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Application of Machine Learning Algorithms in Predicting Rheological Behavior of BN-diamond/Thermal Oil Hybrid Nanofluids

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Abstract: The use of nanofluids in heat transfer applications has significantly increased in recent times due to their enhanced thermal properties. It is therefore important to investigate the flow behavior and, thus, the rheology of different nanosuspensions to improve heat transfer performance. In this study, the viscosity of a BN-diamond/thermal oil hybrid nanofluid is predicted using four machine learning (ML) algorithms, i.e., random forest (RF), gradient boosting regression (GBR), Gaussian regression (GR) and artificial neural network (ANN), as a function of temperature (25–65 °C), particle concentration (0.2–0.6 wt.%), and shear rate (1–2000 s^{-1}). Six different error matrices were employed to evaluate the performance of these models by providing a comparative analysis. The data were randomly divided into training and testing data. The algorithms were optimized for better prediction of 700 experimental data points. While all ML algorithms produced R^2 values greater than 0.99, the most accurate predictions, with minimum error, were obtained by GBR. This study indicates that ML algorithms are highly accurate and reliable for the rheological predictions of nanofluids.

Keywords: artificial neural network; gradient boost regression; Gaussian regression; machine learning; nanofluids; random forest; rheology

Citation: Ali, A.; Noshad, N.; Kumar, A.; Ilyas, S.U.; Phelan, P.E.; Alsaady, M.; Nasir, R.; Yan, Y. Application of Machine Learning Algorithms in Predicting Rheological Behavior of BN-diamond/Thermal Oil Hybrid Nanofluids. *Fluids* **2024**, *9*, 20. https://doi.org/10.3390/fluids9010020

Academic Editors: D. Andrew S. Rees and Rajinder Pal

Received: 4 December 2023
Revised: 4 January 2024
Accepted: 5 January 2024
Published: 9 January 2024

1. Introduction

The increase in the significance and demand of thermal management for heat transfer applications led to the introduction of nanofluids, owing to their exceptional thermal properties. Nanofluids are colloidal suspensions formed by dispersing nanoparticles of diameters less than 100 nm into base fluids such as water, ethylene glycol, water, etc. Hybrid nanofluids can be prepared through the dispersion of two or more dissimilar nanoparticles in the base fluid in the form of a composite or a mixture, and they are found to have greater thermal, hydrodynamic, and rheological properties than unitary nanofluids [1,2]. Suspensions of metals, metal oxides, and other compound nanoparticles allow for the enhancement of thermal conductivity. However, other thermophysical properties, such as the nanofluid's density, specific heat, and dynamic viscosity, also play an important role in improving its heat transfer performance in several applications [3,4]. Nanofluids have been utilized in heating and cooling systems, electronics, transportation, and power generation, amongst other applications [5]. The flow behavior of several different nanofluids and the

effect of other parameters such as magnetic field, solar energy, and entropy are now being studied for more advanced applications [6–8].

Viscosity is an essential thermophysical property because of its direct influence on the heat transfer characteristics of a nanofluid [9] and its effect on the pressure drop and pumping power. There is a higher pumping work demand for nanofluids because of their increased viscosity, in comparison to base fluids that do not contain nanoparticles. Consequently, the operating cost of the system increases [10,11]. The viscosity of nanofluids depends on several factors such as the type of base fluid and temperature, size and shape of particles, pH value, shear rate, etc. [12,13].

Several conventional models have been investigated to predict the viscosity of nanofluids. These include the Einstein [14], Brinkman [15], Wang [16], Krieger and Dougherty (K-D) [17], and Batchelor [18] models, among others. However, due to certain limitations, these models do not accurately predict the viscosity of nanofluids [19]. Researchers have also developed mathematical or empirical correlations for viscosity predictions with consideration of more parameters [20]. Recently, there has been a surge in the use of artificial intelligence (AI) and machine learning (ML) algorithms, particularly supervised learning techniques for the prediction of different thermophysical properties [21–23]. Despite being black-box models, the use of AI and ML is found to be fairly useful due to the challenges of processing data for the characterization of nanofluids [24]. Moreover, these predictions are also found to be highly accurate, granted that enough data points are available in the form of experimental data [25].

Amongst the many models available, artificial neural network (ANN) has been the most popular among researchers so far. Studies show that ANN is more accurate than conventional models and empirical correlations for viscosity predictions of nanofluids [26]. Li et al. [27] investigated the thermal performance of Al_2O_3/ethylene glycol nanofluids via a proposed correlation and ANN. The values for the coefficient of determination (R^2) for ANN predictions were found to be 0.9984 and 0.9997 for viscosity and thermal conductivity, respectively, showing more precise results than the correlation used. Davood et al. [28] used ANN to predict the viscosity of (WO_3)-MWCNTs/engine oil hybrid nanofluids as a function of the volume fraction of nanoparticles, shear rate, and temperature. The ANN results showed acceptable accuracy. In another study [29], the ANN prediction for the viscosity of CuO-MWCNT/engine oil hybrid nanofluids with inputs of temperature and volume fraction was found to be accurate and in good agreement with the experimental data. Similar results in favor of the accuracy of ANN compared to data fitting in an empirical correlation for MCWNT/water nanofluids were obtained in another study; ANN produced a maximum deviation of 0.28%, where solid volume fraction and temperature were used as inputs [30]. Thermophysical properties besides viscosity have also been predicted via ANN. Vafaei et al. [31] determined the thermal conductivity ratio of MgO-MWCNT/ethylene glycol hybrid nanofluids with a maximum deviation of 0.8% from the best ANN model. The ANN-predicted results in another study also provided good accuracy in comparison to experimental results for thermal conductivity ratios, density, viscosity ratio, and specific heat [32].

Researchers have also employed ML algorithms such as random forest (RF), multilayer perceptron (MLP), support vector regression (SVR), least-squared support vector machine (LSSVM), gradient boosting regression (GBR), extreme gradient boost (XGBoost), boosting regression trees (BRT), Gaussian regression (GR), decision tree regression (DTR), etc., and have drawn a comparison to determine which of these models exhibits a better performance for that particular nanosuspension. Ilyas et al. [33] employed ANN, RF, and GBR to predict the viscosity of diamond–graphene/mineral oil hybrid nanofluids based on input parameters of temperature, shear rate, and concentration. RF produced more accurate predictions than ANN and GBR. Gholizadeh et al. [34] assessed the predictive performance of RF against that of MLP and SVR, using five input parameters i.e., solid volume fraction, viscosity of the base fluid, temperature, density, and size of nanoparticle. The RF model provided the best prediction for the viscosity of nanofluids (R = 0.989). Bhanuteja et al. [35]

developed viscosity prediction models via four ML algorithms: GBR, RF, Adaboost, and voting regression. RF and GBR models demonstrated the best fit, with an R^2 greater than 0.99 and a maximum deviation of ±4.2%.

A recent study [30] estimated the specific heat capacity of water-based hybrid nanofluids considering the influence of several parameters using the GR, XGBoost, and SVR models. While all three algorithms showed excellent results, XGBoost outperformed the other two models, suggesting a much more feasible alternative to experimental approaches to determine the specific heat capacity of nanofluids. Ning et al. [36] used ANN and LSSVM for the prediction of filtration loss and shear stress of SiO_2/water drilling fluid. Both the models achieved R^2 values greater than 0.99, which demonstrated excellent accuracy. Similar results were obtained through ANN modeling to predict thermal conductivity (with the input parameters being temperature and concentration) and zeta potential (with the inputs being pH and concentration) of Fe_3O_4/water [37]. In another study [38], a GBR predictive model was developed to estimate the density of Al_2N_3, Si_3N_4, and TiN, suspended in ethylene glycol based on mass fraction, size and molecular weights of nanoparticles, and temperature. The proposed model exhibited high precision and was in good agreement with the experimental results. The results of some other studies that utilized ML algorithms for the prediction of thermophysical properties are given in Table 1.

Table 1. Use of ML techniques for high-accuracy predictions.

Nanofluid	Parameters	Inputs	Ranges	ML Techniques	Remarks	Ref.
TiO_2/water	Thermal Conductivity	Size Volume Fraction Temperature Thermal Conductivity	10–51.87 nm 0.002–4% 10–90 °C 0.6–1.455 W/mK	ANN, GBR, SVR, DTR, RF	GBR was found to be the most accurate, with an R^2 value of 0.99 for both testing and training data.	[39]
rGO-Fe_3O_4-TiO_2/ethylene glycol	Density Viscosity	Temperature Nanoparticle Concentration Shear Rate	25–50 °C 0.01–0.25% 1–1000 s^{-1}	BRT, SVR, ANN	R value of BRT for both density (0.9989) and viscosity (0.9979) was higher than that of SVR and ANN.	[40]
20 different Nanofluids	Thermal Conductivity	Temperature Volume Concentration Particle Size Mixture Ratio Acentric Factor of Base Fluid Thermal Conductivity Nanoparticle Density	20–70 °C 0–3.5 1.5–70 nm 0.15–0.85 0.343–0.659 0.16–1.44 W/mK 1000–10,500 kg/m^3	MLP-ANN, SVR	R^2 values of 0.99997 and 0.99788 were obtained by ANN and SVR, respectively.	[41]
ZrO_2/water	Viscosity	Temperature Concentration	10–65 °C 0.0125–0.2%	MLP-ANN	R^2 value of 0.99858 was obtained by ANN, demonstrating high-accuracy predictions.	[42]
ZnO-MWCNT (30:70)/W30 engine oil	Viscosity	Volume Fraction Temperature Shear Rate	0.05–1% 5–55 °C 50–1000 rpm	ANN	ANN produced high-accuracy predictions (compared to correlations), with an R^2 value of 0.9973.	[43]

ML algorithms have also been utilized for other applications besides evaluating the thermal performance of nanofluids, e.g., in the energy and environment sectors. Nie et al. [44] proposed a prediction model for electrical energy consumption in buildings using GBR. In another study [45], GR performed well compared to BRT in evaluating the performance of a small-scale solar organic Rankine cycle system. Cai et al. [46] used GBR for the prediction of net ecosystem carbon exchange (NEE), and RF for identifying the significant parameters influencing NEE. Comparison with three other models concluded that GBR performed high-accuracy predictions.

There is scarcely any literature available using some of the more recent ML algorithms, let alone on the predictions of thermophysical properties, particularly viscosity, despite being significantly influential to thermal transfer, which is the value added by this research. In

this study, the viscosity of a boron nitride (BN)–diamond (1:1)/thermal oil hybrid nanofluid was predicted via four models, i.e., random forest (RF), gradient boosting regression (GBR), Gaussian regression (GR), and artificial neural network (ANN), using 700 experimental data points. The rheological properties of BN-diamond nanofluids have not been subjected to any prior predictive investigation via machine learning techniques or otherwise. A comparative analysis of the four algorithms is presented to evaluate the performance and the accuracy of each model.

2. Methodology

2.1. Experimental Dataset

A BN-diamond/thermal oil hybrid nanofluid was employed as the experimental dataset for the prediction of viscosity in this study [47]. The nanomaterials included spherical diamond nanoparticles with a diameter of 3–10 nm and purity > 98.3%, as well as hexagonal BN with a size of 70–80 nm and 99.8% purity. The nanomaterials were mixed in equal-mass proportions (1:1) to form a hybrid system. The base fluid used was commercial thermal oil, used to disperse the hybrid nanomaterials. The details are included in reference [47].

The nanofluid was prepared using the two-step method, which involved the formation of a homogeneous suspension by adding the nanoparticles in thermal oil, i.e., the base fluid, in a 1:1 ratio, as it was stirred continuously. An inorganic surfactant (Span-85) was added to stabilize the nanofluids [47]. In reference [47], the rheology of BN-diamond/thermal nanosuspensions was evaluated as a function of temperature, particle concentration, and shear rate ranging from 25 to 65 °C, 0.2 to 0.6 wt.%, and 1 to 2000 s^{-1}, respectively.

In this study, BN-diamond/thermal oil was subjected to rheological predictions via four machine learning techniques i.e., random forest (RF), gradient boosting regression (GBR), Gaussian regression (GR), and artificial neural network (ANN), using 700 experimental data points, with inputs of temperature, particle concentration, and shear rate. The distribution of the 700 data points used, with respect to the three input parameters over their experimental ranges (25–65 °C, 0.2–0.6 wt.%, and 1–2000 s^{-1}), is illustrated in a violin plot (Figure 1). The distribution of data points was even for temperature and particle concentration, while shear rate and viscosity (the output of the models) showed more variation, with medians in the lower region. Experimental results showed that there was a significant change in viscosity for shear rates under 100 s^{-1} (where the data points are largely concentrated), and a Newtonian behavior was observed [47].

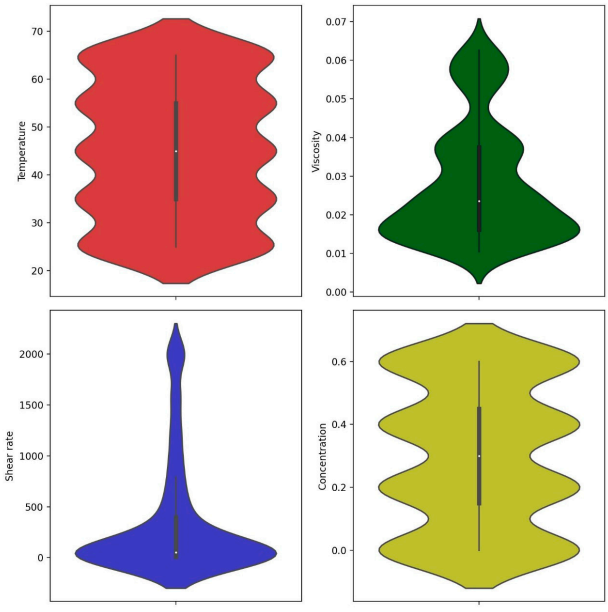

Figure 1. Violin plot of the experimental dataset used for modeling.

The accuracy of these predictions was evaluated by comparison with the measured viscosity from the aforementioned study. (An overview of the methodology is presented in Figure 2.) Six error matrices i.e., coefficient of determination (R^2), mean absolute error (MAE), root mean square error (RMSE), bias, Legate and McCabe Index ($E_{L,M}$) and Willmot Index of Agreement (I_A), were used for this purpose, and they are given in Equations (1)–(6), respectively [33].

$$R^2 = 1 - \frac{\sum_1^n (y_i - \hat{y}_i)^2}{\sum_1^n (y_i - \overline{y}_i)^2}. \quad (1)$$

$$MAE = \frac{1}{N}\sum_1^n |y_i - \hat{y}_i| \quad (2)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{N}} \quad (3)$$

$$bias(\hat{\theta}) = E_\mu(\hat{\theta}) - \theta \quad (4)$$

$$E_{L,M} = 1 - \frac{\sum_{i=1}^{i=N} |y_i - \hat{y}_i|}{\sum_{i=1}^{i=N} |y_i - \overline{y}_i|} \quad (5)$$

$$I_A = 1 - \frac{\sum_{i=1}^{i=N} (y_i - \hat{y}_i)^2}{\sum_{i=0}^{i=N} (|y_i - \overline{y}_i| + (\hat{y}_i - \overline{y}_i))^2} \quad (6)$$

where y_i is the given data point, $\overline{y}_i$ is the mean of all the data points, $\hat{y}_i$ denotes the predicted values, and N is the number of observations.

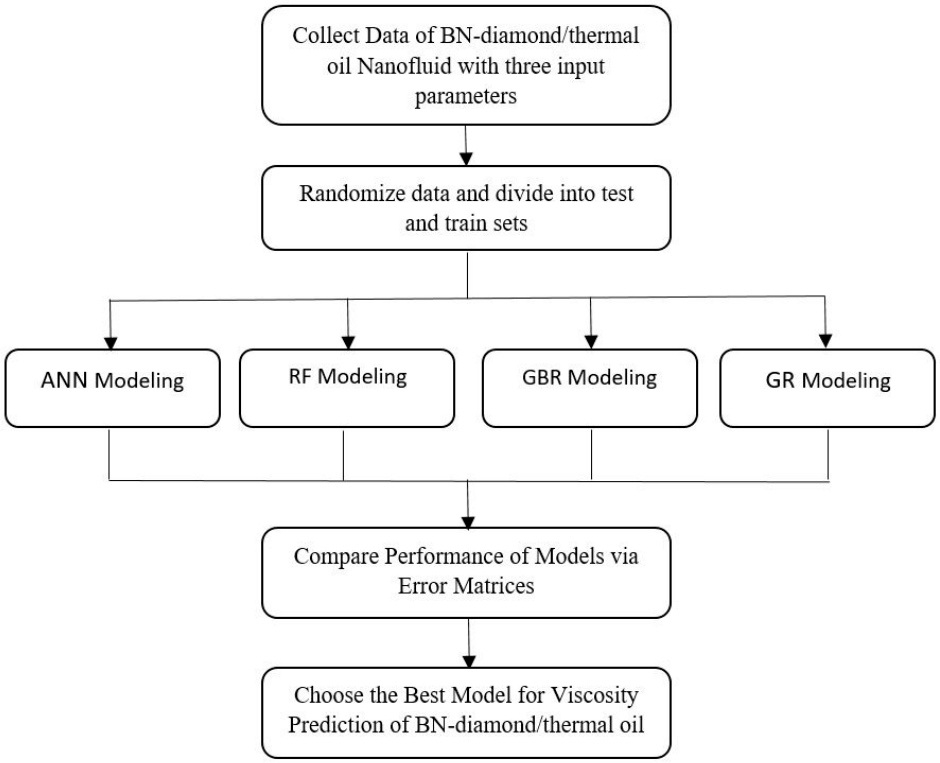

Figure 2. An overview of the methodology applied for predicting rheology via machine learning algorithms.

2.2. Predictions via Random Forest (RF)

Random Forest (RF) is a fast and reliable model that makes decisions based on the characteristics of several decision trees. The more diverse these trees are, the more consistent the RF model is [39]. It utilizes a statistical technique called bagging.

2.3. Predictions via Gradient Boosting Regression (GBR)

In gradient boosting regression, the learning procedure sequentially and consecutively adds new models to the ensemble, which produces an accurate prediction of the response variable [48]. Gradient boosting regression utilizes an algorithm that minimizes the amount of loss that occurs [49] by fitting a regression tree on the negative gradient of a specified loss function [39]. The loss function applied can be arbitrary, which allows GBR to be flexible for a particular dataset.

2.4. Predictions via Gaussian Regression (GR)

GR is a probabilistic regression-based model, i.e., it is associated with learning a continuous function from training data. Several covariance functions can be integrated with GR to obtain optimized results from testing data. The relationship between inputs and outputs in GR can be described as shown in Equation (7) [50].

$$y = f(x) + \xi\xi \sim N\left(0, {v_n}^2\right) \tag{7}$$

where N is the number of pairs of feature vectors and ξ is distributed with zero mean noise.

2.5. Predictions via Artificial Neural Network (ANN)

ANN models contain a hidden layer which includes the number of neurons, the activation function, the number of layers, and a training algorithm. ANN finds the connection between the data provided to the model; the output depends on the back propagation of the randomly initialized weights of the input data [39]. The neural network in this study was modeled using the Levenberg–Marquardtt training algorithm with three hidden layers. It was modeled using a number of neurons ranging from 2 to 12. For proper optimization, the errors were all generated for different numbers of neurons. As demonstrated in Figure 3, the least error (in accordance with all error matrices) was detected at 12 neurons.

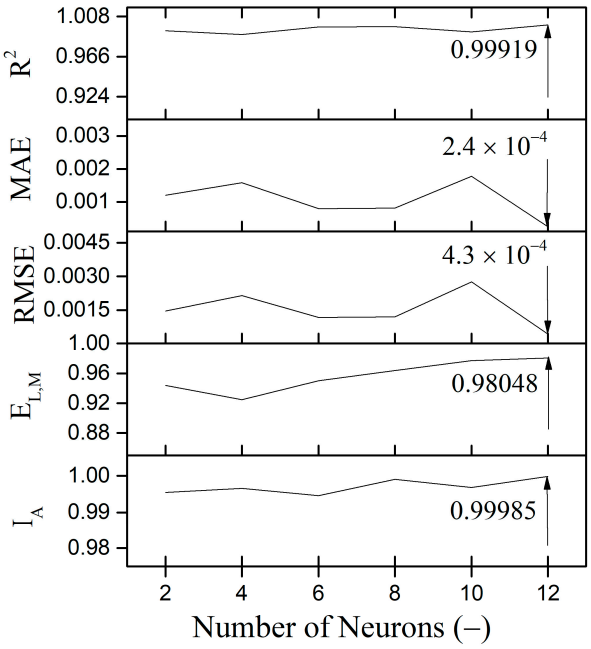

Figure 3. Error analysis to find the optimum number of neurons for ANN.

3. Results and Discussion

The rheology of BN-diamond/thermal oil nanosuspensions was predicted via random forest (RF), gradient boosting regression (GBR), Gaussian regression (GR), and artificial neural network (ANN) machine learning algorithms as a function of three input parameters: temperature, particle concentration, and shear rate.

The data points were randomized and divided into testing and training data. It is important to note that all data points were used for modeling the algorithms. The original experimental data (taken from [47]) were not refined or normalized and no data points were excluded for rheological predictions. This signifies that the errors generated also include data points which may show a certain degree of deviation.

3.1. Random Forest (RF)

RF showed the most deviation in data and the least accurate predictions amongst the four ML algorithms. The distribution of the data points for RF against absolute difference, which is the relative error between the testing and training data, is shown in Figure 4. Data far from the origin represent more deviation. It is noticeable from the figure that data points are significantly scattered for the both training and testing sets, and they are less concentrated around nil absolute difference.

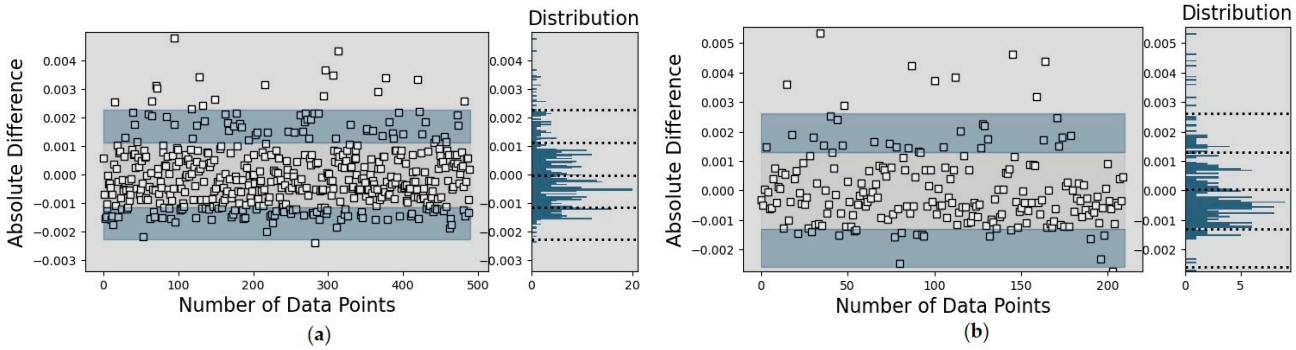

Figure 4. Distribution of data points for (**a**) RF training data and (**b**) RF testing data.

One of the key matrices used to validate the performance of the algorithms is the coefficient of determination (R^2), which represents the relationship between the predicted and the experimentally measured viscosity; an R^2 value close to 1 indicates accuracy in the predictions. Although all four ML algorithms produced good predictions, with an R^2 greater than 0.99 for the testing and training data, the least effective of them is RF, i.e., R^2_{train} = 0.994368 and R^2_{test} = 0.99258 (Figure 5).

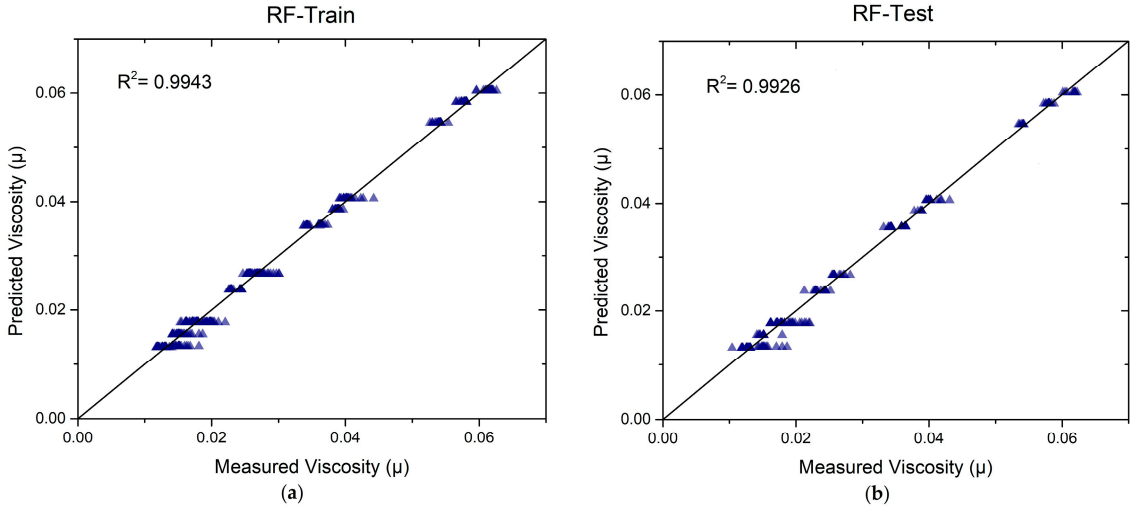

Figure 5. Measured vs predicted viscosity for (**a**) RF training data and (**b**) RF testing data.

3.2. Gradient Boosting Regression (GBR)

GBR training and testing data, illustrated in Figure 6, both show high accumulation of data at absolute difference of zero. Very few data points lie outside the ranges of −0.00025 up to 0.00025 and −0.0005 up to 0.0005 for the training and testing data, respectively. The

most accurate predictions for the viscosity of the BN-diamond/thermal oil nanofluid were obtained by GBR, with R^2 values of R^2_{train} = 0.999939 and R^2_{test} = 0.99953. The plots in Figure 7 are well accumulated to the 45° reference, exhibiting an excellent fit to the model. Predicted data scarcely show any deviation from the experimentally measured viscosity, demonstrating the high precision and accuracy of the rheological behavior predictions and the reliability of the GBR model. This was enabled by the iterative boosting of a weaker learner into a stronger learner.

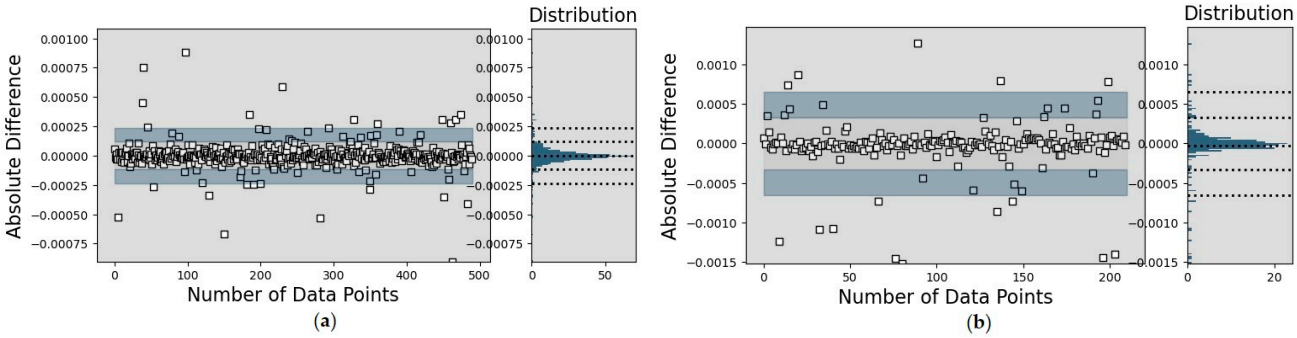

Figure 6. Distribution of data points for (**a**) GBR training data and (**b**) GBR testing data.

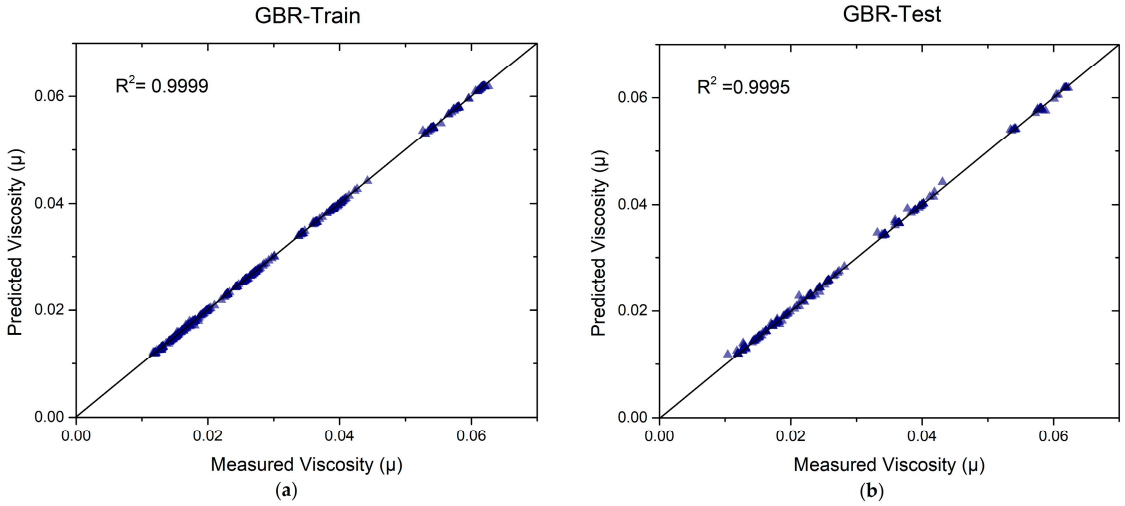

Figure 7. Measured vs. predicted viscosity for (**a**) GBR training data and (**b**) GBR testing data.

3.3. Gaussian Regression (GR)

Rheological predictions via GR were good, but not the most accurate out of the algorithms used. More convergence of data was observed in the training set (plots accumulated between −0.001 and 0.001) than in the testing set, as seen in Figure 8. This reflects on the greater deviation shown in Figure 9, where the R^2 value of the testing set, i.e., 0.994911 was lower than that of the training set, i.e., 0.998587. This result of GR may be attributed to its potential to not scale very well with an increased number of data points.

3.4. Artificial Neural Network (ANN)

ANN produced the second most accurate predictions, after GBR. The absolute difference ranged from −0.001 to 0.003, with plots more concentrated up to 0.001, as illustrated in Figure 10; a higher level of convergence of data was observed in comparison to GR and RF. From the regression plot depicted in Figure 11, a little more deviation from the reference line in the testing set is observed. However, the R^2 values for both the training and testing data (R^2_{train} = 0.999193 and R^2_{test} = 0.998561) were found to be satisfactory. ANN is a highly reliable model owing to its ability to optimize data by selecting the number of neurons

by trial and error. Optimization techniques reduce error, thus increasing the accuracy of the predictions.

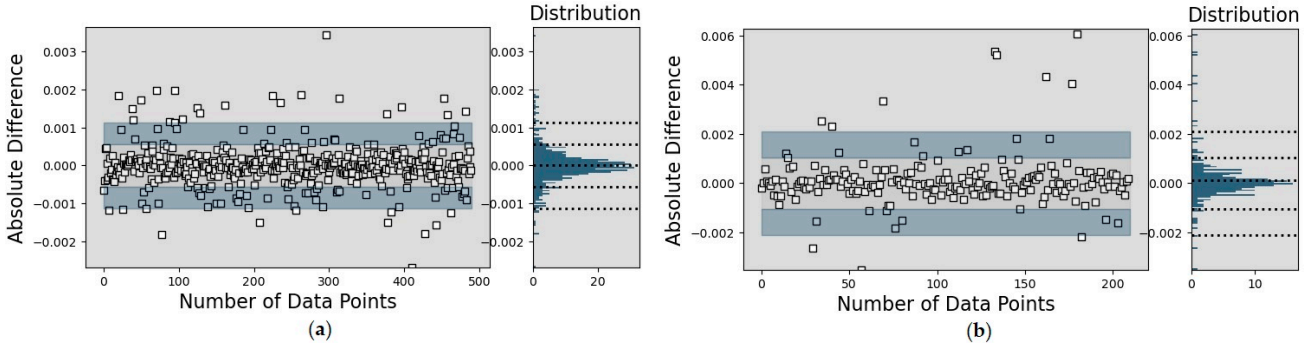

Figure 8. Distribution of data points for (**a**) GR training data and (**b**) GR testing data.

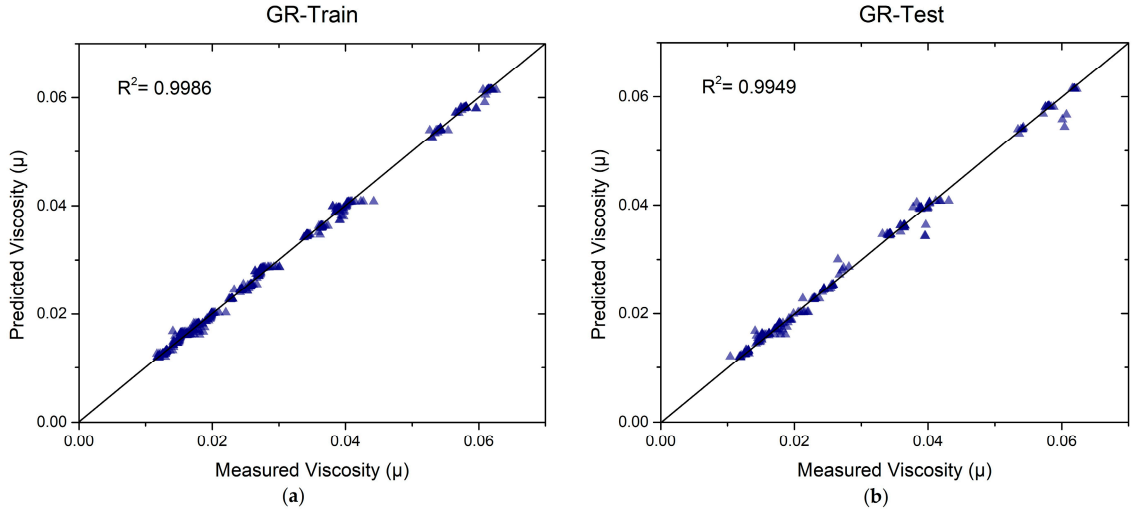

Figure 9. Measured vs predicted viscosity for (**a**) GR training data and (**b**) GR testing data.

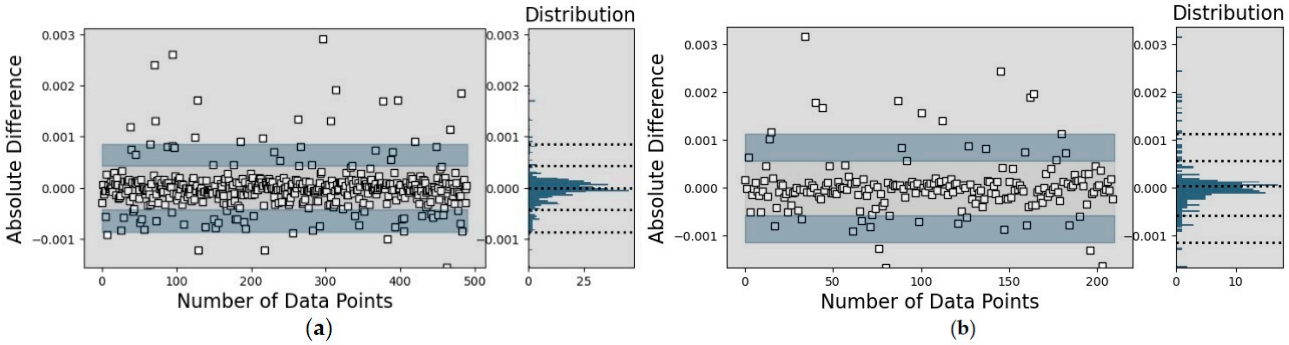

Figure 10. Distribution of data points for (**a**) ANN training data and (**b**) ANN testing data.

These results were further verified by using five other error matrices, i.e., mean absolute error (MAE), root mean square error (RMSE), bias, the Legate and McCabe Index ($E_{L,M}$), and the Willmot Index of Agreement (I_A). The comparison of these error matrices (and R^2) with RF, GBR, GR, and ANN for testing and training data is presented in Figure 12. MAE is the average variance between the significant and projected values of the same dataset, RMSE is the average difference between the experimentally measured and the predicted values, and bias refers to the error between the average predictions and the measured values. $E_{L,M}$ and I_A are measures of how well the model fits. Higher values of

MAE, RMSE, and bias errors and lower values of $E_{L,M}$ and I_A indicate less accuracy in the predictions obtained by the ML algorithms. It can be observed from Figure 12 that errors in RF were much greater in number than those in GR, ANN, and GBR (in the same order), and GBR had the least errors and the highest values of $E_{L,M}$ and I_A, i.e., 0.9952 and 0.99998 for training data and 0.98755 and 0.99988 for testing data, respectively.

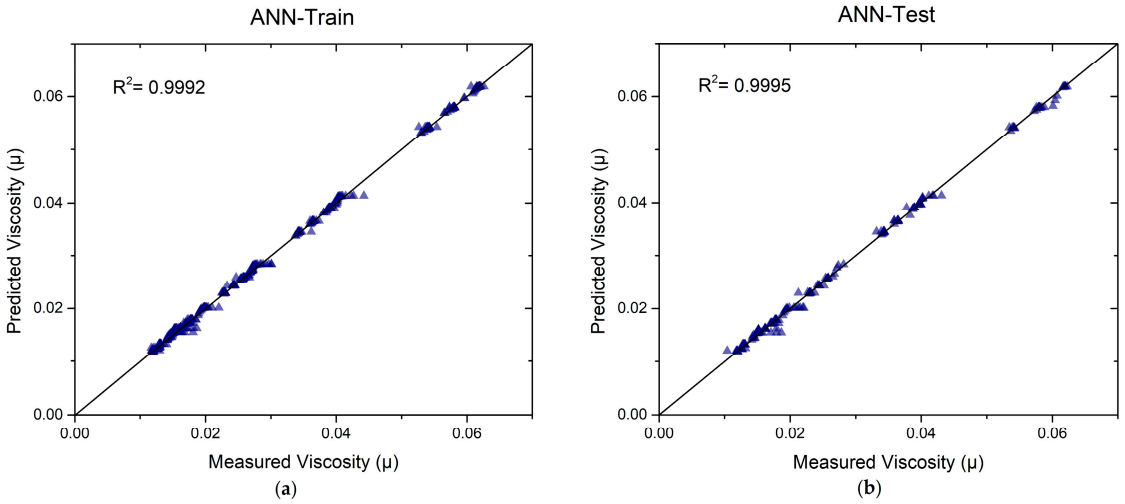

Figure 11. Measured vs predicted viscosity for (**a**) ANN training data and (**b**) ANN testing data.

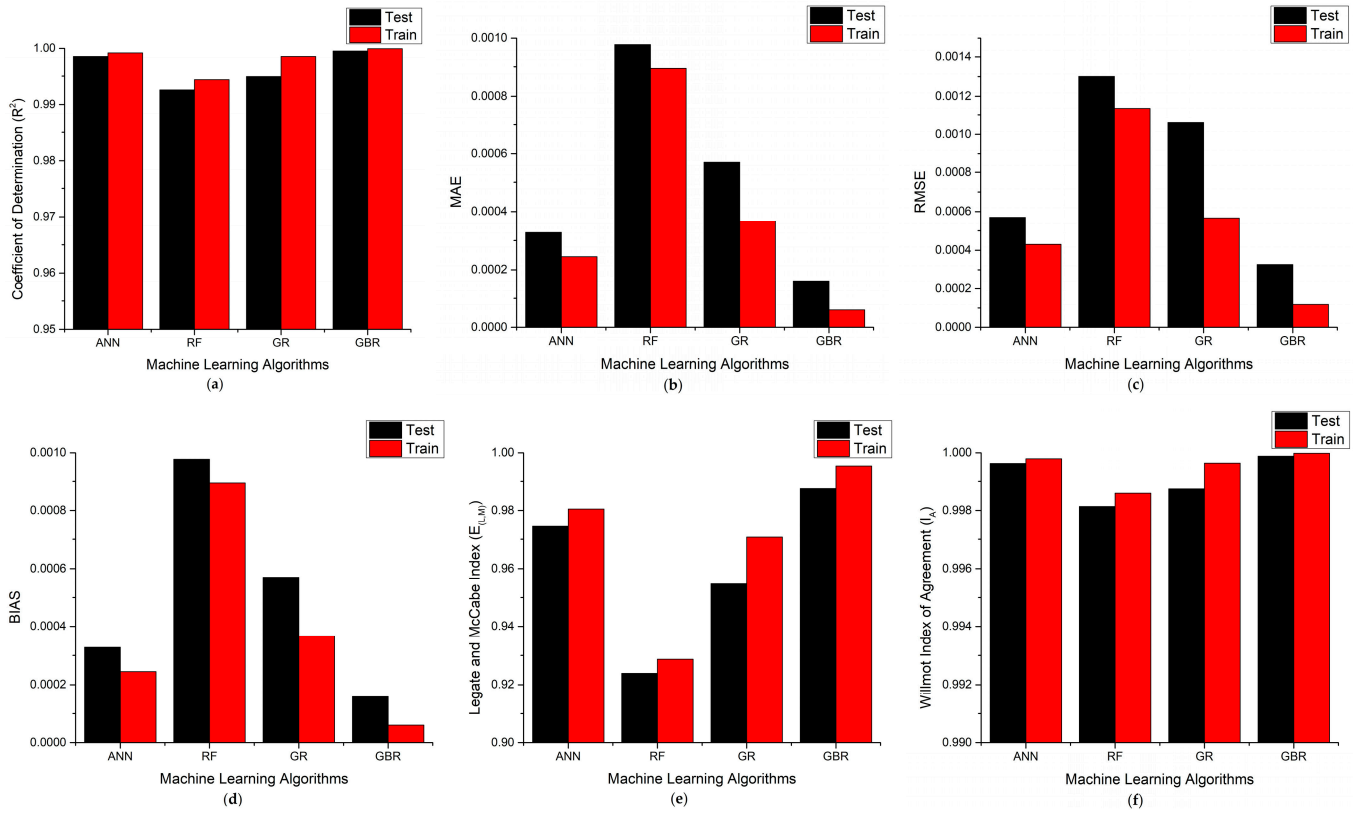

Figure 12. Comparison of error matrices between testing and training data of RF, GBR, GR, and ANN. (**a**) Coefficient of determination (R^2); (**b**) mean absolute error (MAE); (**c**) root mean square error (RMSE); (**d**) bias; (**e**) Legate and McCabe Index ($E_{L,M}$); (**f**) Willmot Index of Agreement (I_A).

4. Conclusions

In light of the limited studies available on the rheological behavior predictions of hybrid nanofluids, especially via machine learning (ML) algorithms, this study aimed to predict the viscosity of BN-diamond/thermal oil using four different ML algorithms, i.e., random forest (RF), gradient boosting regression (GBR), Gaussian regression (GR), and artificial neural network (ANN). Temperature, particle concentration, and shear rate were the three input parameters of the models, with the output being viscosity. The performance of these models was evaluated using six error matrices, namely, coefficient of determination (R^2), mean absolute error (MAE), root mean square error (RMSE), bias, the Legate and McCabe Index ($E_{L,M}$), and the Willmot Index of Agreement (I_A). Results showed that all R^2 values were greater than 0.99; the highest R^2 was obtained using GBR, followed by ANN, GR, and RF (which showed the most deviation from the experimentally measured viscosity). Overall, ML algorithms were found to be highly accurate and reliable for rheological predictions, specifically in comparison to conventional and empirical models.

Author Contributions: Conceptualization, S.U.I., P.E.P. and Y.Y.; Data curation, S.U.I.; Formal analysis, A.A., N.N., A.K. and M.A.; Funding acquisition, A.A.; Investigation, M.A. and R.N.; Methodology, A.A., A.K., S.U.I., P.E.P., M.A. and Y.Y.; Resources, S.U.I. and M.A.; Software, A.K.; Supervision, P.E.P. and Y.Y.; Validation, A.K. and S.U.I.; Visualization, N.N. and R.N.; Writing—original draft, A.A. and N.N.; Writing—review and editing, P.E.P. and Y.Y. All authors have read and agreed to the published version of the manuscript.

Funding: This work was funded by the University of Jeddah, Jeddah, Kingdom of Saudi Arabia, under grant No. UJ-21-ICI-13.

Data Availability Statement: The data can be available on request.

Acknowledgments: The authors acknowledge the University of Jeddah, KSA, for technical and financial support.

Conflicts of Interest: The authors declare no conflicts of interest.

Nomenclature

Symbols	
E_{LM}	Legate and McCabe Index, LM Index (-)
I_A	Willmot Index of Agreement, W Index (-)
N	Number of observations in Equations (1)–(7)
R^2	Coefficient of determination (-)
T	Temperature (°C)
y_i	Given data point in Equations (1)–(6)
$\hat{y}_i$	Predicted values in Equations (1)–(6)
$\overline{y}_i$	Mean of the given values in Equations (1)–(6)
Greek Symbols	
φ	Nanomaterial concentration (%)
γ	Shear rate (1/s)
μ	Viscosity (Pa·s)
Abbreviations	
AI	Artificial intelligence
ANN	Artificial neural network
BRT	Boosting regression trees
DTR	Decision tree regression
GBM	Gradient boosting machine
GR	Gaussian regression
LSSVM	Least squared support vector machine
MAE	Mean absolute error
ML	Machine learning
MLP	Multilayer perceptron
RF	Random forest

RMSE	Root mean square error
R^2_{test}	Coefficient of determination for testing set
R^2_{train}	Coefficient of determination for training set
SVR	Support vector regression
XGBoost	Extreme gradient boost

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