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Research Article

Predicting Thermophysical Property of Aluminum Oxide/Ethylene Glycol-Water Nanofluid: A Machine Learning Approach

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ABSTRACT

Nanofluids are used in industrial thermal applications because of their significant thermal characteristics. Machine learning algorithms have recently advanced to the point that they can properly anticipate the thermophysical properties of nanofluids. The literature study provides the data needed to train the models. The gathered data will be separated into groups for testing and training according to 20% and 80% ratios. The thermophysical characteristics of the water-EG base fluid at various percentages mixed with Al_2O_3 nanoparticles are analyzed in this work. The thermophysical properties were predicted using several machine-learning algorithms. The mean square error and coefficient of determination (R^2) were used to compare the models' accuracy. According to the study's findings, machine learning models are the most accurate and quick ways to forecast thermophysical parameters. The accuracy of the model was found to be 99%. The MSE and R^2 value of the XGBoost algorithm was found to be 0.0001 and 0.99 respectively. An XGBoost machine learning model was proposed in this study to forecast the thermophysical characteristics of the Al_2O_3/water_EG nanofluid. This work's novelty lies in the powerful, data-driven alternative that machine learning techniques offer, enabling real-time, high-accuracy predictions of thermal conductivity based on simulation or experimental datasets. This method improves the design and optimization of nanofluids for specific thermal applications, fills in data gaps through substitute modeling, and drastically lowers experimental effort and expense.

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1. Introduction

Machine learning (MI) is one form of artificial intelligence (AI) that allows computers to predict the future without writing any program or coding. In machine learning two major components are signal and response. The output by the combinations of input data can be easily predicted by ML. The suspension of nanoparticles in the base fluid like water or Ethyl Glycol (EG) is called nanofluids. Nanofluids enhance the heat transfer performance of thermal devices. The performance

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of the nanofluids depends on volume fraction, temperature, types of nanoparticles, and their size. The prediction of the performance at different combinations is difficult to determine. Therefore either experimental methods or simulations are used to determine optimal performance. Conducting experiments or simulation methods is expensive and time-consuming. Therefore, machine learning is found to be one of the efficient methods to predict the thermophysical properties of nanofluid. Many experimental and theoretical studies have been done to propose the correlation between the input parameters like volume fraction, temperature, mixture percentage, and type of nanoparticles to predict the thermal conductivity and viscosity of the nanofluid. However, accurate correlations are not available to predict the exact properties of the nanofluid at various conditions. Palash et al. [1] developed machine-learning models to predict the thermal conductivity of titania-water nanofluid using ANN, GBR, SVR, DTR, and RFA algorithms. They found that GB is the best algorithm compared to all other algorithms in terms of accuracy. Ekene Onyiriuka [2] used a model of model approach to predict the thermal conductivity of the nanofluid. They compared the experimental results with model-predicted results and found good agreement between them. Abulhassan Ali et al. [3] used machine learning algorithms to predict the thermal behavior of BN-diamond/thermal oil nanofluids using different algorithms and a 700 experimental data set. The GBR algorithm proved better than all other algorithms. Hamid et al. [4] experimentally investigated the viscosity of Al_2O_3/EG-water nanofluid. They found that nanofluid viscosity depends on concentration, temperature, and volume fraction. The viscosity and thermal conductivity of Al_2O_3/EG-water nanofluid were experimentally determined by Sundar et al. [5]. They proposed different correlations to find the viscosity and thermal conductivity at different volume fractions, temperatures, and base fluid concentrations. Chiam et al. [6] studied the viscosity and thermal conductivity of Al_2O_3/EG-water nanofluid taking different ratios of the base fluid. They found that a decrease in the base fluid percentage mixture enhanced the viscosity of the nanofluid. Gallego et al. [7] experimentally measured the viscosity and thermal conductivity of Al_2O_3/EG-water nanofluid at different concentrations of nanoparticles. They compared the experimental results with theoretical models and found good agreement. Empirical correlations for viscosity and thermal conductivity of Al_2O_3/EG-water nanofluid were developed by Sawicka et al. [8]. The study concluded that the results of the correlation and the literature properly match each other. The thermal conductivity of EG-water nanofluid with varying percentages of different nanoparticles was experimentally investigated by Yashawantha and Vinod [9]. The prediction was done by ANN modeling and found to be in good agreement with the proposed correlations. The cooling performance of Al_2O_3/EG-water nanofluid in hot press applications was investigated by Lim et al. [10]. The results show that the life of the die is enhanced by using nanofluid as a coolant. Esfe et al. [11] developed correlations to predict the thermal conductivity of $Mg(OH)_2$–EG nanofluid using experimental results. The results were compared with ANN model predictions and it was found that ANN models can perfectly predict the properties of the nanofluid. An ANN model was developed by Sadeghzadeh et al. [12] to predict TiO_2–Al_2O_3/water nanofluid thermophysical properties. The model accuracy was around 0.98, which was within the acceptable limit. Different machine learning algorithms were compared to predict the viscosity of nanofluids by Shateri et al. [13]. The analysis shows that DT models predict more accurately compared to other models. Bakthavatchalam et al. [14] used AI to predict the thermal properties of MWCNT nanofluids. They found that the modeling method reduces the cost and time of experimentation. Sayantan Mukherjee et al. [15] explored nanofluid thermal conductivity, noting that kinetic theory and Brownian motion both contribute to its increase with temperature. Experimental results supported this, showing that thermal conductivity is also affected by surfactants, stability, and volume fraction. Ali et al. [16] examined the effects of nanoparticle size and volume fraction concentration on thermal conductivity using a transient hot-wire laser displacement method. Their findings indicated that increasing volume fraction concentration optimizes thermal conductivity. This trend was also observed in a study of the volume fraction effects of Al and Al_2O_3 nanoparticles suspended in distilled water, ethylene glycol, and ethanol, with results showing that thermal conductivities and diffusivities of these nanofluids increase as particle volume fraction rises. Ali et al. [17] noted similar results, while Mohammed Hemmat Esfe et al. [18] conducted studies at volume fractions of 0.2% to 0.5% and temperatures from 24°C to 50°C, demonstrating a marked enhancement in thermal conductivity as concentration and temperature rose. Azmi et al. [19] experimented with different Al_2O_3 (0.2% to 1.0%) nanofluid volume concentrations in various EG-water ratios (60:40, 50:50, and 40:60), finding that both thermal conductivity and viscosity of the nanofluids were consistently higher than those of the base fluid. Pravin Kumar et al. [20] conducted experiments on water-based fly ash-Cu hybrid nanofluid to determine heat transfer coefficient, friction factor, and pressure drop at various Reynolds number flow rates. The study found that pressure drops in the fly ash nanofluid and hybrid nanofluid increased with higher Reynolds numbers. Kazem et

al. [21] compared and evaluated the performance of ANN models with experimental results. Al-Waeli et al. [22] presented an ANN and mathematical model for nano-PCM cooling. They found that linear models predict accurate results. GA and ANN models used by Topal et al. [23] predict the viscosity of nanofluids accurately. Erdogan et al. [24] used the ANN method to measure the viscosity of water-based nanofluids with different nanoparticles. Mukherjee et al. [25] used MLP modeling and experimental methods to find the heat transfer ability of silica-ethylene glycol nanofluid. Goncalves et al. [26] performed a review on the challenges and controversies of thermal conductivity prediction models. They concluded their work by stating that nanofluids have wide applications in nanomedicine and renewable energies. Moolya et al. [27] performed a numerical analysis to predict the MHD and aspect ratio effect on double diffusive mixed convection using an LR model. From the literature, it is found that various researchers have developed correlations to predict the thermophysical properties of nanofluids using some experimental data. The experimental setup required to get the required results is very expensive and time-consuming. The developed correlations work only for specific conditions. Much work has been done to develop machine learning models to predict the properties of nanofluids containing nanoparticles with water as the base fluid. In this work, an attempt is made to develop an accurate model to predict the thermal conductivity of a hybrid nanofluid. Different ML algorithms were used to develop models for prediction, and their accuracy was compared. Statistical methods were used to compare the accuracy of the models. Several machine-learning methods were used to predict the thermophysical properties of nanofluids. This work attempts to develop a machine-learning model that can accurately predict the hybrid nanofluid's thermal conductivity using a range of ML methods. The objective of this work is to cut down on experimentation time and expense; this effort aims to identify a substitute technique for predicting the thermophysical characteristics of nanofluids.

2. Methodology

In this work, the thermophysical properties of the Al_2O_3/EG-water nanofluid are predicted using machine learning algorithms. The selected properties are viscosity and thermal conductivity at various temperatures, volume fractions, and EG-water mixing percentages. The required data for testing and training the models have been collected from the literature. These data are from experiments, simulations, and correlations. The data are stored in a data bank in Excel CSV format. The collected data were then split into testing data and training data. 80% of the data collected is used for training the model and 20% is used for testing the model. After segregating the data into training and testing, the next step is the selection of models. In this work, Linear Regression (LR), Decision Tree (DT), Random Forest (RF), and Gradient Boosting (GB) models were used for prediction modeling. All the models were trained and tested for prediction using 865 different data points for all the selected combinations. The models were evaluated using R^2 values. The accuracy of the models was compared using mean absolute error, mean squared error, and root mean squared error.

3. Description of Data Stream and Models

The data required to train the machine learning models were collected from eight articles. In this work, machine learning models were developed to predict the dependent variable, thermal conductivity, using three independent variables: EG-water ratio, temperature, and volume fraction. LR, DT, RF, and GB models were trained and tested to predict thermal conductivity. Table 1 shows the data collected for Al_2O_3/EG-water nanofluid to train and test the model.

3.1. Linear Regression

This algorithm shows the best performance when the relationship between the variables is linear. Linear regression is a fundamental and widely used supervised learning algorithm in machine learning. It is mainly used in this study to predict the thermal conductivity of Al_2O_3/EG-water nanofluid at different volume fraction ratios, temperatures, and base fluid concentrations. This works on the following representation, as shown in Eq. (1).

$$y = w_1x_1 + w_2x_2 + w_3x_3 + \cdots + w_nx_n + b + \epsilon \quad (1)$$

where:

$$w_n = weights$$

$$b = bias$$

$$\epsilon = error$$

The main objective of this method is to determine a best-fit line to minimize the prediction error. This algorithm is simple and efficient for using medium-sized data points. Figure 1 shows the flow diagram of the linear regression process.

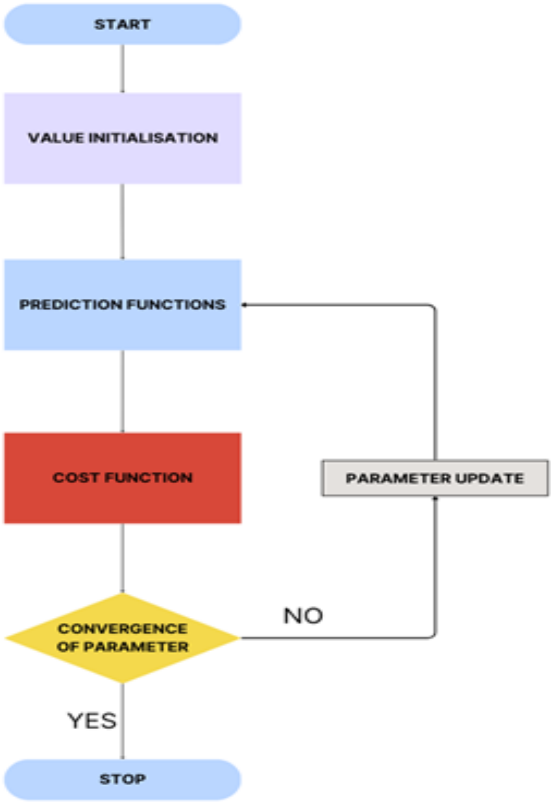


Fig. 1. Linear Regression flow diagram

3.2. Decision Tree

For classification and regression-type projects, decision trees are a powerful supervised learning algorithm. A tree-like structure is modeled, as shown in Fig. 2, on decisions and their possible effects, making it easy to learn and interpret. The root node, internal node, and leaf node are structured in the form of a tree. The growth of the tree continues until the maximum depth is reached, the minimum samples per leaf are satisfied, and no further improvement in predictions is possible. This algorithm is easy to understand and handles problems with nonlinear relationships between the dependent and independent variables.

3.3. Linear Gradient Boosting

This is a powerful supervised learning algorithm used for regression and classification-type problems. It prepares a set of weak learners in a consecutive way, as shown in Fig. 3, where each new learner corrects the errors of its predecessor. The predictive accuracy of this algorithm is very high. It also handles complex patterns of data. Gradient boosting algorithms are mainly used in research and development due to their accurate and robust model development capacity.

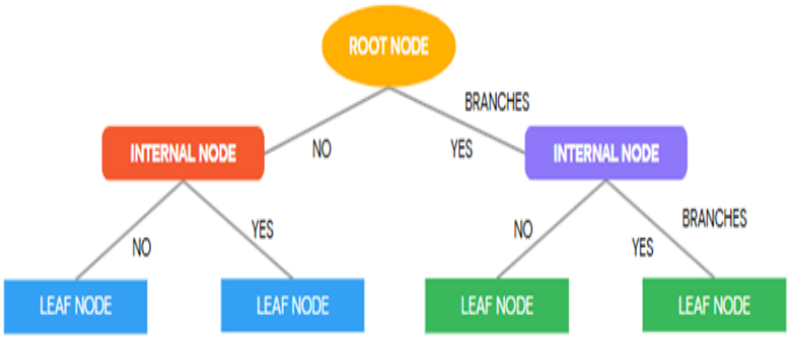


Fig. 2. Decision Tree flow diagram

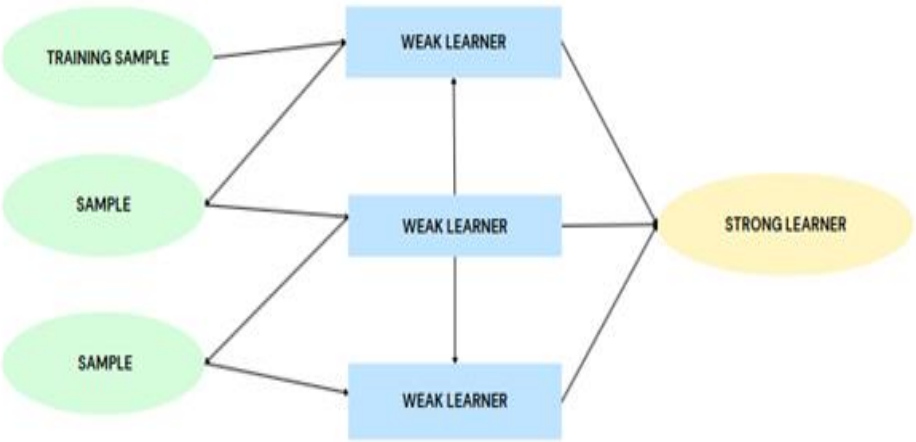


Fig. 3. Linear gradient boosting flow diagram

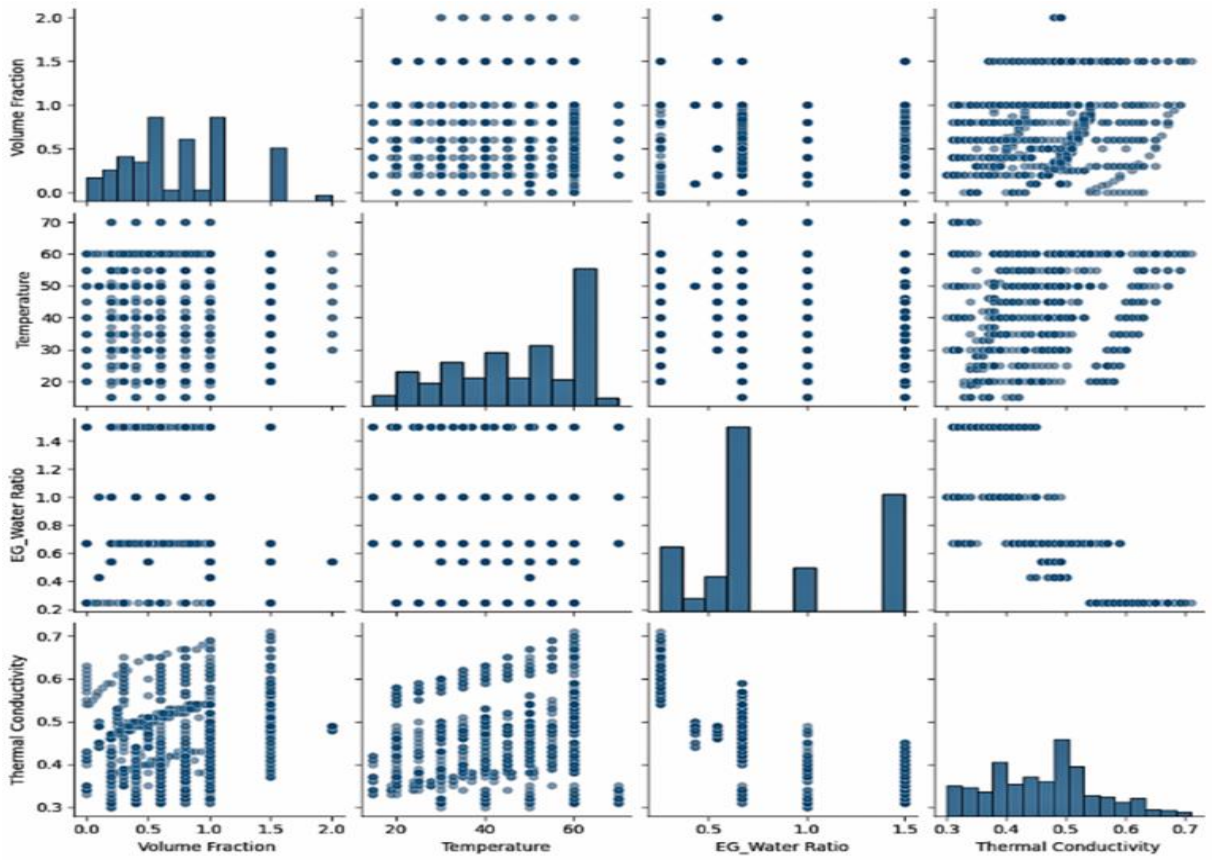


Fig. 4. Pair plot

Table 1. Data source for model training and testing

Nanoparticle	Base Fluid	Data points	Source	Nanoparticle	Base Fluid	Data points	Source
Al_2O_3	EG_Water	172	[4]	Al_2O_3	EG_Water	33	[8]
Al_2O_3	EG_Water	266	[28]	Al_2O_3	EG_Water	15	[29]
Al_2O_3	EG_Water	75	[9]	Al_2O_3	EG_Water	64	[6]
Al_2O_3	EG_Water	150	[10]	Al_2O_3	EG_Water	90	[5]

3.4. Support Vector Regression Algorithms

These algorithms are derived from support vector machines (SVM) and are supervised learning algorithms used for regression tasks. The function was derived and used to estimate the target values within an indicated perimeter of tolerance. It does not aim to minimize error but seeks to fit the data within a margin around the true value. Loss functions are used to penalize the data points which fall outside the margin. The main aim is to keep the prediction error within the tolerance margin. It works well with both linear and nonlinear regression problems using kernels. It balances underfitting and overfitting with appropriate hyperparameter tuning.

4. Results and Discussion

The thermal conductivity of Al_2O_3/EG-water nanofluid was predicted using different machine learning algorithms. Three input parameters—EG-water concentration, temperature, and volume fraction of the nanoparticle—were used as the major input parameters to predict thermal conductivity. The models used to predict the thermophysical properties were trained and tested using a sufficient number of data points to obtain accurate and valid results.

4.1. Data Set Analysis

In the pair plot shown in Fig. 4, the diagonal histogram shows that thermal conductivity has a skewed distribution, while a more uniform distribution is observed for volume fraction. A positive correlation was observed between volume fraction, temperature, and thermal conductivity, but no relationship was observed between the EG-water ratio and thermal conductivity. A total of 865 data points were used for the analysis. The values of skewness and kurtosis are in the acceptable

range, showing the quality of data selected to design prediction models. The statistical parameters chosen for the study are shown in Table 2.

4.2. Linear Regression (LR)

The linear regression model was first used to predict the result by fitting the best-fit line. Fig. 5 shows the scatter plot and the best-fit line for the developed model's predicted values. The factors used to determine the accuracy of the model are R^2, RMSE, MSE, and MAE. The R^2 value for the developed model using the linear regression algorithm is 0.64, the RMSE value is 0.0316, the MSE is 0.003, and the MAE is 0.04. In this algorithm, accuracy was found to be 64%.

Because the scatter plot shown in Fig. 4 does not show a strong linear relationship between thermal conductivity and the selected variables, it was decided to use a decision tree algorithm for further analysis. Fig. 5 shows the regression line and predicted thermal conductivity for the test data using the LR algorithm.

Table 2. Statistics of the data used to develop prediction models

Variables	Total data	Mean	Std. Deviation	Skewness	Kurtosis
Volume Fraction	865	0.729	0.433	0.607	-0.024
Temperature	865	45.06	14.267	-0.401	-1.040
EG_Water ratio	865	0.838	0.432	0.496	-1.05
Thermal Conductivity	865	0.463	0.089	0.285	-0.453

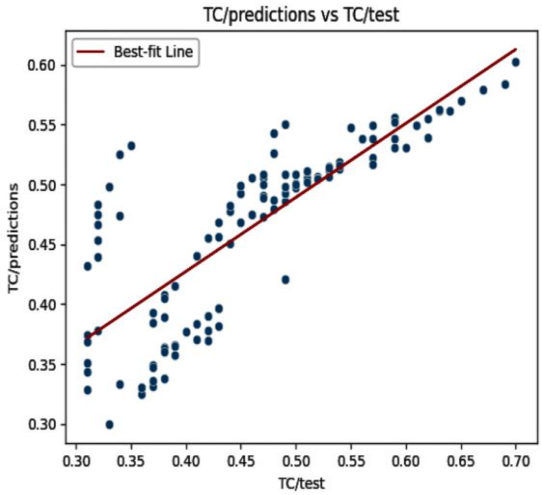


Fig. 5. Predicted value by Linear Regression

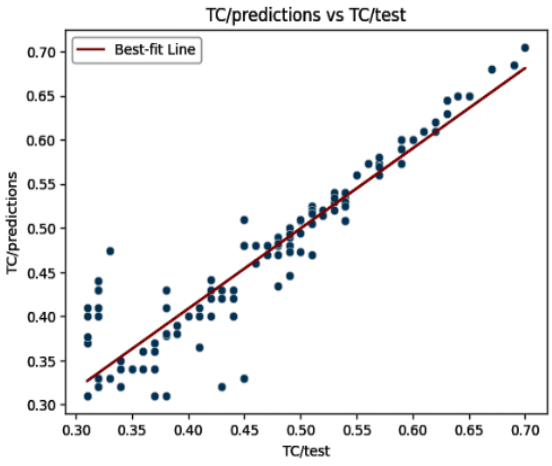


Fig. 6. Predicted value by DT

4.3. Decision Tree (DT)

A decision tree is a powerful supervised machine learning method. Decision trees are helpful for making predictions about unconditional outputs. From the analysis, it was found that the accuracy of this algorithm is slightly better than that of the linear regression algorithm. The R^2 value for the model developed using DT is 0.87, the RMSE value is 0.034, the MSE is 0.001, and the MAE is 0.018. The prediction accuracy for this algorithm was found to be 87%, and it was decided to use an RF algorithm for further analysis. Fig. 6 shows the regression line and predicted thermal conductivity for the test data using the DT algorithm. A total of 23% improvement in prediction accuracy was obtained with the DT model.

4.4. Random Forest (RF)

This algorithm is similar to DT, in which several decision trees are constructed to obtain accurate predictions during the training stage. This approach essentially combines many distinct models to make a final decision. Each model makes a valuable contribution to the prediction. Therefore, this algorithm is more accurate than DT. The R^2 value for the model developed using RF is 0.88, the RMSE value is 0.032, the MSE is 0.001, and the MAE is 0.019. With this algorithm, accuracy increased by 1%, and it was found that the RF algorithm is comparatively better for the selected problem. Figure 7 shows the regression line and predicted thermal conductivity for the test data using the RF algorithm.

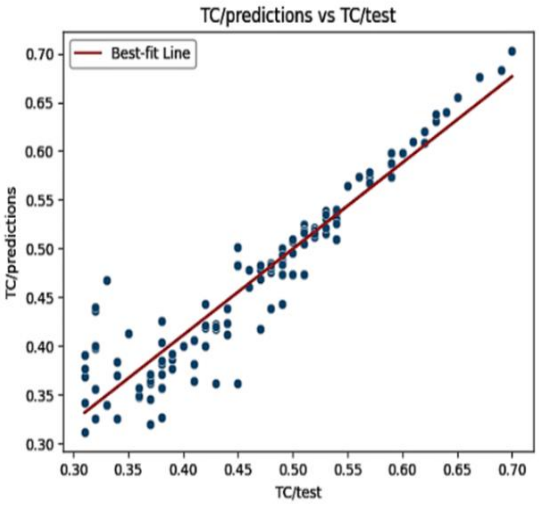


Fig. 7. Predicted value by RF

4.5. Gradient Boosting (GB) and XGBoost Algorithms

Gradient boosting algorithms are powerful algorithms for predictive-type problems. In this method, the loss function is optimized by using weak learners that focus on the error residuals from the preceding models to produce accurate estimations. The R^2 value for the model developed using GB is 0.92, the RMSE value is 0.0276, the MSE is 0.0007, and the MAE is 0.017. With this algorithm, accuracy increased by 4%, and it was found that the GB algorithm is comparatively better for the selected problem.

Figure 8 shows the regression line and predicted thermal conductivity for the test data using the GB algorithm.

Table 3 compares the accuracy of the models based on MAE, MSE, RMSE, and R^2 values. The GB algorithm is a comparatively more accurate algorithm than the previously discussed algorithms for the prediction of Al_2O_3/EG-water nanofluid thermal conductivity. A further increase in accuracy was achieved using the XGBoost algorithm.

Figure 9 shows the cluster of data points around the best-fit line. This shows that the XGBoost model has comparatively high accuracy in predicting the thermal conductivity. The R^2 value of this model is 0.9841, which is within the acceptable limit. Therefore, it is concluded from this analysis that the XGBoost algorithm can be used to predict the thermal conductivity of Al_2O_3/EG-water nanofluid at any given temperature, volume fraction, and EG-water mixing ratio.

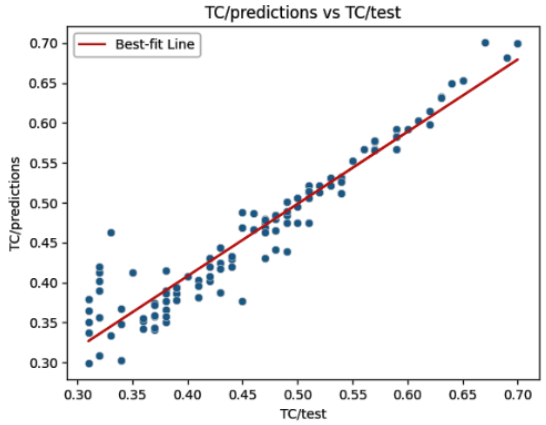


Fig. 8. Predicted value by GB

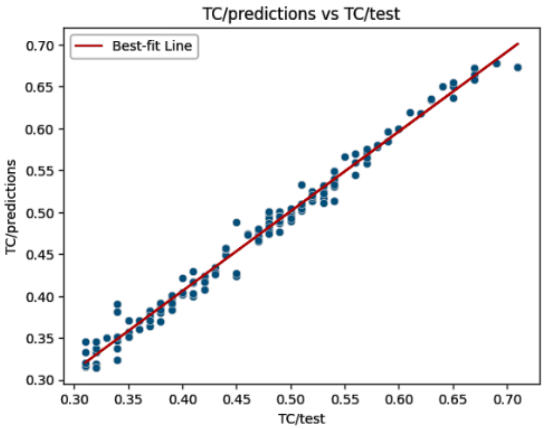


Fig. 9. Predicted value by XGB

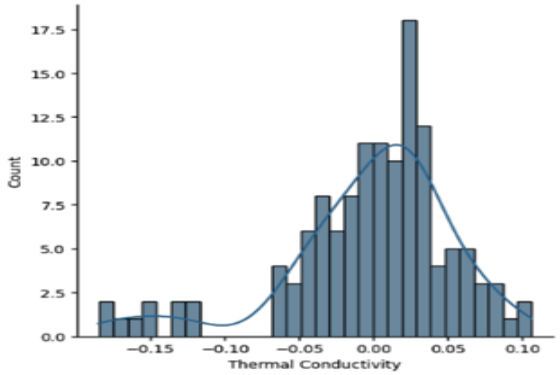
Table 3. Summary of the accuracy of algorithms.

Models	MSE	RMSE	R^2
LR	0.0031	0.056	0.65
DT	0.0011	0.034	0.87
RF	0.0010	0.032	0.89
GB	0.0007	0.002	0.92
XGBoost	0.0001	0.011	0.99

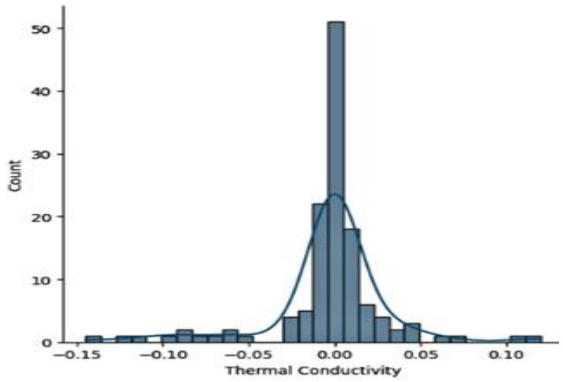
4.6. Validation of results

The accuracy of the model is determined by the residuals in statistical analysis. The difference between the actual value and the predicted value is the residual. In the regression analysis, some residuals were found to be positive and some were found to be negative, which indicates whether the predicted value is greater than or less than the actual value.

Figures 10 (a), 10 (b), 10 (c), and 10 (d) show the histograms of residuals and the probability plots for the LR, DT, RF, and GB models. All residuals are within the acceptable limit.



(a)



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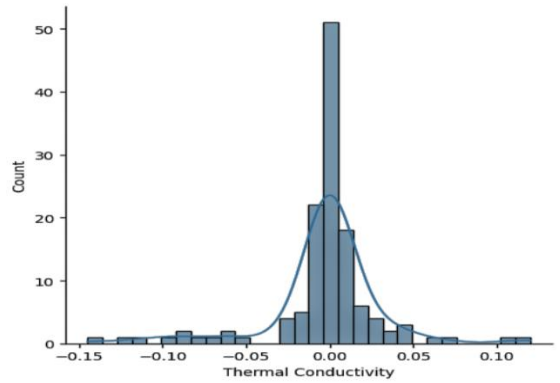
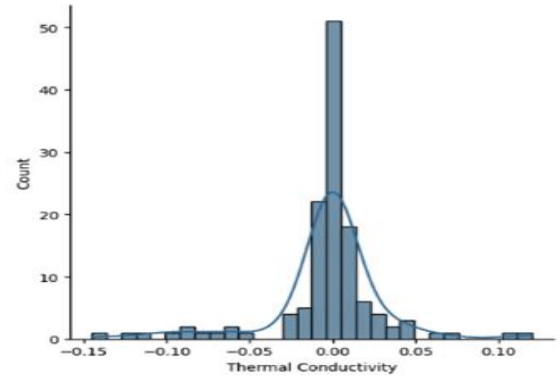


(c)



(d)

Fig. 10. Histograms of residuals (a) LR. (b) DT, (c) RF, and (d) XGB

Figure 11 compares the experimental results of [5] with the thermal conductivity predicted using the models. The predicted results show excellent agreement with the experimental data, demonstrating the model's high accuracy and reliability. The close match validates the model's ability to capture the complex nonlinear relationships between temperature, nanoparticle concentration, and thermal conductivity. Additionally, statistical performance metrics such as R^2, RMSE, and MSE confirm the strength and generalization capability of the models. The strong correlation highlights the potential of the proposed ML model as a reliable tool to predict thermal conductivity. This model can also serve as an alternative to experimental studies.

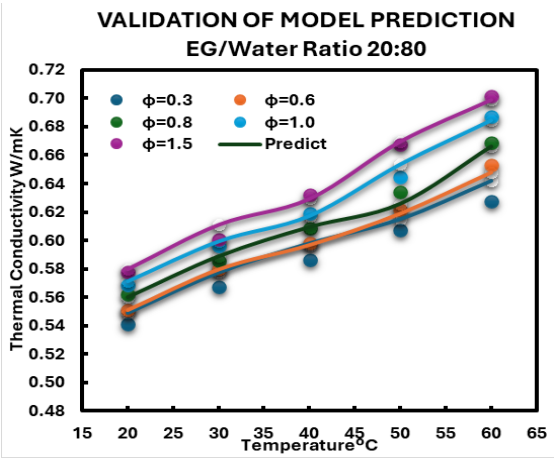


Fig. 11. Comparison of Predicted thermal conductivity with the Experimental result [5]

5. Conclusions

In this study, an attempt is made to predict the thermal conductivity of Al_2O_3/EG-water nanofluid using machine learning algorithms. Different machine learning algorithms (LR, DT, RF, and GB) are compared for their accuracy in predicting the thermal conductivity of Al_2O_3/EG-water nanofluid. The input parameters used are the volume fraction of nanoparticles, temperature, and the EG-water mixing ratio to predict thermal conductivity. Different statistical metrics such as MAE, MSE, RMSE, and R^2 are used for the comparison of the developed models.

- From the analysis, it is found that the XGBoost algorithm is the best for predicting the thermal conductivity of the nanofluid in terms of its accuracy.
- The predicted results accurately match the experimental results. This model can be used for the prediction of the thermal conductivity of Al_2O_3/EG-water nanofluids.
- The residuals of the predicted values are found to be within the acceptable limit.

- The MSE and R^2 values of the XGBoost algorithm are 0.0001 and 0.99, which are within the acceptable limit.
- The accuracy of the predicted result using XGBoost is 99%.
- These models can be used for the design of thermal devices.
- The cost and time of experiments can be reduced by using machine learning models.

Future research might concentrate on broadening the model's applicability by including other thermophysical characteristics, such as density, specific heat, and viscosity, using similarly varied datasets. Future research can investigate validation against recently published experimental data to further confirm the model's generalizability, even though the current study uses 865 data points from various literature sources and shows strong predictive accuracy through validation with one representative study. Other kinds of hybrid nanofluids with various base fluids or nanoparticle combinations can also be included in the model. Lastly, practical adoption in industrial and research applications would be facilitated by the creation of an intuitive software tool or interface based on the trained model.

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Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this article.

Authors Contribution Statement

Suvarna Kulal: Software editing, conceptualization, methodology and Writing the first draft. Shivananda Moolya: Validation, postprocessing, , supervision.
Yahya Al-Hashmi: Data collection. Omar Al Kiyumi: He oversees data administration and reference formatting for this study.
Tariq Al Rashdi: His responsibilities include modifying software and helped in creating the report's initial draft.

Nomenclature

ANN	Artificial Neural Networks
MSE	Mean Square Error
MHD	Magneto Hydro Dynamic
LR	Linear Regression
DT	Decision tree
RF	Random Forest
GB	Gradient Boosting

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