



Research article

Regression analysis for thermal properties of Al₂O₃/H₂O nanofluid using machine learning techniquesP.C. Mukesh Kumar^{a,*}, R. Kavitha^b^a University College of Engineering, Dindigul, 624 622, Tamilnadu, India^b Parisutham Institute of Technology and Science, Thanjavur, 613 005, Tamilnadu, India

ARTICLE INFO

Keywords:

Computer science
 Mechanical engineering
 Nanotechnology
 Computing methodology
 Fluid mechanics
 Heat exchanger
 Heat transfer
 Gaussian process regression
 Viscosity
 Kernel function
 Predictor variable
 Thermal conductivity
 Nanofluids

ABSTRACT

Nanofluids possess higher thermal properties than the other conventional base fluids. Many investigators suggested that the nanofluids have the potential to apply in various engineering fields. In real time situation it is challenging to determine the thermal conductivity of nanofluids with accuracy as they have many depending factors. Moreover, numerous experimental tests are required to acquire the thermal conductivity of nanofluids accurately. In this research paper, thermal conductivity ratio and dynamic viscosity ratio of Al₂O₃/H₂O nanofluid are predicted accurately by using Gaussian Process Regression (GPR) methods. The input predictor variables used in this model are temperature, volume fraction and size of the nanoparticles. 222 experimental data sets are taken to predict the thermal conductivity ratio (TCR), dynamic viscosity ratio (DVR) and also the effectiveness of the predictor variables in predicting the response variables are extensively studied and found that the temperature is the crucial factor to enhance the thermal conductivity ratio. The proposed modeling is performed by using MATLAB software. The predictions were evaluated by various evaluation criterions. It is observed that an optimized Gaussian process regression (GPR) method with matern kernel function shows an accurate agreement with experimental data with Root Mean Square Error (RMSE) value of 0.000126 for TCR and squared exponential kernel function show good agreement with experimental data with Root Mean Square Error (RMSE) value of 0.000045 for DVR. Regression coefficient value (R²) is 0.99; nearer to one hence the predicted results are reliable.

1. Introduction

Diffusion of nano-sized particles, dimensions vary from 1 nm to 100 nm into base fluids like water, ethylene glycol, engine oil and transformer oil leads to the formation of nanofluids. Nanofluids possess high thermal and transport properties, due to its uniqueness in enhancing the thermal conductivity, it succeeded in various applications. The necessary dependent factors which help to enhance the thermal conductivity are temperature, volume fraction, size of the nanoparticle, shape of the nanoparticle, base fluid, and method of fabrication of nanoparticles [1]. Many researchers have experimentally studied to the factors which influence the thermal conductivity of nanofluids. Das et al. [2], Hojjat et al. [3], Vajjha et al. [4] and Tajik et al. [5] have clearly stated that increase in temperature raises the thermal conductivity of nanofluids. Importance of volume fraction in terms of increasing the thermal conductivity of nanofluids studied by Battira et al. [6], Tajik et al. [5] and Aminreza et al. [7] suggested that the temperature and volume fraction are the most vital factors to increase the thermal conductivity of nanofluids. M. Beck et al.

[8], Murshed et al. [9], Uddin et al. [10] and Reza et al. [11] tested and revealed that increase in size of nano particle increases the thermal conductivity of nanofluids.

Various researchers investigated the significance of dynamic viscosity for heat transfer coefficient, Masuda et al. [12], Putra et al [13] and Pak and Cho [14] experimentally studied that increase in particle concentration leads to increase the viscosity of nanofluids. Alawi et al. [15] through investigation found that increase in temperature and increase in size of the nano particle decreases the dynamic viscosity of nano fluid. Hemmat Esfe et al. [16] stated that decrease in the nano particle size will increase the viscosity. Alawi et al. [15] and Srivastava [17] discussed about the shape of the nano particle and its importance in the determination of dynamic viscosity of nanofluid. There are so many theoretical correlations and experiments were found and conducted to find the thermal conductivity and dynamic viscosity of nanofluid but there is very little accordance between them and it is tiresome. Data mining is an important process in knowledge discovery. Data mining techniques are used to extract the hidden pattern knowledge from large dataset. Data

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mining techniques can be performed using soft computational tool it is an effective one with machine learning algorithms for prediction with ease and accurate.

Machine learning system is the basic to artificial neural networks, fuzzy systems, simulated annealing, rough sets, and genetic algorithms to learn and predict the hidden patterns from the unstructured large data sets. Algorithms like linear regression (LR), multivariate linear and non linear regression (MLR and MNR), back propagation neural network (BP-NN), support vector regression (SVR) and the Gaussian process regression (GPR) methods are available in the machine learning techniques. Many researchers were used Multi layer perceptron Artificial Neural Network (MLP-ANN) with back propagation algorithm for prediction. Tahani et al. [18] proposed an ANN modeling to predict the thermal conductivity of nanofluids and the result is promising with the experimental values. Dalkilic et al [19] performed the prediction of dynamic viscosity by using ANN method. The enhancement in the heat transfer of a nanofluid depends mainly on different values of volume fraction stated by Arman Safdari et al. [20]. The effect of size of the nanoparticle and values of volume fraction in TiO₂ nanofluid studied by Hosseini et al. [21] and stated that, increase in volume fraction lead to increase in viscosity of nanofluid. Giovanni et al. [22], Ariana et al. [23] and Khosrojerdi et al. [24] used ANN methodology to predict the thermal conductivity of various nanofluids. Hemmat Esfe et al. [16] and Heidari et al. [25] predicted the viscosity of various nanofluids using ANN techniques.

Very few researchers used Support Vector Machine and Regression methods for prediction of thermal conductivity and viscosity of nanofluids. Zanty et al. [26] used support vector machine for classification, Support Vector Regression (SVR) is an non linear generalization algorithm using VC theory stated by Vapnik [27], Ibrahim et al. [28] predicted the thermal conductivity of nanofluid by using ANN and SVR method and concluded that SVR method has more accuracy than ANN method for prediction of thermal conductivity of nanofluids. Khairul et al. [29] studied experimentally the prediction of heat transfer coefficient and friction factor of CuO/H₂O nanofluid using fuzzy logic expert system. The temperature and volume fraction data were used to predict the thermal conductivity of nanofluids in most of the research works. From the literature review, it seems that a very little research work was done by using Gaussian process to predict the thermal conductivity and dynamic viscosity of nanofluids. Hence in this investigation, Gaussian Process Regression model (GPR) has been used to predict the thermal conductivity ratio and dynamic viscosity ratio of Al₂O₃/H₂O nanofluids. As an input data, predictor variables such as temperature, volume fraction and size of the nanoparticles are used. It is observed in this paper, the behavior of different kernel functions and the accuracy in prediction. In addition the effectiveness and interaction between the predictor variables were also studied. The proposed model is optimized with hyper parameters and compares the predicted data with the experimental data. There is a good accordance between the experimental values and predicted values by the GPR model.

2. Description of GPR model

A Gaussian process is a collection of random variables, any finite number of which has a joint Gaussian distribution. A Gaussian process is specified by its mean function and covariance function otherwise called as kernel function. It is represented mean function $m(x)$ and the kernel function $k(x, x')$ of a real process $f(x)$ in Eqs. (1), (2), and (3).

$$m(x) = E[f(x)] \tag{1}$$

$$k(x, x') = E[(f(x) - m(x))(f(x') - m(x'))] \tag{2}$$

$$f(x) \approx gp(m(x), k(x, x')) \tag{3}$$

Where $m(x)$ represents mean function, $k(x, x')$ denotes covariance function and (x, x') are random variables [30].

Rasmussen [30] reported GPR as given best performance in prediction when compared with Linear Regression (LR), Rigid Body Dynamics (RBD) and Locally Weighted Projection Regression (LWPR). Few authors [5, 23] discussed about the prediction of thermal conductivity of alumina water based nano fluids by using Multilayer Perceptron model (MLP-ANN) whereas in this research article, the prediction of thermal conductivity of Al₂O₃/H₂O modeled by Gaussian process regression methods because with limited data set, MLP-ANN suffers local optima and slow convergence. This limitation is overruled by GPR method. Hence in this paper GPR method is used for prediction. The objective of using Gaussian process Regression (GPR) is to predict the output data with minimum error value.

Kernel function is the important component in a Gaussian process. Kernel functions in Gaussian process regression are Exponential function, γ -Exponential function, Squared Exponential function, Rational Quadratic, Matern class of covariance function and Neural network function, the mathematical formulation are given in Eqs. (4), (5), (6), (7), (8), (9), (10), and (11) respectively. In this paper we used Squared Exponential function, Rational Quadratic, Matern $\nu = 5/2$ class of kernel function.

$$Exponential = \exp\left(-\frac{r}{\ell}\right) \tag{4}$$

$$\gamma - Exponential = \exp\left(\left(-\frac{r}{\ell}\right)^\gamma\right) \text{ for } 0 < \gamma \leq 2 \tag{5}$$

$$k_{SE}(r) = \exp\left(-\frac{r^2}{2\ell^2}\right) \tag{6}$$

$$k_{RQ}(r) = \left(1 + \frac{r^2}{2\alpha\ell^2}\right)^{-\alpha} \tag{7}$$

$$Matern = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{\ell} r\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}}{\ell} r\right) \tag{8}$$

$$k_{\nu=3/2}(r) = \left(1 + \frac{\sqrt{3}r}{\ell}\right) \exp\left(-\frac{\sqrt{3}r}{\ell}\right) \tag{9}$$

$$k_{\nu=5/2}(r) = \left(1 + \frac{\sqrt{5}r}{\ell} + \frac{5r^2}{3\ell^2}\right) \exp\left(-\frac{\sqrt{5}r}{\ell}\right) \tag{10}$$

$$k_{NN} = \sin^{-1}\left(\frac{2\tilde{x}^T \sum \tilde{x}'}{\sqrt{(1 + 2\tilde{x}^T \sum \tilde{x})(1 + 2\tilde{x}'^T \sum \tilde{x}')}}\right) \tag{11}$$

Where, $\tilde{x} = (1, x_1, \dots, x_d)^T$ \tilde{x} is augmented input vector r denotes $|x - x'|$, ν is positive integer.

The proposed model further optimized by using hyper parameters, Hyper parameters plays a vital role by directly controlling the behavior of the training algorithm and maximize the performance of the trained model.

3. Evaluation criteria

In this research paper, a various evaluation criterion are used to evaluate the GPR model. The criteria are Mean Square Error (MSE), Root Mean Square Error (RMSE), Normalized Mean Square Error (NMSE), Mean Absolute Error (MAE), Regression coefficient value (R²) and Absolute Average Relative Deviation percentage (AARD%). The mathematical formulations of criteria are shown in Eqs. (12), (13), (14), (15), (16), and (17) respectively.

$$MSE = \frac{1}{n} \sum_{i=1}^n (k_p - k_a)^2 \tag{12}$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (k_a - k_p)^2} \tag{13}$$

$$NMSE = \frac{MSE}{\text{var}(k_a)} \tag{14}$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |k_a - k_p| \tag{15}$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (k_a - k_p)^2}{\sum_{i=1}^n (k_a - \bar{k}_a)^2} \tag{16}$$

$$AARD\% = \frac{1}{n} \sum_{i=1}^n \left| \frac{k_a - k_p}{k_a} \right| \times 100 \tag{17}$$

Where k_p , k_a denote thermal conductivity ratio of predicted data and experimental data respectively, \bar{k}_a is the mean value of thermal conductivity of experimental data for ‘n’ data values, ‘n’ denotes the total number of data samples. k_p , k_a are replaced by μ_p , μ_a to determine the dynamic viscosity ratio. $\bar{\mu}_a$ is mean value of dynamic viscosity ratio of experimental data. An adjusted response function is used to explore the effect of the predictor variables temperature, volume fraction and size of the nanoparticles on thermal conductivity ratio (TCR) and also in dynamic viscosity ratio (DVR) of Al_2O_3/H_2O nanofluids. These criteria values are used to compare the accordance between experimental values and predicted values.

4. Results and discussions

The experimental values used for training the GPR model and the predictor variable values have been taken from [15] and [31]. Size of the nanoparticles, volume fraction and experimental thermal conductivity ratio values of Al_2O_3/H_2O nanofluids have been taken to train the GPR model with different kernel function which consists of 70 sample dataset. 45 sample dataset based on the size of the nanoparticles, volume fraction and experimental dynamic viscosity ratio have been taken to predict the dynamic viscosity ratio of Al_2O_3/H_2O nanofluid. 107 sample dataset were used to predict the effectiveness of the predictor variables like temperature, volume fraction and size of the nanoparticles to find the thermal conductivity ratio. It is studied that the crucial factor to enhance thermal conductivity of nanofluids is temperature than the volume fraction and size of the particle.

4.1. Prediction of TCR and DVR

The GPR model is trained with different kernel functions namely Squared Exponential, Rational Quadratic and Matern class of covariance with ‘v’ take the value as 5/2. GPR model with cross validation, it partition the dataset into number of fold to perform cross validation thereby to protect the data from over fitting problem and possess generalization ability. In this proposed model, the dataset where

partitioned into 5 fold, 10 fold and 15 fold and the results were compared using RMSE evaluation criterion.

In the prediction of TCR, the Matern kernel function produces less RMSE value when compared with other two kernel functions, whereas in the prediction of DVR, the Squared exponential kernel function gives less RMSE value than the Matern and Rational Quadratic, the same is shown in the Table 1. Table 2 consist of all the evaluation criteria of Matern kernel function with $v = 5/2$ for TCR and Squared exponential kernel function for DVR.

Observed that there is a good accordance between the experimental values and predicted values by Gaussian process regression model. It is shown that predictions of TCR by matern 5/2 kernel function are more accurate than the prediction by other two kernel functions. Figure 1 depicts the Prediction of TCR using GPR- Matern Kernel Method with $v = 5/2$ value. The GPR model with matern 5/2 further optimized by using the hyper parameters, Figure 2 represents the comparison between without hyper parameter and with hyper parameter optimization of Gaussian process regression model.

Figure 3 represents the Prediction of DVR using GPR Squared Exponential kernel function. The GPR model with Squared Exponential further optimized by using the hyper parameters, Figure 4 represents the comparison between without hyper parameter and with hyper parameter optimization of Gaussian process regression model. In Table 3, the optimization is noticeably shown in terms of RMSE value of Matern kernel function for TCR prediction and squared exponential kernel functions for DVR prediction with hyper parameters.

4.2. Effects of predictor variables in prediction of TCR

4.2.1. Effect of volume fraction and size of the nano particle

Effect refers the effect of two selected predictors on response. The Figure 5 represents an effects of both size of the nanoparticles and volume fraction on TCR by changing one of the predictor values with other predictor values held fixed. Increase in the size of the nano particle from 11nm to 108nm decreases the TCR values by 0.05 and increasing the volume fraction from 0.01 to 0.05 increases the TCR by 0.125 values. The optimum values of size of the nanoparticles and volume fraction are 59.5nm and 0.03 respectively.

An adjusted response function describes the relationship between the fitted response and a single predictor, with the other predictors averaged out by averaging the fitted values over the data used in the fit. A regression model for the predictor variables (x_1, x_2, \dots, x_p) and the response variable y has represented in the Eq. (18).

$$y_i = f(x_{1i}, x_{2i}, \dots, x_{pi}) + r_i \tag{18}$$

Where ‘f’ is a fitted regression function and ‘r’ is a residual. The subscript ‘i’ represents the observation number. The adjusted response function for the first predictor variable x_1 , it is depicted in the Eq. (19).

$$g(x_1) = 1/n \sum_{i=1}^n f(x_{1i}, x_{2i}, \dots, x_{pi}) \tag{19}$$

Where ‘n’ is the number of observations. The adjusted response data value is the sum of the adjusted fitted value and the residual for each observation. Thus the adjusted TCR values are calculated by varying the values of one of the predictor values with other predictor values held fixed. Keeping fixed number of various volume fractions for different

Table 1. Comparison of RMSE value with different number of fold for predicted TCR and DVR.

Kernel Functions	TCR			DVR		
	Values of Root Mean Square Error					
	5 fold	10 fold	15 fold	5 fold	10 fold	15 fold
Rational Quadratic	0.0049437	0.0049875	0.0050531	0.024712	0.022956	0.020176
Squared Exponential	0.0048204	0.0048729	0.0049447	0.024475	0.021711	0.019119
Matern (v = 5/2)	0.004779	0.004826	0.0049337	0.025269	0.023832	0.021021

Table 2. Evaluation of Covariance Functions for predicted TCR and DVR.

Evaluation	MSE	RMSE	R ²	MAE	NMSE	AARD%
Matern (v = 5/2) for TCR	0.000024	0.004779	0.99	0.0035878	0.000021	0.004195
Squared Exponential for DVR	0.000482	0.021711	0.99	0.015508	0.000327	0.019064

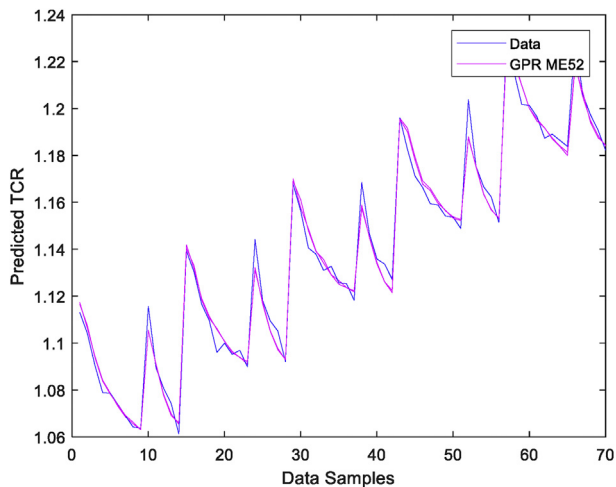


Figure 1. Prediction of TCR using GPR- Matern Kernel Method with $v = 5/2$ value.

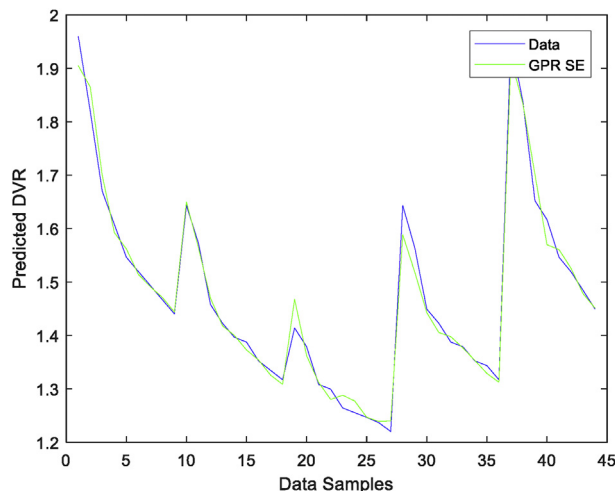


Figure 3. Prediction of DVR using GPR- Squared Exponential Method.

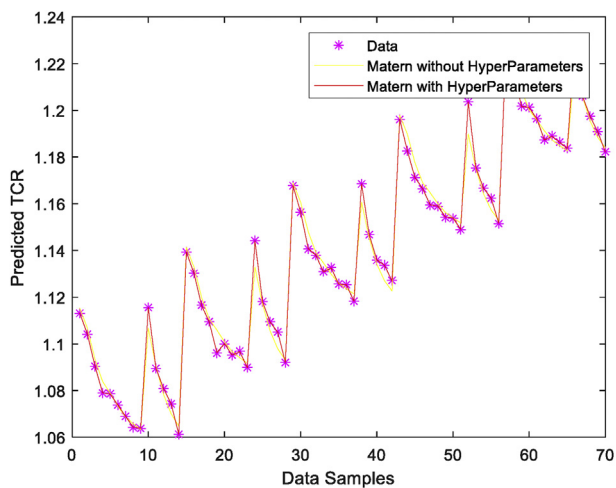


Figure 2. Comparison in Prediction of TCR using GPR - Matern Kernel Method with $v = 5/2$ value without and with hyper parameters.

values of size of nanoparticles the highest volume fraction shows the enhancement in the TCR. For various fixed number of size of particles and different values of volume fraction, smallest size of the nanoparticles shows enhancement in TCR it as shown in Figure 6 and in Figure 7 respectively.

4.2.2. Effect of size of the nano particle and temperature

The effect of temperature and size of the nanoparticles were shown in the Figure 8. Increasing the temperature from 293K to 323K increases the TCR values by 0.175 and decreasing the diameter from 80 nm to 11 nm increases the TCR by 0.04 values. The optimum values of size of the nanoparticle and temperature are 36nm and 308K respectively. In Figure 9 for fixed number of various size of the nanoparticles and different temperature values, the diameter of 36nm shows a precise enhancement in TCR, for various fixed number of temperature values and

different diameter of the nanoparticles, the maximum temperature shows an enhancement in TCR it is represented in the Figure 10.

4.2.3. Effect of volume fraction and temperature

The effects of temperature and volume fraction were shown in the Figure 11. Increasing the temperature from 293K to 325K increases the TCR values by 0.15 and increases the volume fraction from 0.0011 to 0.05 increases the TCR by 0.25 values. The optimum values of volume fraction and temperature are 0.03 and 310K respectively. Very low volume fraction values decreases the TCR values also shown in the Figure 11. In Figure 12 and in Figure 13, the highest values of volume fraction and highest temperature values shows the enhancement in the TCR values respectively.

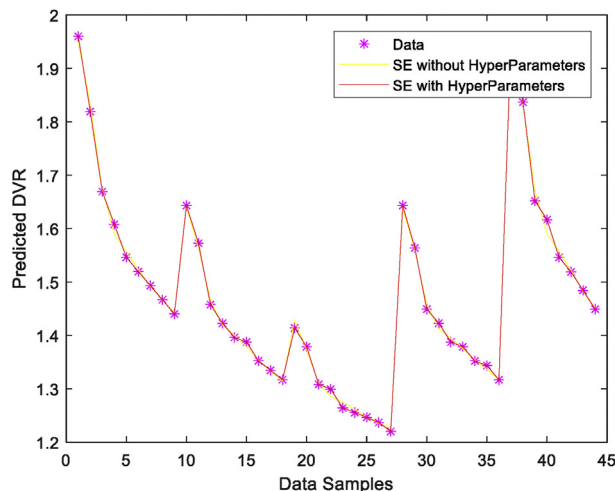


Figure 4. Comparison in Prediction of DVR using GPR – Squared Exponential without and with hyper parameters.

Table 3. Comparison of RMSE values without and with hyper parameters for predicted TCR and DVR.

Evaluation	TCR	DVR
	Matern (5/2)	Squared Exponential
RMSE without hyper parameter	0.004328	0.00874
RMSE with hyper parameter	0.000126	0.000045

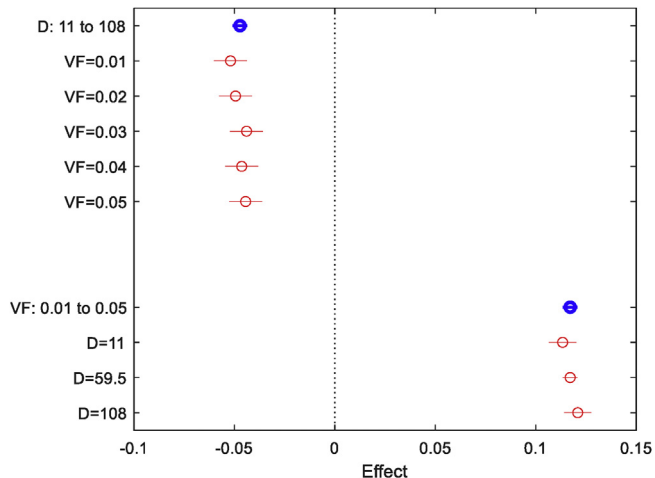


Figure 5. Effect of volume fraction and size (nm) of the nanoparticles.

4.3. Effects of predictor variables in prediction of DVR

4.3.1. Effect of volume fraction and temperature

The effects of temperature and volume fraction on response DVR are shown in the Figure 14. Increasing the temperature from 293K to 324K decreases the DVR values by 0.6 and increases the volume fraction from 0.01 to 0.05 increases the DVR by 0.6 values. The optimum values of volume fraction and temperature are 0.03 and 310K respectively. In Figure 15 for fixed number of various volume fraction and different temperature values, the volume fraction of 0.05 shows a precise enhancement in DVR. DVR value is higher for temperature having lower value it is represented in the Figure 16.

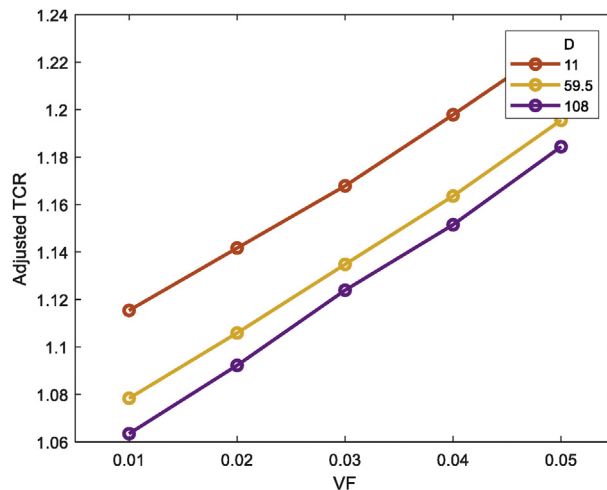


Figure 7. Effect of various fixed size (nm) and different values of volume fraction in the Prediction of TCR.

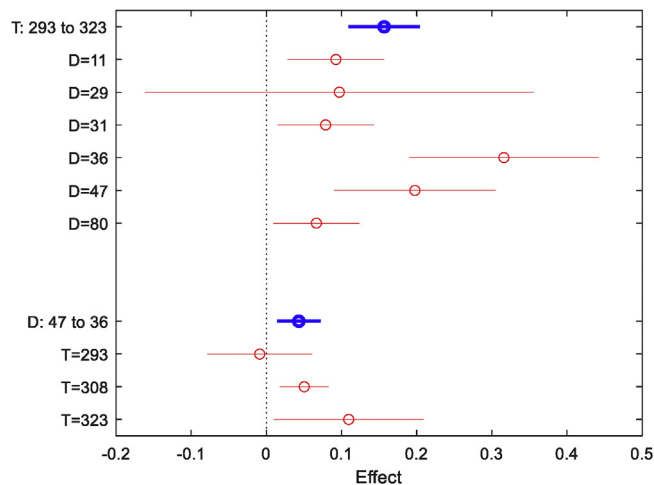


Figure 8. Effect of temperature (K) and size (nm) of the nanoparticles.

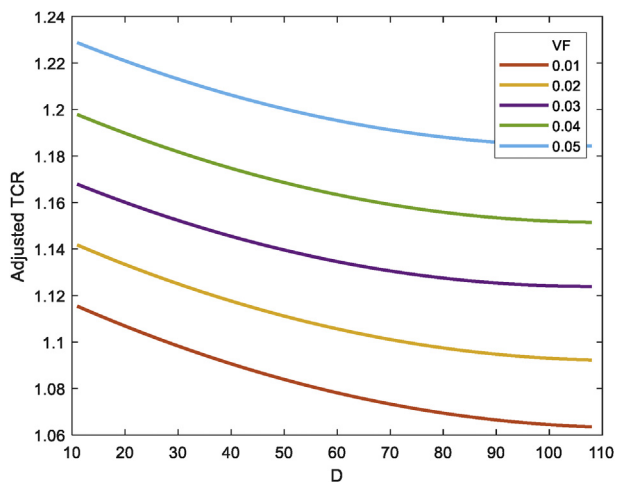


Figure 6. Effect of various fixed volume fraction and different size (nm) in the Prediction of TCR.

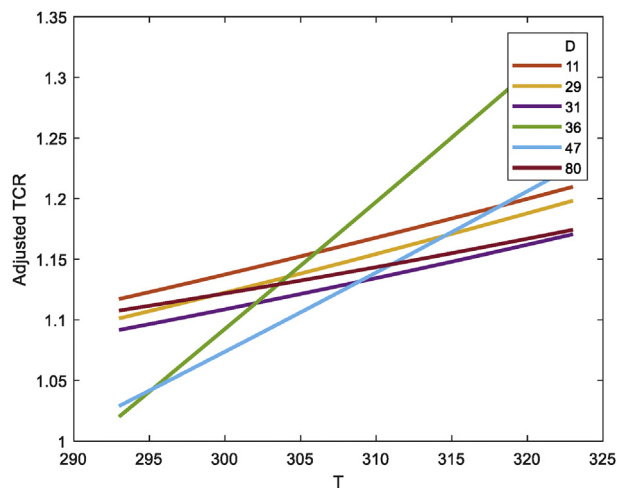


Figure 9. Effect of various fixed diameter (nm) and different temperature (K) values in the Prediction of TCR.

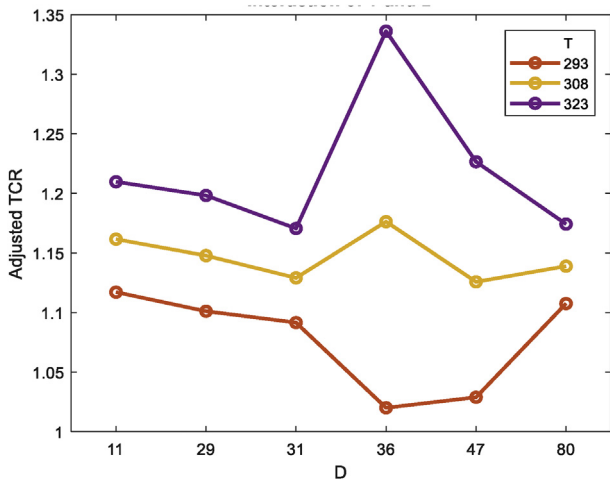


Figure 10. Effect of various fixed temperature (K) values and different diameter (nm) values in the Prediction of TCR.

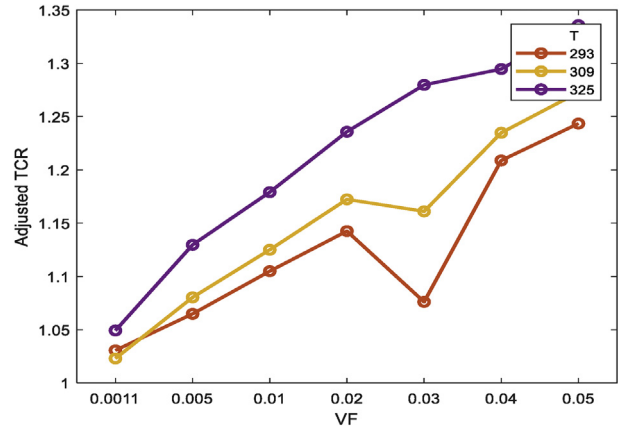


Figure 13. Effect of various fixed temperature (K) values and different values of volume fraction in the Prediction of TCR.

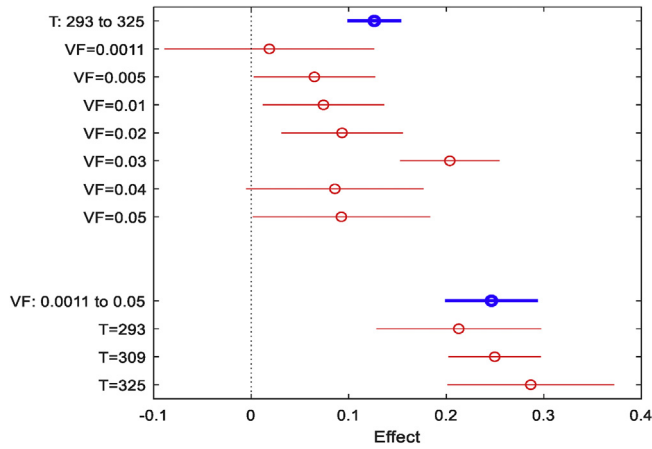


Figure 11. Effect of temperature and volume fraction.

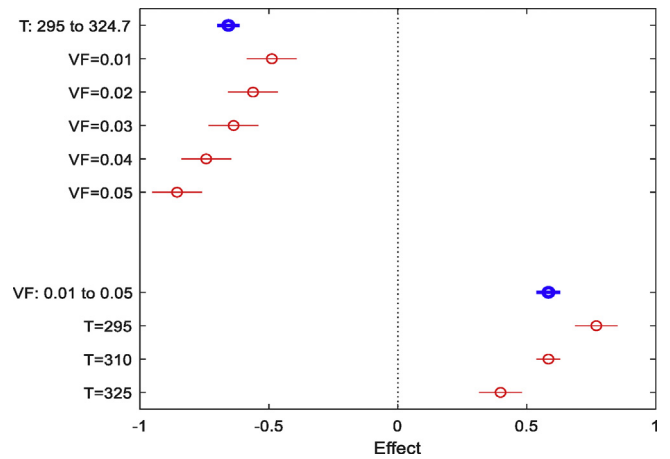


Figure 14. Effect of temperature and volume fraction.

5. Conclusions

In this research paper, 222 sample datasets have been used for the predictions of the thermal conductivity ratio and dynamic viscosity ratio of Al_2O_3/H_2O nanofluids by using Gaussian process regression (GPR) method. Temperature, volume fraction and size of the nanoparticles parameters were used as predictor variables. The thermal conductivity

ratio and dynamic viscosity ratio are taken as response variable in the proposed modeling. The effectiveness of the predictor variables in predicting the response variables are extensively studied. It is studied that the temperature of nanofluids plays a major role than the volume fraction and size of the nanoparticles to enhance thermal conductivity of nanofluids. The proposed GPR methods were modeled with different kernel functions and different number of fold to cross validate the dataset to

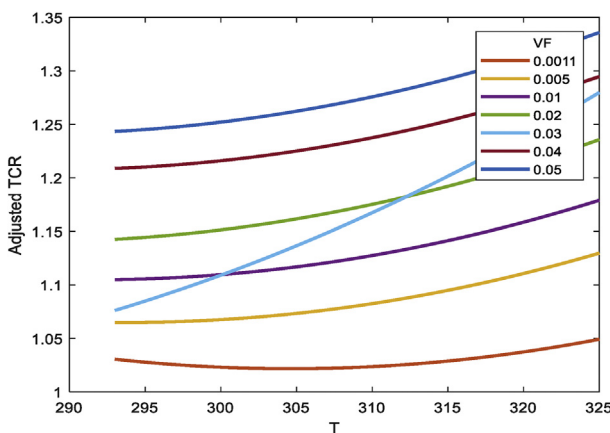


Figure 12. Effect of various fixed volume fraction and different temperature (K) values in the Prediction of TCR.

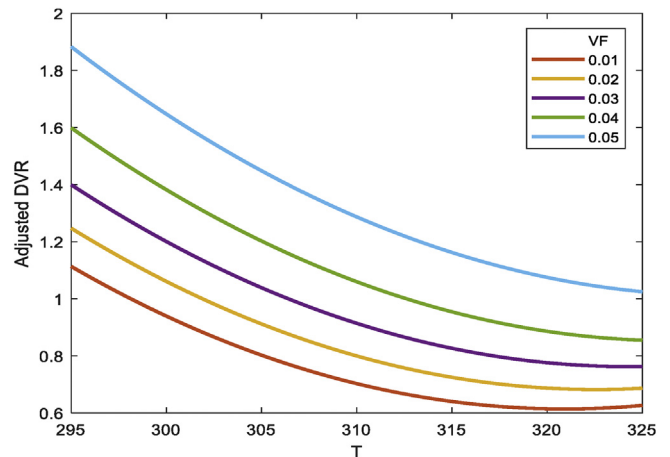


Figure 15. Effect of various fixed volume fraction and different temperature (K) values in the Prediction of DVR.

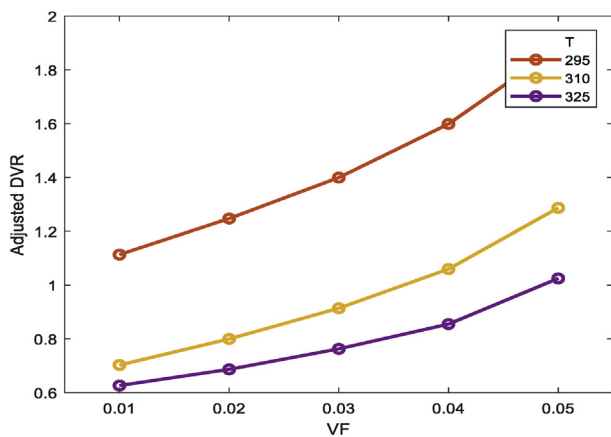


Figure 16. Effect of various fixed temperature (K) values and different values of volume fraction in the Prediction of DVR.

evade over fitting problem. Found that the Matern kernel function and squared exponential kernel function exhibit accurate prediction of thermal conductivity ratio and dynamic viscosity ratio respectively. The proposed model were optimized by using hyper parameters and the Root Mean Square Error (RMSE) values of thermal conductivity ratio by matern kernel function and dynamic viscosity ratio by squared exponential kernel function are 0.000126 and 0.000045 respectively. Found that the Regression coefficient value (R^2) for overall data is 0.99. Therefore, Gaussian process regression (GPR) method accurately predicts the thermal conductivity ratio and dynamic viscosity ratio of Al_2O_3/H_2O nanofluids.

Declarations

Author contribution statement

P. C. Mukesh Kumar: Conceived and designed the experiments; Wrote the paper.

K. Rajan: Analyzed and interpreted the data; Wrote the paper.

Funding statement

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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