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Prediction of nanofluid viscosity using multilayer perceptron and Gaussian process regression

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Abstract
More than a decade, a numerous experimental and theoretical studies of thermophysical properties of nanofluids are conducted to reveal its heat transfer characteristics. Due to nanofluid unique thermal properties, it is broadly used in various applications from automobile applications to biomedical applications. Despite that various experimental and theoretical studies of nanofluids are developed, the accordance between them is very little and also it is tiresome and expensive. To predict the thermal properties in an easy way, soft computing tools are utilized. In this research work, dynamic viscosity ratio of Al_2O_3/H_2O is predicted using machine learning techniques like multilayer perceptron and Gaussian process regression. In the proposed multilayer perceptron—artificial neural network model, varying a range of neurons in the hidden layer and using Levenberg–Marquardt as training function, it is found that 6 neurons in the hidden layer give less root mean square error value of 0.01118. Different kernel functions are opted to train the proposed Gaussian process regression model, and it is found that Matern kernel function shows the best performance with less root mean square error value of 0.018, and regression coefficient value of both the models is 0.99. This research work will reduce the experimental test run cost, and the models are accurate in prediction.

Keywords Nanofluids · Temperature · Artificial neural network · Multilayer perceptron · Gaussian process regression

List of symbols

GPR	Gaussian process regression
DVR	Dynamic viscosity ratio
MLP	Multilayer perceptron
ANN	Artificial neural network
H_2O	Water
Al_2O_3	Alumina oxide
RMSE	Root mean square error
NMSE	Normalized mean square error
MAPE	Mean absolute percentage error
R^2	Regression coefficient value
MSE	Mean squared error
MAE	Mean absolute error
μ_p	Dynamic viscosity ratio of predicted data
μ_a	Dynamic viscosity ratio of experimental data
$\bar{\mu}_a$	Mean value of dynamic viscosity ratio of experimental data
n	Total number of data samples
T	Temperature (K)
ϕ	Volume fraction
D	Size of nanoparticle (nm)
σ	Standard deviation

Introduction

The exemplary growth in various fields by the nanofluids is because of its unique thermophysical properties. The most important properties of nanofluids are thermal conductivity, viscosity, specific heat, density, convective heat transfer and pressure drop. There are many dependent factors like volume fraction, dimensions of nanoparticle, shape of the nanoparticle, temperature that influence to determine the thermophysical properties of nanofluids. High enhancement of thermal conductivity and Newtonian behavior with good stability made nanofluids as best fluid in cooling technology stated by Das et al. [1].

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The applications of nanofluids are broader from automobile sector to cancer therapy affirmed by Mukesh et al. [2]. Adelekan et al. [3] extensively studied about TiO_2 nanofluids and concluded that TiO_2-based nanolubricants play a vital role in domestic refrigerator. Karen cacua et al. [4] stated that there is an enhancement of thermal conductivity in nanofluids compared with conventional base fluids, namely water, ethylene glycol and engine oil, and revealed that temperature plays an important role in increasing thermal conductivity of nanofluids and high temperature conditions are significant in cooling applications. Farhad and Jalali [5] experimented using copper oxide–thermal oil (CuO–HTO) nanofluid in inclined circular tube and revealed that enhancement of convective heat transfer is more than pressure drop by the nanofluid with 1.5% of nanoparticle volume fraction and 387 as Prandtl number in an inclined angle of 30 °C.

Keshteli and Sheikholeslami [6] revealed that combination of the nanoparticles and fin has shown significant improvement in the rate of solidification. Barewar et al. [7] have studied extensively about thermophysical properties of ZnO nanofluids, and further, the author customized the nanofluids by adding Ag nanoparticle and compared both the ZnO nanofluid and Ag/ZnO hybrid nanofluids. The author observed that thermal enhancement is higher in the hybrid nanofluid than in the normal nanofluid. Convective heat transfer rate of two different nanofluids in different materials like copper, aluminum and stainless steel is experimentally investigated by the authors Solangi et al. [8], and they stated that tube made up of copper has shown significant thermal conductivity than aluminum and stainless steel.

Theoretical analyses, mathematical models and experimental test runs were developed to analyze the physical properties of nanofluids. Theoretical models to predict viscosity are developed first by Einstein [9], and further improvement is made by [10, 11], using particle volume fraction viscosity model developed by [12, 13]. Several theoretical models using temperature as dependant variable are developed by [14–16]. Classical models and models derived from classical models to predict the viscosity of nanofluids are studied by Mukesh et al. [17], and they further stated that various theoretical formula found are fair in accuracy and discrepancies exist between experimental results and theoretical model results.

Artificial intelligence techniques are highly supported to model complex systems of high nonlinearity. Among the techniques, knowledge discovery of data (KDD) is used to extract the hidden pattern knowledge from large dataset. KDD can be implemented using soft computing tools. It is mainly for accurate estimations with ease; many machine learning algorithms like linear regression, multivariate linear regression, multilayer perceptron neural network with back propagation, support vector regression, Gaussian process regression are utilized for accurate prediction.

To predict the thermophysical properties of nanofluids accurately, various researchers opted artificial intelligence techniques. [18, 19] used single-walled and multiwalled carbon nanotubes to predict the thermal behavior of nanofluids using artificial neural network and revealed that the prediction is accurate and possesses good agreement with the experimental data. Predictions of thermophysical properties of metallic oxides are determined by Longo et al. [20] using artificial neural network. Feedforward structure of neural network is modeled by Vaferi [21] to predict the thermal behavior of nanofluids. Esfe and Kamyab [22] stated that raise in temperature decreases the viscosity of the nanofluids.

Multilayer perceptron with feedforward propagation method is modeled by Ebrahim [23] to predict the thermal behavior of various metallic oxides, and they stated the prediction by the proposed model is accurate. To predict the thermal conductivity of magnetic nanofluid Fe_3O_4, Afrand et al. [24] designed an optimal artificial neural network model and affirmed that the proposed model is accurate in prediction. Ali aminan [25] designed cascade forward neural network model to predict effective thermal conductivity of different nanofluids and revealed that model proposed for prediction possesses good accordance with experimental data.

Fuzzy C-Means adaptive neuro-fuzzy inference system (ANFIS) with probabilistic neural network model is designed by Adewale et al. [26], and fuzzy logic expert system is modeled by Khairul et al. [27] to analyze and predict the heat transfer coefficient of CuO/H_2O nanofluids. Dinesh et al. [28] studied the correlation between dependent variables and independent variables using response surface methodology (RSM) and Grey relational analysis (GRA) for prediction of thermal properties of nanofluids.

Salehi et al. [29], modeled an ANN and optimized the model using genetic algorithm (GA) for Ag/H_2O nonofluids, and the author found the prediction by the model is accurate. Two different machine learning techniques, namely ANN methodology and SVR methods, are used for prediction of thermophysical properties of nanofluids by Ibrahim et al. [30], and further, the author stated that SVR method is exceptional in prediction. Kavitha and Mukesh Kumar [31] developed models using machine learning techniques, namely MLP and SVR, to predict the thermal conductivity ratio of CNT/H_2O nanofluids and reported that SVR model is suitable for prediction than MLP for limited data sets.

From the literature review, it seems that a Gaussian process regression methodology to predict the thermal behavior of nanofluids is not extensively studied. Hence, in this research paper, in addition to MLP–ANN model, Gaussian process regression method (GPR) has been used to predict the thermophysical property such as viscosity in terms of dynamic viscosity ratio of $Al2O3/H_2O$ nanofluids.

Temperature and volume fraction are used to predict the viscosity of nanofluids. Due to the limitation of MLP model like overfitting, GPR methods with cross-validation are introduced and possess better generalization than MLP model. The results obtained by the proposed model have good accordance with the experimental data.

Methodology

MLP–ANN model

Artificial neural networks acquire knowledge by learning the historical data and are capable of accurate prediction of the future outcome. Feedforward with back propagation, feedbackward, cascade—forward with back propagation, layered recurrent, generalized regression, radial basis function and self-organizing map are the types of networks in artificial neural networks. MLP is a machine learning approach. It is one of the network categories of artificial neural network called as feedforward network. It uses the supervised learning and training algorithm. In this research, a model of multilayer perceptron with back propagation is developed, general schematic of MLP–ANN is input layer comprising of the input variables, and it may consist of one or more hidden layers, and output layer comprising the output variable. The MLP–ANN trains the network, and the errors are backpropagated to adjust the masses and biases to obtain the desired output with minimum error.

Several researchers developed MLP—ANN model to predict the thermal properties of nanofluid and stated the accordance between the predicted data and experimental data is excellent. The dependent factors to influence the viscosity of nanofluids are studied by few researchers. Kulkarini et al. [32] revealed the decrease in viscosity and increase in temperature. Masoumi et al. [33] asserted that viscosity of nanofluids depends upon size of the nanoparticle, particle concentration and density of nanoparticle; in addition, viscosity of base fluid needs to be considered stated by Zhao et al. [34]. Juneja and Gangacharyulu [35] experimentally studied that most important parameter to determine the viscosity is temperature and volume fraction. Increase in volume fraction in turn will increase the relative viscosity stated by Tavman et al. [36]. Shape of the nanoparticle influences the enhancement in viscosity affirmed by Srivastava [37]. Qui et al. [38] revealed that increase in temperature in the nanofluids in turn increases the intermolecular distance between the nanoparticles and results in decrease in dynamic viscosity values. Further, the author observed that drag effect of nanofluids increases with nanoparticle volume fraction values which in turn increase the dynamic viscosity values of nanofluids.

The log-sigmoid and tan-sigmoid are transfer function used in multilayer perceptron neural network. Log-sigmoid helps the network to relate the predictor and response variables with any complexity. The value of 'x' ranges between 0 and 1. In tan-sigmoid, the value of x is between -1 and $+1$.

Equations (1)–(3) represent the mathematical formulation of transfer functions used in the MLP-NN model.

$$\text{Logsig}(x) = 1/(1 - \exp(-x)) \tag{1}$$

$$\text{Tansig}(x) = 2/(1 + \exp(-2x)) - 1 \tag{2}$$

$$\text{Purelin}(x) = x \tag{3}$$

Training algorithms are applied to train the networks; the selection of the training algorithms depends upon the selected inputs. Few training functions are gradient descent gradient descent with momentum, Bayesian regularization, scaled conjugate gradient and Levenberg–Marquardt; among these algorithms, Levenberg–Marquardt training is comparatively accurate with less elapsed time and will utilize more memory space than any other algorithms. In the proposed MLP–ANN model, temperature and volume fraction are taken as predictor variables and dynamic viscosity ratio is the response variable; it is represented in Fig. 1.

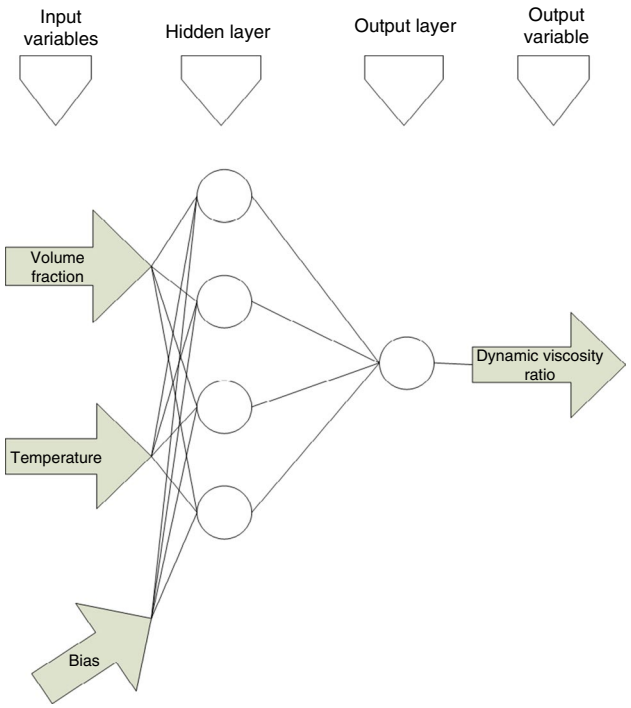

Fig. 1 Representation of proposed MLP–ANN Model

The proposed MLP—artificial neural network model, the input layer, which comprises of explanatory variables, temperature (T in K) and volume fraction (ϕ), the hidden layer where the number of neurons and mass between neurons are adjusted to get the desired output and the output layer, consists of response variable, dynamic viscosity ratio of Al_2O_3/H_2O.

In MLP–ANN model, the input data are partitioned as 70% for training and 15% each for test and validation phase; training functions are compared among themselves and Levenberg–Marquardt algorithm is chosen as training function, and in the same way activation function is compared and Tansig function has been chosen. Numbers of neurons are initially set in the hidden layer, and the performance of the model is validated by the evaluation criteria, root mean square error (RMSE) is the point of reference, till the value of RMSE is less, the numbers of neurons in the hidden layer are adjusted and the model is trained to give the best performance; the flow of the MLP–ANN model is shown in Fig. 2.

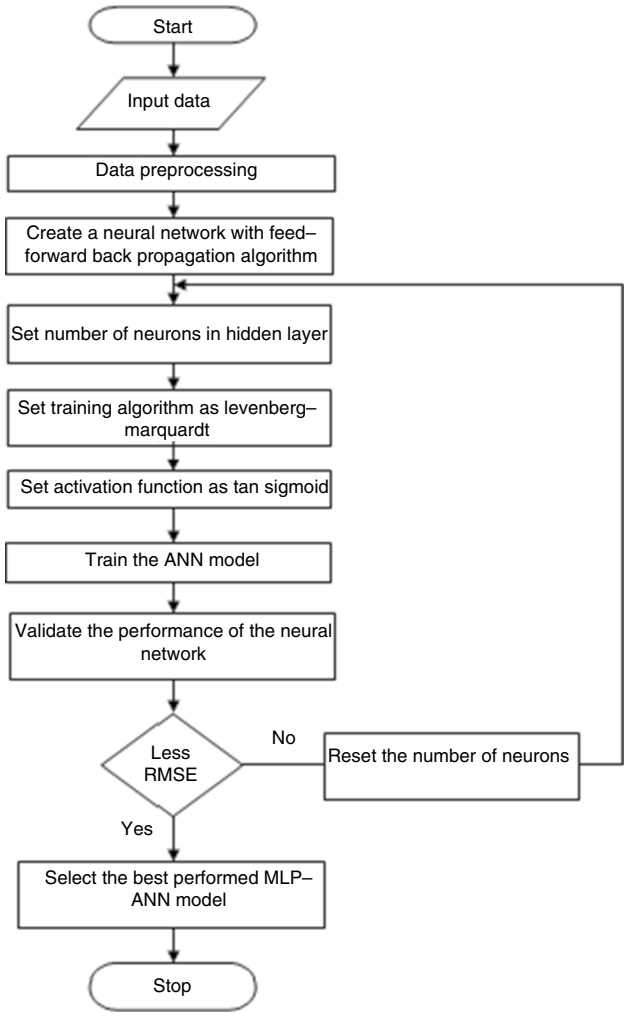

Fig. 2 Flow diagram of the proposed MLP–ANN

GPR model

A Gaussian process is like an infinite-dimensional multivariate Gaussian distribution; it defines a distribution over functions, $p(f)$, where f is a function mapping some input space χ to $\mathfrak{R}$ denoted in Eq. (4).

$$f : \chi \to \mathfrak{R} \tag{4}$$

Gaussian processes (GPs) are parameterized by a mean function, $m(x)$ and a covariance function, $k(x, x')$ is mentioned in Eq. (5).

$$f(x) \sim \mathrm{GP}\big(m(x), k(x, x')\big) \tag{5}$$

Gaussian noise, $\epsilon - N(0, \sigma^2)$, now the Gaussian process with noisy function is denoted by Eq. (6).

$$y \sim \mathrm{GP}\big(m(x), k(x, x') + \delta ij\sigma_{\mathrm{n}}^2\big) \tag{6}$$

Gaussian process regression is nonparametric that is not limited by a functional form and used to calculate the probability distribution of parameters of a specific function. GPR is derived from Bayesian linear regression and calculates the probability distribution over all permissible functions that fit all the data points. Gaussian process regression (GPR) predicts the output data accurately with minimum error value stated by Rasmussen [39].

Kernel functions in Gaussian process regression are exponential function, squared exponential function, rational quadratic and Matern class of covariance function; the mathematical formulation is given in Eqs. (7)–(12), respectively.

$$\text{Exponential} = \exp\left(-\frac{r}{l}\right) \tag{7}$$

$$k_{\mathrm{SE}}(r) = \exp\left(-\frac{r^2}{2l^2}\right) \tag{8}$$

$$k_{\mathrm{RQ}}(r) = \left(1 + \frac{r^2}{2\alpha l^2}\right)^{-\alpha} \tag{9}$$

$$\text{Matern} = \frac{1}{2^{\nu-1}\Gamma(\nu)}\left(\frac{\sqrt{2\nu}}{l}r\right)^{\nu} K_{\nu}\left(\frac{\sqrt{2\nu}}{l}r\right) \tag{10}$$

$$k_{\nu=3/2}(r) = \left(1 + \frac{\sqrt{3r}}{l}\right)\exp\left(-\frac{\sqrt{3r}}{l}\right) \tag{11}$$

$$k_{v=5/2}(r) = \left(1 + \frac{\sqrt{5r}}{l} + \frac{5r^2}{3l^2}\right) \exp\left(-\frac{\sqrt{5r}}{l}\right) \tag{12}$$

where $\tilde{x} = \left(1, x_1, \ldots, x_d\right)^T$, $\tilde{x}$ is augumented input vector, r denotes $|x - x'|$, v is the positive integer.

In this research paper, we predicted the DVR of Al_2O_3/H_2O using the following kernel functions squared exponential function, rational quadratic and Matern class of kernel function; among this, Matern $v = 5/2$ shows the best accuracy; the illustration of the GPR model is shown in Fig. 3. The experimental data sets (106) comprise of temperature, volume fraction and one of the thermophysical properties of nanofluid named as viscosity its subclass dynamic viscosity ratio (DVR) of Al_2O_3/H_2O values. The first two are used as predictor variables to predict the response variable DVR of Al_2O_3/H_2O nanofluids.

In the proposed GPR model, to avoid overfitting of the trained model, the input data are partitioned by different numbers of folds using cross-validation method. The performance of the proposed model is evaluated by various criteria; the vital criterion is RMSE value. The data value predicted by the proposed model is compared with experimental values; both possess good accordance between the models.

Evaluation criteria

In this research paper, various evaluation criteria are used to evaluate the MLP–ANN and GPR model. The criterions are root mean square error (RMSE), regression coefficient value (R^2), mean absolute percentage error (MAPE), mean squared error (MSE), normalized mean square error (NMSE) and mean absolute error (MAE). The mathematical formulations of criterions are shown in Eqs. (13)–(18), respectively.

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\mu_a - \mu_p\right)^2} \tag{13}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(\mu_a - \mu_p\right)^2}{\sum_{i=1}^{n}\left(\mu_a - \bar{\mu}_a\right)^2} \tag{14}$$

$$\text{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{\mu_p - \mu_a}{\mu_a}\right| \times 100 \tag{15}$$

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(\mu_p - \mu_a\right)^2 \tag{16}$$

$$\text{NMSE} = \frac{\text{MSE}}{\text{var}\left(\mu_a\right)} \tag{17}$$

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|\mu_a - \mu_p\right| \tag{18}$$

where μ_p and μ_a denote dynamic viscosity of predicted data and experimental data, respectively, $\bar{\mu}_a$ is the mean value of dynamic viscosity of experimental data for 'n' data values, 'n' denotes the total number of data samples. These criteria values are used to compare the accordance between experimental values and predicted values.

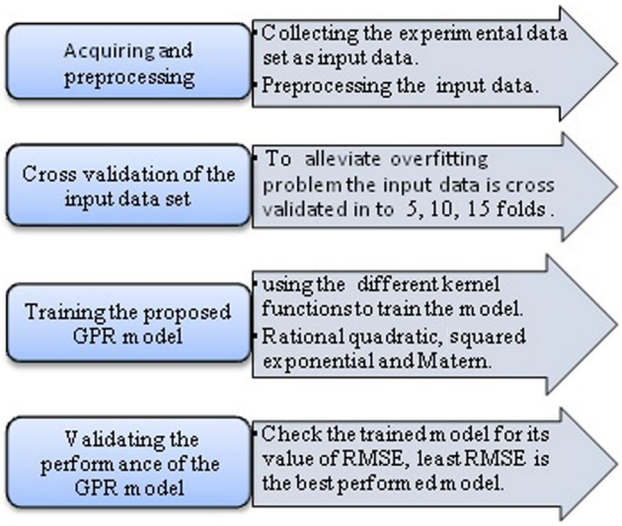

Fig. 3 Illustration of proposed GPR model

Results and discussion

The experimental data sets (106) used for training the MLP–ANN and GPR model have been taken from Alawi [40].

Prediction of DVR by MLP–ANN model

Generally in MLP–ANN model, the data sets split into three different sets to train the model namely training, testing and validation data sets and the percentage of data sets in each are 70, 15 and 15, respectively. In the proposed MLP–ANN, the experimental data sets of 106 samples are taken, and it is split into 74, 16 and 16 data samples in training, testing and validation data sets, respectively. The proposed model is modeled by varying neurons in the hidden layer. Various training functions are applied in the model; they are scale conjugate gradient, gradient descent and Levenberg–Marquardt training functions; among all LM shows the best fit; it is shown in Table 1

Table 1 MLP–ANN model performance with different training functions

Training functions	Performance	Performance		
		Training	Validation	Testing
Scaled conjugate gradient	0.0055	0.0043	0.0061	0.0107
Gradient descent	0.0223	0.0205	0.0291	0.0240
Levenberg–Marquardt	0.000171	0.00018	0.0000964	0.0001

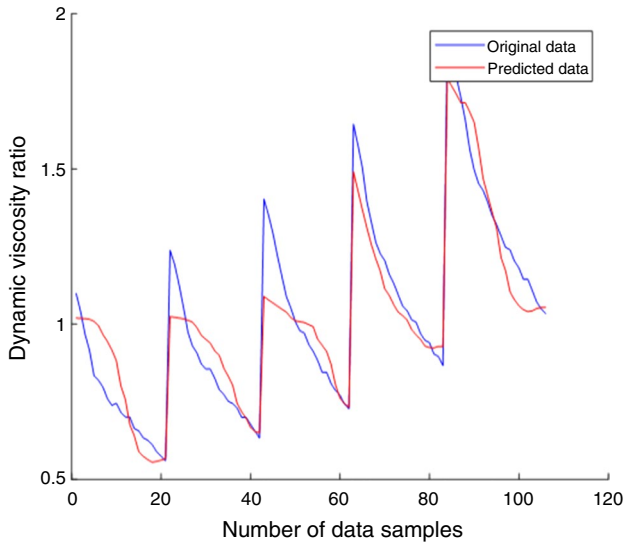

Fig. 4 Prediction of DVR using SCG

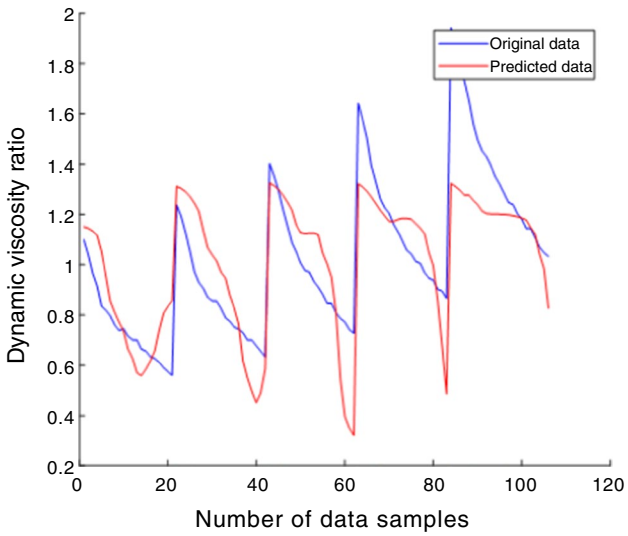

Fig. 5 Prediction of DVR using GD

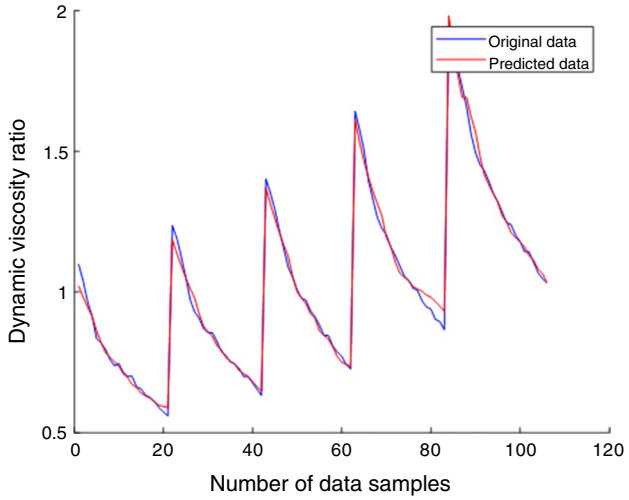

Fig. 6 Prediction of DVR using LM

Table 2 MLP–ANN model with a range of hidden neurons

Number of neurons	MSE	RMSE	R^2	MAE	NMSE	MAPE
5	0.00023	0.01530	0.9972	0.0270	0.00023	0.0626
6	**0.00013**	**0.01118**	**0.9992**	**0.0093**	**0.00012**	**0.04833**
7	0.00033	0.01811	0.9992	0.0166	0.00032	0.07361
8	0.00054	0.02326	0.9987	0.0112	0.00052	0.20496
9	0.00064	0.02532	0.9973	0.0093	0.00062	0.00272
10	0.00023	0.01500	0.9982	0.0092	0.00022	0.10809

Number of neurons in the hidden layer of MLP-ANN model is varied. Six neurons in the hidden layer has shown least MSE values compared with other number of neurons and it is highlighted and has shown in Table 1.

and in Figs. 4–6 representing the accordance between the experimental values and predicted values of various training functions.

The performance of MLP network with a range of neurons in hidden layer is shown in Table 2. The initial masses are made as default random values in order to ensure all the training starts with same initial random masses in the hidden layer. The RMSE value in 6 neurons in the hidden layer is less compared with other range of

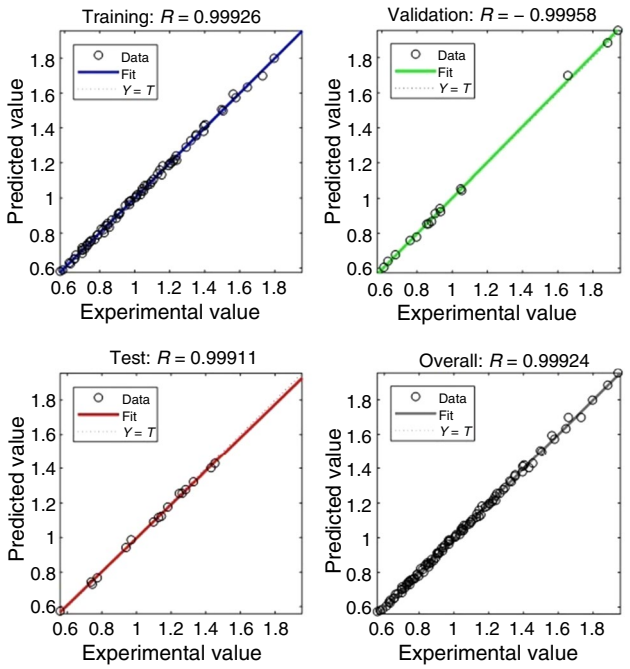

Fig. 7 Overall regression values for 6 hidden neurons

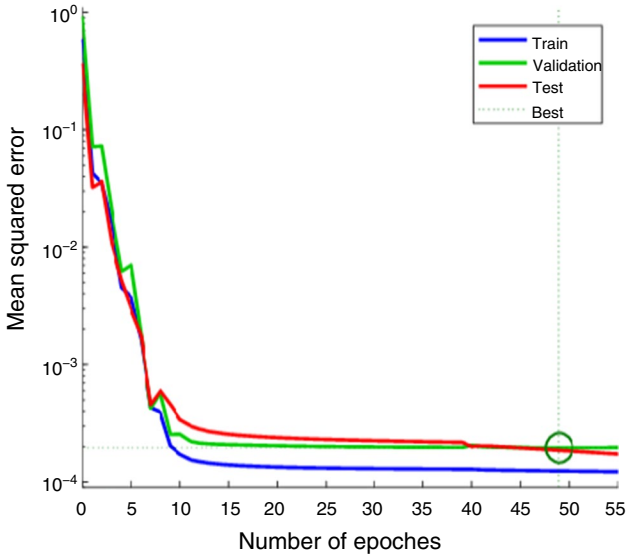

Fig. 8 Proposed MLP–ANN performance diagram

neurons, and the value is 0.01118. The regression diagram, best validation performance and error histogram with 6 neurons in the hidden layer are represented in Figs. 7–9, respectively.

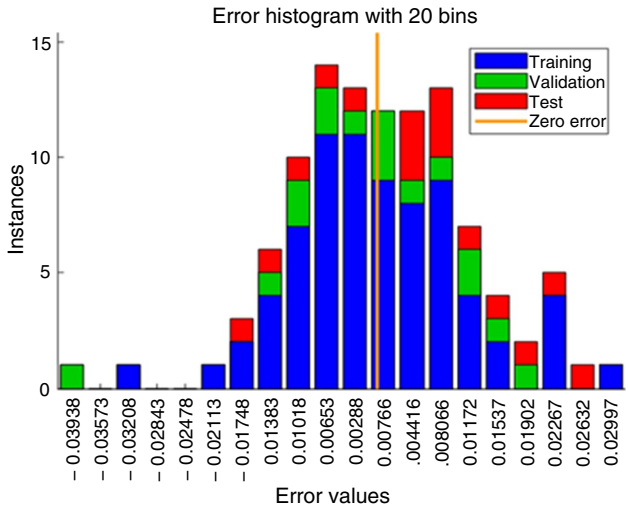

Fig. 9 Proposed MLP–ANN error diagram

Prediction of DVR by GPR method

The proposed Gaussian process regression model is trained with many covariance functions. Common covariance functions are exponential, γ-exponential, squared exponential, rational quadratic and Matern class of covariance with 'v' take the value as 5/2 and 3/2. In this proposed model, rational quadratic squared exponential and Matern class of covariance with 'v' as 5/2 value are used to train the model. Local optima and slow convergence of the trained model are safeguard by using cross-validation; it divides the dataset into number of folds like 5, 10, 15, and it is found that the data set with fold 10 gives less RMSE compared with other folds; it is shown in Tables 3–5.

In the prediction of DVR using covariance function of GPR, the Matern function gives less RMSE value when compared with other kernel functions, and at the same time, prediction speed and training time are optimal in squared exponential covariance function.

The agreement between the experimental data and the predicted data using Matern 5/2 kernel function is good, and it is shown in Fig. 10 and it is more accurate in prediction; it is represented by the regression diagram shown in Fig. 11. Response diagram denotes the closeness between the experimental and predicted values; it is shown in Fig. 12 and the error diagram shows the deviation between the experimental and predicted values and it is shown in Fig. 13.

Table 3 Evaluation of kernel function with fivefold

Fivefold	MSE	RMSE	R^2	MAE	NMSE	MAPE
Rational quadratic	0.00042	0.0204	0.99	0.0148	0.00041	0.00749
Squared exponential	0.00044	0.0209	0.99	0.0154	0.00043	0.00765
Matern 5/2	0.00038	0.0193	0.99	0.0139	0.00036	0.00708

Table 4 Evaluation of kernel function with tenfold

Tenfold	MSE	RMSE	R^2	MAE	NMSE	MAPE
Rational quadratic	0.00038	0.01952	0.99	0.01490	0.00037	0.00711
Squared exponential	0.00041	0.02022	0.99	0.01541	0.00040	0.00745
Matern 5/2	0.00035	0.01871	0.99	0.01416	0.00034	0.00691

Table 5 Evaluation of kernel function with 15-fold

15-fold	MSE	RMSE	R^2	MAE	NMSE	MAPE
Rational quadratic	0.00049	0.02207	0.99	0.01568	0.00047	0.00740
Squared exponential	0.00052	0.02271	0.99	0.01653	0.00050	0.00758
Matern 5/2	0.00045	0.02114	0.99	0.01492	0.00043	0.00710

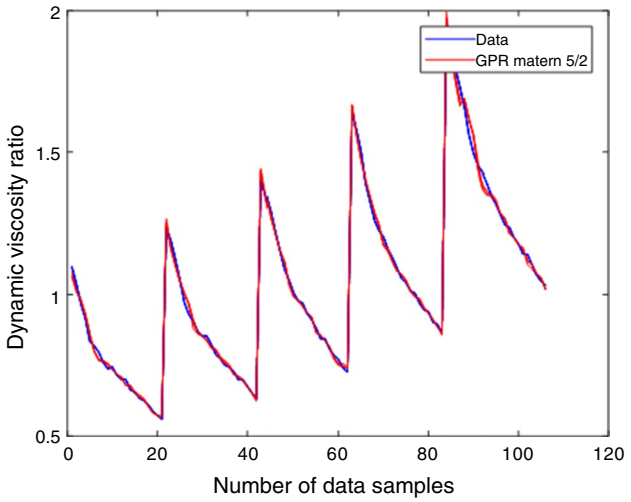

Fig. 10 Prediction of DVR using GPR—Matern Kernel function with $v = 5/2$ value

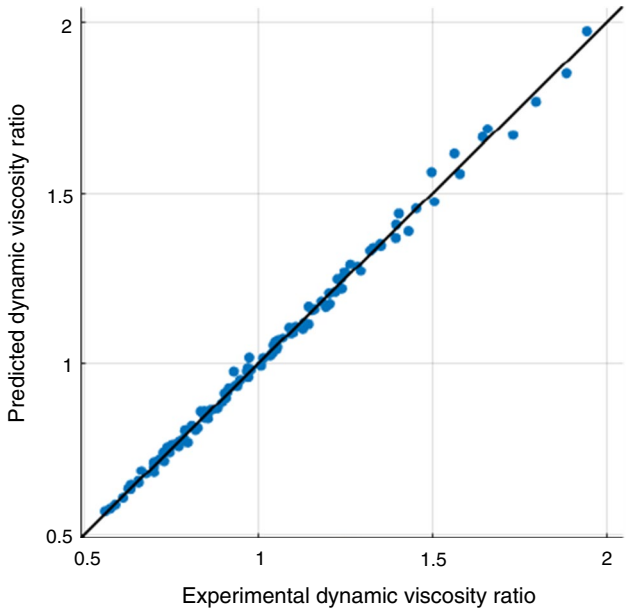

Fig. 11 Regression diagram of GPR—Matern Kernel

Significance of predictor variables in prediction of DVR

Correlation between volume fraction, temperature and dynamic viscosity ratio

The finest values of volume fraction and temperature are 0.04 and 310 K, respectively. Increase in volume fraction and decrease in temperature enhance the dynamic viscosity ratio of Al_2O_3/H_2O nanofluids. It is found that increase in volume fraction from 0.01 to 0.05 increases the DVR by 0.6 values. In Fig. 14, it denotes that high value of volume with low value of temperature gives high value of dynamic viscosity ratio. The effectiveness of predictor variable, temperature in prediction of DVR, is shown in Fig. 15. With low value of temperature, it gives rise to dynamic viscosity ratio; in other words, if the temperature increases from 295 to 325 K, the DVR reduces to 0.3 values.

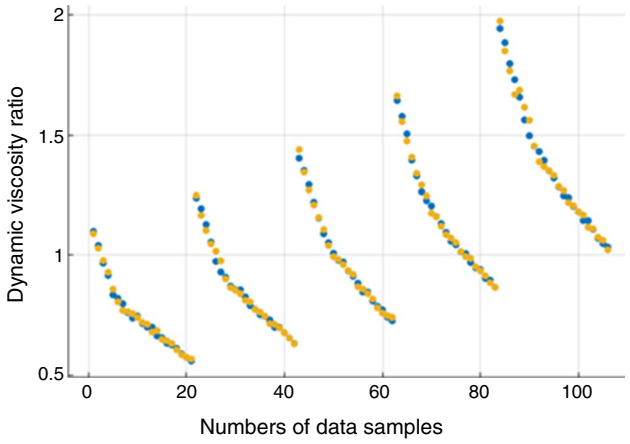

Fig. 12 Response diagram of GPR—Matern Kernel

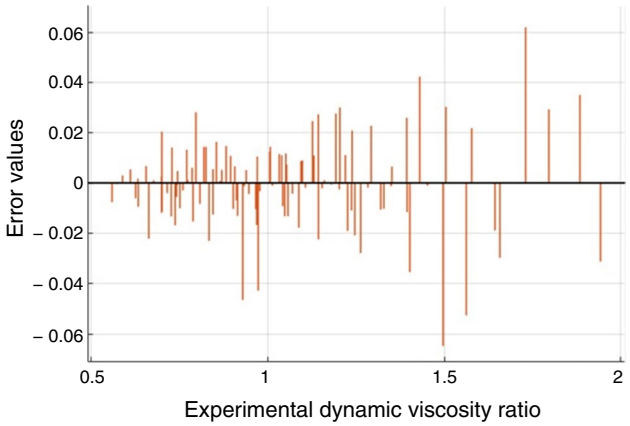

Fig. 13 Error diagram of GPR—Matern Kernel

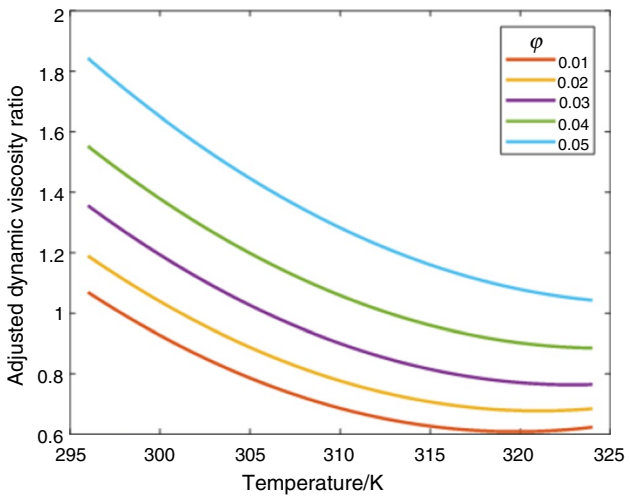

Fig. 14 Effect of volume fraction in prediction of DVR

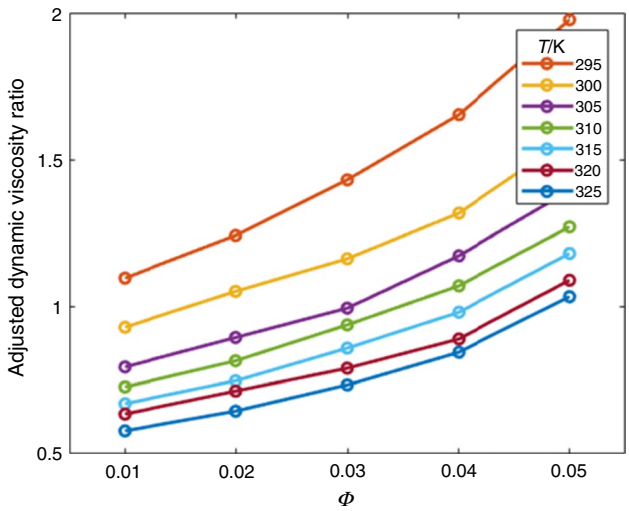

Fig. 15 Effect of temperature in prediction of DVR

Conclusions

One of the major thermophysical properties of nanofluids is viscosity. Dynamic viscosity ratio is subclass of viscosity. Prediction of dynamic viscosity ratio of Al_2O_3/H_2O nanofluids is implemented by using machine learning techniques; in this research work, 106 experimental data sets are used to perform it. Temperature and volume fraction are used as predictor variables to predict the response variable dynamic viscosity ratio (DVR). The proposed models are MLP–ANN and GPR models. The MLP is modeled with a range of 6 neurons in the hidden layer using Levenberg–Marquardt as training function and tan-sigmoid as activation function; the performance is validated. Root mean square error value of 0.01118 and the regression coefficient value (R^2) for overall data are 0.99. With limited datasets, MLP–ANN may suffer with local optima and slow convergence problem; to evade it GPR methods are used to possess generalization ability even with limited datasets. GPR is modeled with different kernel functions, and it is found that Matern class kernel function with value = 5/2 exhibits accurate prediction of dynamic viscosity ratio with less RMSE value of 0.018, and the Regression coefficient value (R^2) is 0.99. This research work will ease the prediction of thermophysical properties of nanofluids, reduce the test run cost and is accurate in prediction.

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