research, 600 073 Chennai, Tamilnadu, India
[*] Corresponding author, e-mail: manikandan-jrf@nitpy.ac.in

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Abstract
In this paper, the effectiveness of artificial neural networks (ANN) and response surface methodology (RSM) models in predicting the thermophysical properties ratio of graphene nanoplatelet (GNP)-ethylene glycol (EG)/water nanofluid has been discussed. Volume concentration (0.1%–0.5%) and temperature (−15 °C to 15 °C) were considered as inputs to train the models to predict the thermophysical properties ratios, including density, viscosity, thermal conductivity, and specific heat capacity. The ANN model with the Levenberg–Marquardt (trainlm) algorithm is used to get the best network by varying the number of 9 neurons in the hidden layer. In addition, an RSM, a three-dimensional surface plot techniques technique, was employed on the data points to obtain the new mathematical correlation for predicting thermophysical properties. Eventually, the mean squared error (MSE), regression coefficient (R^2), and percentage of errors from both techniques were compared. The proposed ANN and RSM models show that the MSE, R^2, and percentage of errors are 2.1239×10^{-5}, 0.998, −1.42 to 1.28, and 0.761, above 0.945, −1.46 to 0.97, respectively. The results revealed both techniques are sorely suitable for predicting the thermophysical properties ratio of GNP-EG/water nanofluid.

Keywords
nanofluid, thermophysical properties, ANN, RSM

1 Introduction

The heat transfer process is vital in many energy sectors and industrial applications [1, 2]. The convective heat transfer process is widely used in many thermal systems for heating and cooling applications [3]. For the past decades, to enhance thermal systems heat transfer performance, researchers have increased the temperature difference between solid surfaces and fluids and increased surface area [4, 5]. In the last few years, because of the miniaturization of compact thermal systems, researchers have focused on the impact of incorporating nanoparticles in the existing heat transfer fluids, such as water [6], ethylene glycol (EG) [7], a mixture of water and EG [8], and oils [9, 10], to improve the heat transfer performance of these systems. Also, many researchers [11] conducted experimental studies and found that incorporating the nanoparticles into existing heat transfer fluids improves the thermal performance of the systems by enhancing thermophysical properties such as density, viscosity, thermal conductivity, and specific heat capacity [12–14]. It is often time-consuming and expensive to conduct experimental studies. Hence, it is important to minimize the number of experiments while maximizing the outcomes. Artificial intelligence (AI), a broad field focused on simulating human intelligence processes using computers, is among the most effective tools for predicting various properties from experimental data [15]. Researchers have used a variety of algorithms to estimate and optimize different parameters like genetic algorithms [16], fuzzy logic [17], particle swarms [18], support vector regression (SVR), the Levenberg-Marquardt algorithm [19], the Bayes

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algorithm [20], and the scaled conjugate gradient algorithm [21]. As AI technology advances, novel prediction approaches that outperform traditional ones have been presented. One of the most often used approaches is artificial neural networks (ANN), which has significant drawbacks, such as the requirement for many control parameters, the difficulty in producing a sustainable output, and overfitting issues. Because of the presence of such flaws, better models have improved the ANN model [22]. These algorithms have great promises and perform well in real-world situations. Table 1 [15, 23–36] provides an overview of recently published studies that use neural networks and response surface methodology (RSM) to predict various nanofluids thermophysical properties. Previous studies have shown that the ANN and RSM approaches are effective in predicting the thermophysical properties of various nanofluids. Klazly and Bognár [37] investigated and developed a new model for calculating the viscosity of Al_2O_3/water nanofluids with varying particle sizes (13 nm and 28 nm) and volume concentrations. They found that viscosity enhancement is influenced by volume concentration, particle size, and Brownian motion.

This study evaluates and compares the performance of ANN and RSM models in predicting the thermophysical properties of graphene nanoplatelet (GNP)–EG/water nanofluids based on experimental data. In the ANN model, temperature and nanoparticle volume concentration are used as input variables, while the thermophysical properties are predicted as outputs. Utilizing ANN and RSM for such analysis enables highly accurate predictions of nanofluid heat transfer characteristics while significantly reducing the cost and effort associated with experimental procedures.

2 Methods

Section 2 addresses the data selection process for modeling, the modeling techniques used, and the evaluation criteria applied to develop the models.

2.1 Data selection

This study develops a prediction model for the thermophysical properties of a mixture of EG and water (50:50 volume ratio) base fluids in the presence of GNP. In this modeling, to investigate the effects of two independent variables, such as volume concentration and

Table 1 The summary of recently published studies for predicting thermophysical properties of nanofluid

References	Base fluid	Nanoparticle	Method	Studied properties
Manikandan and Nanthakumar [23]	SAE10W oil	GNP	ANN and RSM	Thermal conductivity
Komeilibirjandi et al. [24]	EG, water, and engine oil	CuO	Correlation and ANN	Thermal conductivity
Manikandan and Nanthakumar [25]	Damper oil	GNP	ANN and curve fitting	Dynamic viscosity
Rostami et al. [26]	Liquid paraffin	MWCNT*	ANN and RSM	Thermal conductivity
Alade et al. [27]	Diesel oil	GNP, MWCNT	ANN and SVR	Density
Manikandan and Nanthakumar [28]	SAE10W oil	Cu	Curve fitting	Density, viscosity, thermal conductivity, and specific heat capacity
Manikandan and Nanthakumar [29]	SAE10W oil	GNP	ANN and curve-fitting	Specific heat capacity
Yashawantha and Vinod [30]	EG–water (35:65 volume%)	CuO, Al_2O_3, and TiO_2	ANN and correlation	Thermal conductivity
Mirsaeidi and Yousefi [31]	Water, EG and water–EG mixture (60:40 volume%)	Carbon quantum dots	ANN and curve fitting	Density, viscosity, and thermal conductivity
Kishore P V R et al. [32]	Water–EG mixture (60:40 volume%)	GNP, Al_2O_3, and CuO	ANN	Viscosity, and thermal conductivity
Asadi et al. [15]	Engine oil	MWCNT-ZnO (25–75 volume%)	SVR	Dynamic viscosity, and thermal conductivity
Sharma et al. [33]	Water	TiO_2	ANN	Thermal conductivity
Çolak et al. [34]	Water	Cu-Al_2O_3	ANN	Specific heat capacity
Borode et al. [35]	EG and engine oil	GNP and Fe_2O_3	ANN	Viscosity, and thermal conductivity
Hemmat Esfe et al. [36]	EG	TiN50, TiN20	ANN and RSM	Density, thermal conductivity, and specific heat capacity

* Multiwalled carbon nanotube

temperature, on thermophysical properties, laboratory data for density, viscosity, thermal conductivity, and specific heat capacity were collected from the data presented by Dhayanidhi and Selvam [38]. The authors prepared the nanofluids using a two-step method by incorporating GNP (<4 nm) into an EG/water mixture (50:50 volume%). The prepared nanofluid stability was analyzed using zeta potential analyzer. The stability of the prepared nanofluids was analyzed using a zeta potential analyzer. The zeta potential was found to be −33.70 mV at 0.5 volume% of GNP, indicating the good stability of the nanofluid. They also measured the thermophysical properties of the GNP–EG/water nanofluids using various instruments: density was measured with a densitometer (DMA 50, Anton Paar, Graz, Austria) with an accuracy of ±2% to ±3%; viscosity was measured using a rheometer (MCR-102, Anton Paar, Graz, Austria) with an accuracy of ±2%; and thermal conductivity and specific heat were measured using a thermal properties analyzer (TPS 2500S, Hot Disk, USA) with an accuracy of ±5%. The collected data were used to calculate the ratio of thermophysical properties of nanofluids, which was then used to train the ANN and RSM models. The data span a volume concentration range of 0.1%, 0.2%, 0.3%, 0.4%, and 0.5%, and a temperature range of −15 °C, −10 °C, −5 °C, 0 °C, 5 °C, 10 °C, and 15 °C.

2.2 Development of prediction model

In this study, prediction models are developed by using two techniques, one is ANN technique and the other is RSM technique. The ANN and RSM models are created using the neural network and curve fitter (3D surface fit) applications in the MATLAB, (2024b) simulation environment [39]. Generally, the ANN architecture consists of three layers: input, hidden, and output layers. These layers contain several neurons and are interconnected with weight coefficients (w_{ij}) and biases (b_i) to transfer data within the layers. In Eq. (1), the mathematics behind the training process of data is presented. The ANN model was trained on datasets randomly selected from the pre-processed dataset. The data sets contain 35 data points for each thermophysical property such as density, viscosity, thermal conductivity, and specific heat capacity. During the ANN modeling process, the dataset was split into three subsets: training (70%), validation (15%), and testing (15%). The input parameters, volume concentration, and temperature were defined, along with the output, which represents the thermophysical properties ratio of the nanofluids. Furthermore, to train the ANN model, the Levenberg–Marquardt (trainlm) training algorithm is used. For the hidden and output layers, the tan-sigmoid and purelin transfer functions are utilized. The mathematical representation of the transfer functions utilized in the ANN model is shown in Eqs. (2) and (3). Varying the number of neurons in the hidden layer of an ANN can significantly influence the model's performance. The ANN structure was finalized based on the configuration that provided the best optimal performance:

$$y_j = f\left(\sum_{i=1}^{n} w_{ij} x_j + b_i\right), \tag{1}$$

$$\text{tansig}\left(x\right) = \frac{2}{1+\exp\left(-2x\right)} - 1, \tag{2}$$

$$\text{purelin}\left(x\right) = x, \tag{3}$$

where y_j is the i^{th} output, f is the activation function, n is the number of the data points, w_{ij} is the weight coefficients, x_j is the j^{th} input and b_i is the bias.

For the development of the RSM model to predict the thermophysical properties of nanofluids, curve fitting (3D surface fit) was used. In this modeling process, the surface fits for the data points of each thermophysical property is based on RSM. We obtain a polynomial equation from the response surface to estimate the thermophysical properties. To obtain the best surface fit, the order of the polynomial equation is varied.

2.3 Evaluation criteria

In this study, the evaluation of the ANN and RSM models was carried out using the following criteria: mean squared error (MSE), regression coefficient (R^2), and percentage error. The mathematical formulations for these criteria are presented in Eqs. (4) to (7), respectively. Generally, the model with the greater R^2 and the smaller MSE shows better performance.

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\text{TCR}_\text{a} - \text{TCR}_\text{p}\right)^2} \tag{4}$$

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(\text{TPP}_\text{p} - \text{TPP}_\text{a}\right)^2 \tag{5}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(\text{TPP}_\text{a} - \text{TPP}_\text{p}\right)^2}{\sum_{i=1}^{n}\left(\text{TPP}_\text{a} - \overline{\text{TPP}}_\text{a}\right)^2} \tag{6}$$

$$Error\left(\%\right) = \left(\frac{\text{TPP}_\text{a} - \text{TPP}_\text{p}}{\text{TPP}_\text{p}}\right) \times 100 \tag{7}$$

In Eqs. (4) to (7), where n represents the total number of data, TCR_a and TCR_p indicates the actual thermal conductivity ratio and predicted thermal conductivity ratio. TPP_a, TPP_p, denotes the thermophysical property ratio of actual experimental measured data and predicted data respectively. $\overline{TPP_a}$ is the mean value of actual measured data.

3 Result and discussion

Section 3 discusses the ANN and RSM models performances in predicting the thermophysical properties ratio of the GNP-EG/water nanofluid concerning volume concentration and temperature. It also discusses the comparison between the ANN and RSM models against experimental data.

3.1 Evaluation of ANN model performance

In the ANN modeling process, 140 sets of experimental data were used to make the prediction model. These sets were then split into 98 sets (70%) for training, 21 sets (15%) for validation, and 21 sets (15%) for testing. In the ANN modeling process, it is assumed that there is enough data to capture the underlying patterns; insufficient data can lead to underfitting or overfitting. Additionally, inputs are typically normalized or standardized, as this scaling helps improve model convergence and stability. Assumes a functional (possibly nonlinear) relationship exists between the inputs and outputs that can be approximated by the network. The input parameters are considered as volume concentration, temperature, and the output parameters are considered as thermophysical properties such as density ratio, viscosity ratio, thermal conductivity ratio, and specific heat capacity ratio, respectively. The model was trained using the trainlm algorithm, the tansigmoid, and the purlin transfer function. Also, change the number of neurons in the hidden layer to get the best network structure. Finally, the best ANN architecture (2–9–1–4) was found to have 9 neurons in the hidden layer. This was determined by using evaluation criteria such as the lowest MSE value and the highest R^2 value. Fig. 1 illustrates the optimal architecture of the ANN model.

Fig. 2 shows the MSE plot of the proposed ANN architecture. The horizontal axis represents the number of epochs as a numerical value, while the vertical axis displays the MSE values. The blue, green, and red color lines, as well as the dotted lines, indicate the train, validation, and test data sets, and the best points, respectively. The green-colored small circle signifies the optimal MSE value. The MSE values rapidly decreased as the number of epochs increased; eventually, the best validation performance was 2.1239×10^{-5}, attained at 39 epochs.

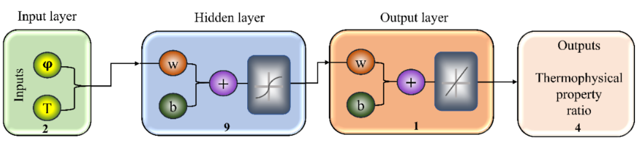

Fig. 1 The best ANN architecture for predicting thermophysical properties of nanofluid

Fig. 3 shows the regression plot of the proposed ANN model for training, validation, testing, and all data sets. The horizontal and vertical axes represent the experimental and ANN-predicted data. The blue, green, red, and black fit lines indicate the bisector lines, the small circle represents the data points, and R represents the regression coefficient values. The R-values for the training (R = 0.99949), validation (R = 0.9925), and test (R = 0.99459) sets are all very

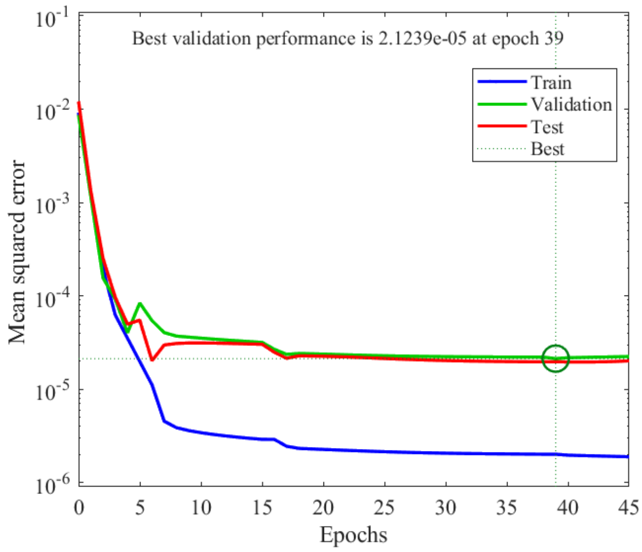

Fig. 2 MSE plot of proposed ANN architecture

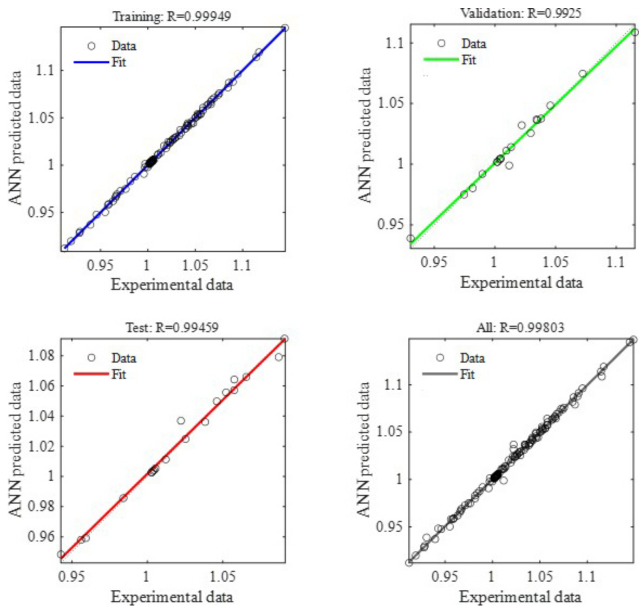

Fig. 3 Regression plot of proposed ANN architecture

high and close to 1. This indicates a strong correlation between the experimental data and the ANN's predictions across all datasets. Based on Fig. 3, the model is neither significantly underfitting nor overfitting. It demonstrates a good fit to the data.

Fig. 4 represents the error histogram of the proposed ANN model with 20 bins. In Fig. 4, the horizontal axis denotes the error values, and the vertical axis represents the number of instances. The blue, green, and red vertical bars indicate the error values concerning the number of instances for training, validation, and test data sets. The orange color vertical line denotes the zero error. From Fig. 4 found that the proposed ANN model has error values ranging between −0.01399 and 0.01211, also most of the data points are very close to the zero-error line. Fig. 5 (a) to (d) shows the agreement between the experimental data and the proposed ANN model predictions with respect to input parameters such as the volume concentration (0.1%–0.5%) and temperature (−15 °C to 15 °C) of the GNP-EG/water nanofluids. The horizontal axis depicts the data samples for each thermophysical property, while the vertical axis represents the thermophysical property, such as density ratio, viscosity ratio, thermal conductivity ratio, and specific heat capacity ratio. The blue color line represented experimental data, while the pink line represented ANN model-predicted data. Fig. 5 (a) to (d) show a good agreement between the experimental and ANN model-predicted data.

3.2 Evaluation of RSM model performance

In the RSM technique, the 3D surface fitting method was used to develop the mathematical model to predict

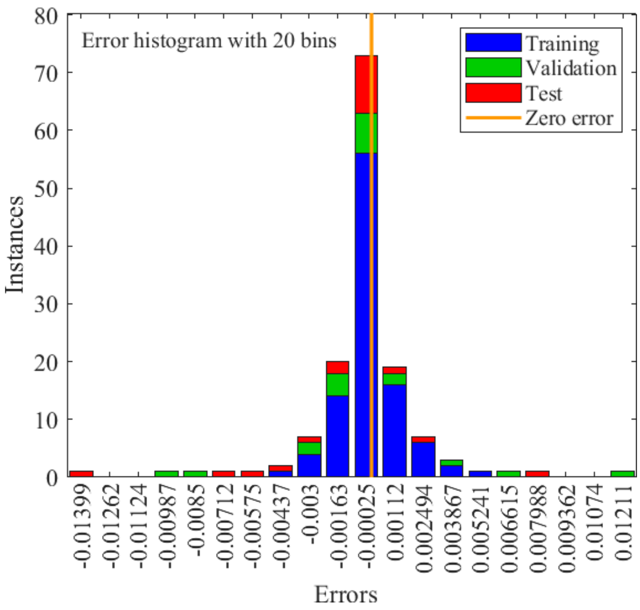

Fig. 4 Error histogram of proposed ANN architecture

the thermophysical properties of nanofluids. The input parameters are volume concentration, temperature, and experimentally measured data. The curve-fitting application in MATLAB [39] was used to develop surface fitting based on input parameters. In this surface-fitting process using polynomial regression to create a mathematical model, the best-fitting polynomial equation is obtained by varying the order of the polynomial equation. The accuracy of the model is evaluated based on MSE and R-squared values. Table 2 presents a mathematical correlation with goodness of fit obtained by RSM for predicting the thermophysical properties of GNP-EG/water nanofluids. These mathematical correlations relate the properties to two variables: volume concentration (φ) and temperature (T). The first equation in Table 2 represents the correlation for the density ratio of GNP/EG nanofluids, with a root mean square error (RMSE) of 0.0014 and a coefficient of determination (R^2) of 1. The second equation in Table 2 corresponds to the viscosity ratio, with an RMSE of 0.0091 and R^2 of 0.9997. The third equation in Table 2 provides the correlation for the thermal conductivity ratio, yielding an RMSE of 0.0074 and R^2 of 0.9895. The fourth equation in Table 2 models the specific heat ratio, with an RMSE of 0.0171 and R^2 of 0.9459. These models are accurate within specific operating conditions. The applicability of the equations in Table 2 is limited to a volume concentration range of 0.1% to 0.5% and a temperature range of −15 °C to 15 °C. Fig. 6 (a) to (d) shows the 3D surface fitting diagram of the thermophysical properties of GNP nanofluids and corresponding residual plots. From Fig. 6 (a) to (d), it was observed that all experimental data points were well-fitted on the surface plot. Consequently, the residual error ranges are 0.5×10^{-5} to 10×10^{-5} for density ratio, −0.01 to 0.01 for viscosity ratio, -4×10^{-3} to 2×10^{-3} for thermal conductivity ratio, and −0.01 to 0.01 for specific heat ratio. It shows the prediction accuracy of these mathematical models. Fig. 7 (a) to (d) represents the accordance between the experimental data and proposed RSM model-predicted data concerning the input parameters such as volume concentration and temperature. The horizontal axis represents the data samples of each thermophysical property, and the vertical axis indicates the thermophysical property, such as density ratio, viscosity ratio, thermal conductivity ratio, and specific heat capacity ratio, respectively. The blue color line indicated experimental data, and the brown color line indicated RSM model predicted data. From Fig. 7 (a) to (d), it is observed that there is good agreement between the experimental and ANN model-predicted data.

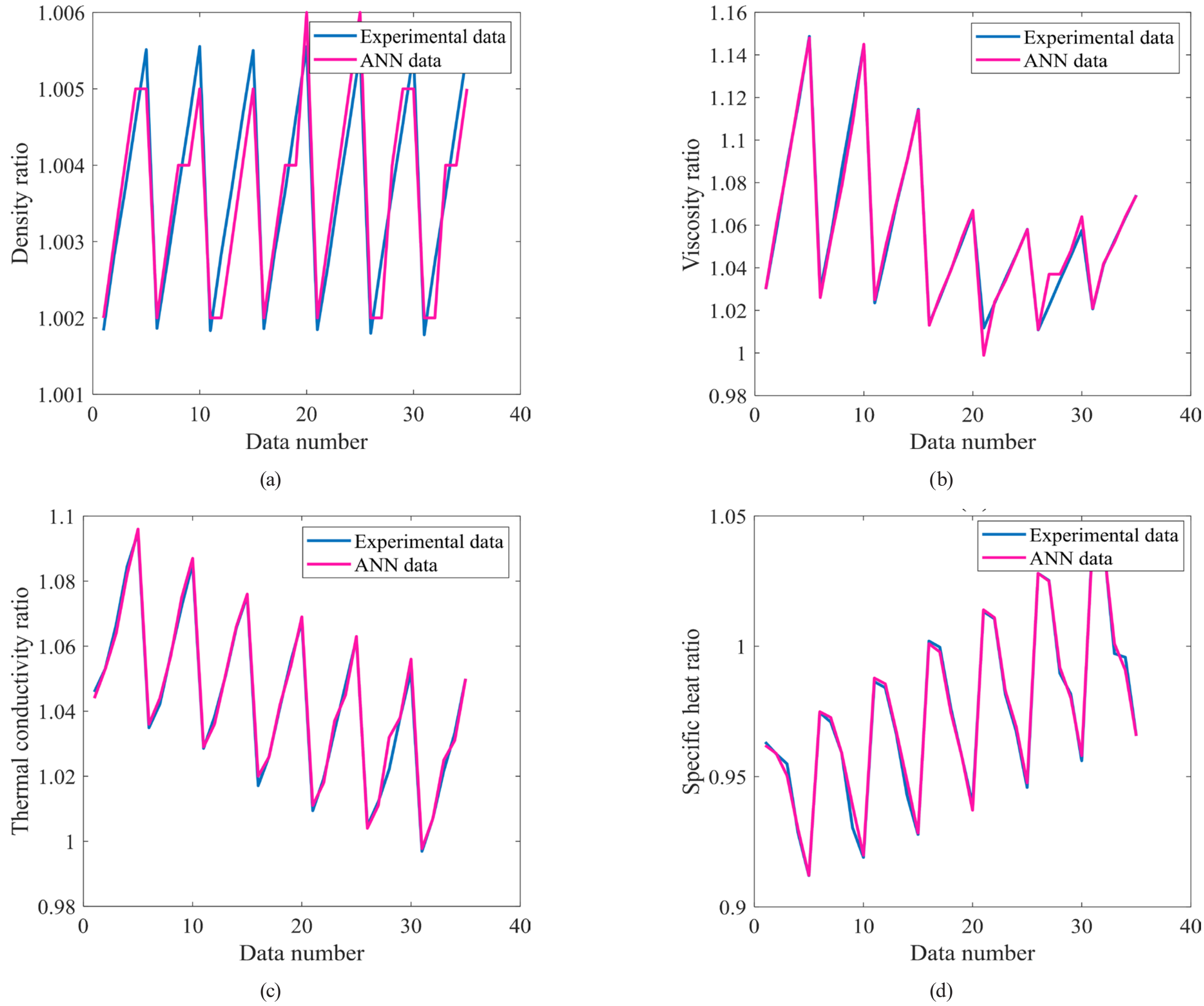

Fig. 5 Comparison of the data obtained by the ANN model and experimental data; (a) Relationship between data number and density ratio; (b) Relationship between data number and viscosity ratio; (c) Relationship between data number and thermal conductivity ratio; (d) Relationship between data number and specific heat ratio

Table 2 Mathematical model obtained by RSM for predicting nanofluid thermophysical properties

Equation No.	Mathematical model	RMSE	R^2
1.	$\frac{\rho_{nf}}{\rho_{bf}} = 1.0037 - 0.0001\varphi + 0.0013T$	0.0014	1
2.	$\frac{\mu_{nf}}{\mu_{bf}} = 1.0471 - 0.0366\varphi + 0.0224T + 0.111\varphi^2 - 0.0100\varphi T - 0.0003T^2 + 0.0112\varphi^3 + 0.0041\varphi^2 T - 0.0008\varphi T^2 + 0.0003T^3$	0.0091	0.9997
3.	$\frac{k_{nf}}{k_{bf}} = 1.0405 - 0.0162\varphi + 0.0184T + 0.0014\varphi^2 + 0.0014T^2$	0.0074	0.9895
4.	$\frac{(C_p)_{nf}}{(C_p)_{bf}} = 0.9770 + 0.0223\varphi - 0.0241T + 0.0011\varphi^2 - 0.0030\varphi T - 0.0041T^2$	0.0171	0.9459

The explanations of the symbols used in Table 2 are as follows:

$\frac{\rho_{nf}}{\rho_{bf}}$: Density ratio; $\frac{\mu_{nf}}{\mu_{bf}}$: Viscosity ratio; $\frac{k_{nf}}{k_{bf}}$: Thermal conductivity ratio; $\frac{(C_p)_{nf}}{(C_p)_{bf}}$: Specific heat ratio; bf: base fluid; nf: nano fluid

3.3 Evaluation of error percentages of prediction models

Figs. 8 and 9 reveal that the error ranges between the predictions and experimental data in the ANN and RSM models. The error percentage was computed using Eq. (6). In Figs. 8 and 9, the horizontal axis indicates the number of data points, and the vertical axis represents the error percentages. Furthermore, the blue, orange, yellow, and

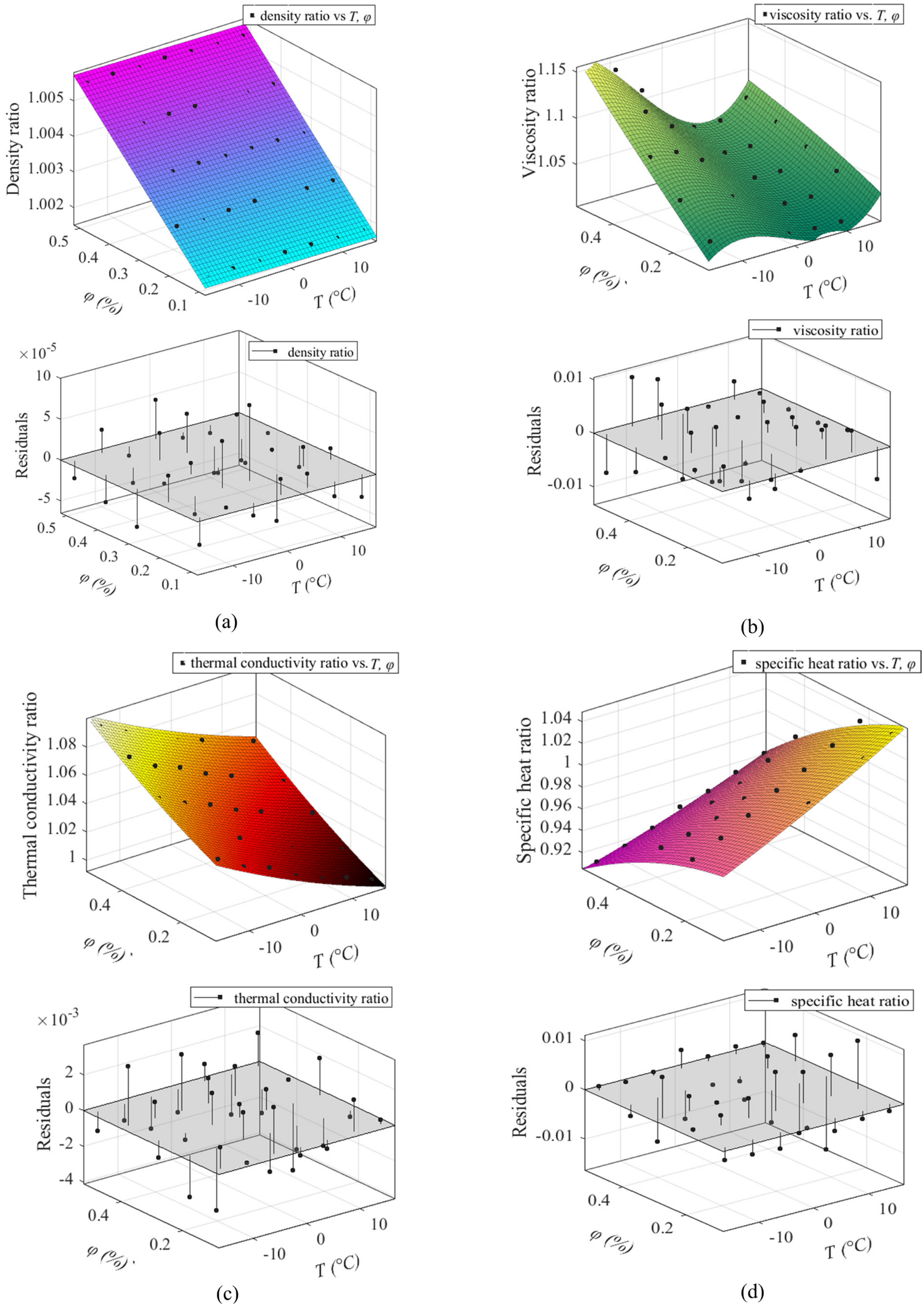

Fig. 6 3D surface fit diagram with residual plot for: (a) density ratio, (b)viscosity ratio, (c) thermal conductivity ratio, (d) specific heat ratio

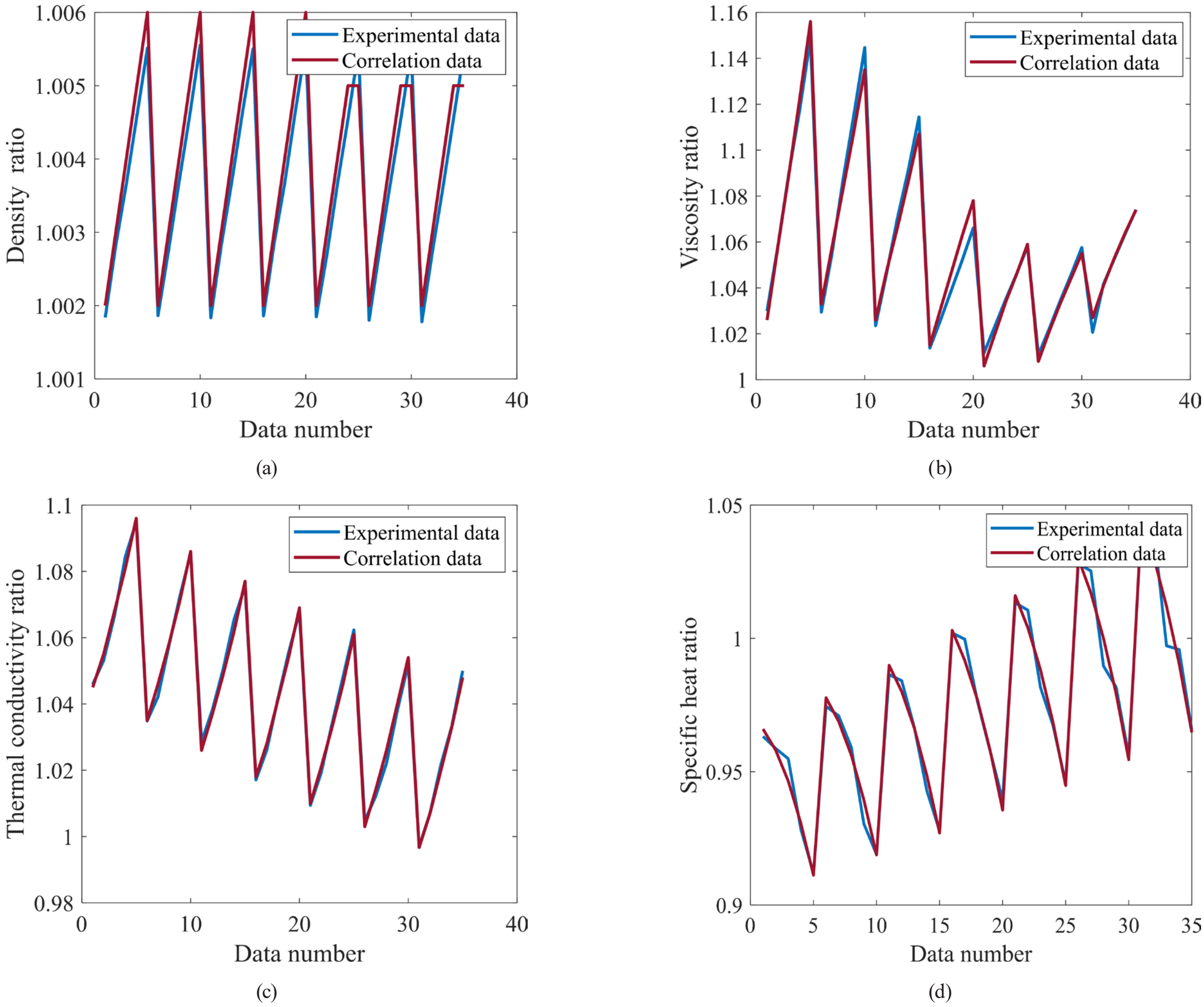

Fig. 7 Comparison of the data obtained by the RSM model and experimental data; (a) Relationship between data number and density ratio; (b) Relationship between data number and viscosity ratio; (c) Relationship between data number and thermal conductivity ratio; (d) Relationship between data number and specific heat ratio

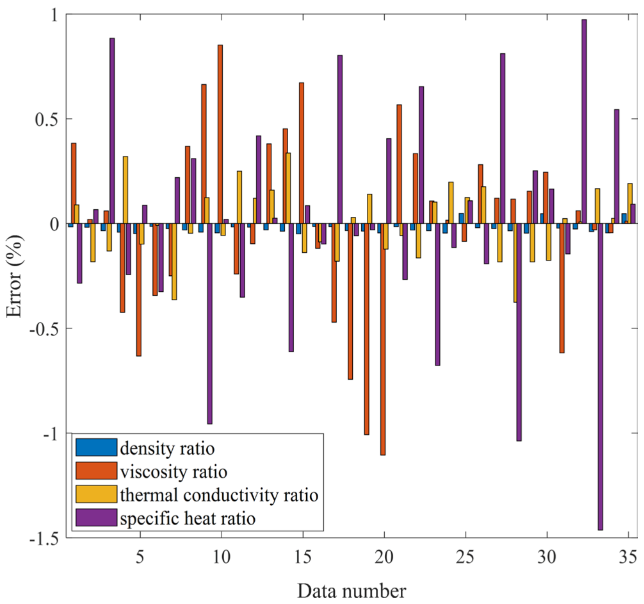

Fig. 8 Percentage of error for ANN predicted data

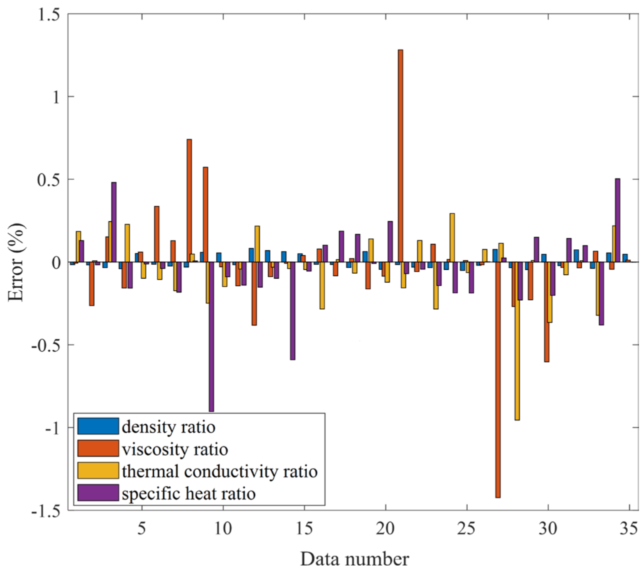

Fig. 9 Percentage of error for RSM model predicted data

purple colors denote the error ranges of ANN and RSM predictions. From Fig. 8, it was observed that the ANN model predictions error ranges were −0.05 to 0.082% for density ratio, −1.42 to 1.28% for viscosity ratio, −0.95 to 0.29% for thermal conductivity ratio, and −0.90 to 0.48 for specific heat ratio. Similarly, Fig. 9 shows that the RSM model prediction error ranges were −0.049 to 0.048% for density ratio, −1.105 to 0.85% for viscosity ratio, −0.33 to 0.36 for thermal conductivity ratio, and 1.46 to 0.97 for specific heat ratio, respectively. Based on these results, the ANN model had an error range of −1.42 to 1.28% for predicting the thermophysical properties of the GNP-EG/water nanofluid, and the RSM model had an error range of −1.46 to 0.97. Therefore, the error percentage of both prediction models is less than 1.5%, which is the acceptable range for predicting the thermophysical properties ratio of the GNP-EG/water nanofluids.

4 Conclusion

In this study, both ANN and RSM models are proposed for predicting the thermophysical property ratio of GNP-EG/water nanofluids. The input and output parameters of these models are volume concentration, temperature, and thermophysical property ratios. The following significant outcomes were derived from these prediction models:

- The implementation of the ANN and RSM techniques was successful for predicting the thermophysical properties ratio of GNP-EG/water nanofluids.
- The best ANN architecture achieved with 9 neurons in the hidden layer. The ANN technique was accurate enough that the MSE and R^2 values for GNP-EG/water nanofluids were 2.1239×10^{-5} and 0.998, respectively. The error reported is less than 1.5%.
- The RSM model yielded MSE and R^2 values of 0.761 and above 0.945, respectively. The percentage of error was below 1.5%.
- The error for both ANN and RSM techniques are below 1.5%. This is in close agreement with the predictions and actual experiments. In conclusion, both models outperformed each other in predicting the thermophysical properties ratio of GNP-EG/water nanofluids.
- As a result, both ANN and RSM models are recommended for researchers to predict the thermophysical properties of GNP-EG/water nanofluids used in heat transfer applications.

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