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Computational Analysis on the Thermo-Physical Properties of Al_2O_3 Nanoparticles Suspended in Different Based Fluids Using Back-Propagated Deep Neural Networks

Maryam Akhwater *
* Department of physics, Faculty of art and science – Almarj, University of Benghazi, Libya

تحليل حسابي للخصائص الفيزيائية الحرارية للجسيمات النانوية لاكسيد الالومنيوم العالقة في سوائل مختلفة باستخدام الشبكات العصبية العميقة ذات الانتشار العكسي

مريم اخويطر *
* قسم الفيزياء، كلية الآداب والعلوم - المرج، جامعة بنغازي، بنغازي، ليبيا

*Corresponding author: maryam.akhwater@uob.edu.ly

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Abstract:
Over the last few years, various nanofluids have been produced by suspending nonmetallic nanometer-sized solid particles (< 100 nm) in heat transfer fluids like water, and ethylene glycol. The thermo-physical properties in terms of thermal conductivity, viscosity, and heat and mass transfer characteristics have been widely investigated for their potential thermodynamic applications. In the present work, different supervised machine learning and back-propagated deep neural network (BDNN) methods were adopted to predict the thermal conductivity and viscosity of Al_2O_3 nanoparticles dispersed in several base fluids of water and ethylene glycol W–EG. The training data were collected from previously reported experimental data to be applied in BDNN and two different machine learning models, polynomial regression model (PRM) and decision tree regression (DTR). In addition, other proposed BDNNs were built up, tested, and evaluated using different numbers of hidden layers and neurons to determine the optimum network architecture in terms of its predictive precision. Furthermore, to assess the accuracy and predictive ability of all three prediction algorithms, statistical indices including root mean square error (RMSE), relative error (r), and regression coefficient R^2 coupling with regression graphs using the training data sets were used. The results indicated that BDNN is the most efficient model in predicting the thermo-physical properties of W–EG Al_2O_3, showing great agreement between simulated and targeted dependent variables with excellent accuracy of up to 996% and 998% for thermal conductivity and viscosity, respectively. In contrast, the PRM has low predictive capability and unsatisfactory performance with higher RMSE values of 0.0132 and 0.0201 for thermal conductivity and viscosity, respectively.

Keywords: Al_2O_3 Nanofluids; Back-Propagated Deep Neural Network; Decision Tree; Polynomial Regression; Thermal Conductivity; Viscosity.

الملخص
على مدى السنوات القليلة الماضية، تم إنتاج العديد من السوائل النانوية عن طريق مزج جزيئات صلبة غير معدنية بحجم النانومتر (100 نانومتر) في سوائل ناقلة للحرارة مثل الماء و الإيثيلين جلايكول. تم فحص الخصائص الفيزيائية الحرارية من حيث الموصلية الحرارية واللزوجة وخصائص انتقال الحرارة والكتلة على نطاق واسع نظرا لتطبيقاتها الديناميكية الحرارية المحتملة. في هذا العمل، تم اعتماد طرق مختلفة للتعلم الآلي الخاضع للإشراف والشبكة العصبية العميقة ذات الانتشار العكسي *(BDNN)* للتنبؤ بالموصلية الحرارية واللزوجة لجسيمات أكسيد الألومنيوم النانوية المختلطة في العديد من السوائل الأساسية للماء والإيثيلين جلايكول *(W-EG)* . في هذه الدراسة تم جمع بيانات التدريب من البيانات التجريبية التي تم نشرها سابقًا ليتم تطبيقها في نماذج *BDNN* ونموذجين اخرين مختلفين للتعلم الآلي وهما: نموذج الانحدار متعدد الحدود *(PRM)* ونموذج انحدار شجرة القرار *(DTR)* . بالإضافة إلى ذلك، تم إنشاء شبكات *BDNN* المقترحة الأخرى واختبارها وتقييمها باستخدام أعداد مختلفة من الطبقات المخفية والخلايا الاصطناعية العصبية لتحديد بنية الشبكة المثلى من حيث الدقة التنبؤية. علاوة على ذلك، لتقييم الدقة والقدرة التنبؤية لجميع خوارزميات التنبؤ الثلاثة، تم استخدام المؤشرات الإحصائية بما في ذلك خطأ الجذر التربيعي المتوسط *(RMSE)* والخطأ النسبي *(r)* ومعامل الانحدار R^2 المقترنة مع الرسوم البيانية للانحدار باستخدام مجموعات بيانات التدريب. أشارت النتائج إلى أن *BDNN* هو النموذج الأكثر كفاءة في التنبؤ بالخصائص الفيزيائية الحرارية لاكسيد الالومنيوم، حيث يُظهر اتفاقًا كبيرًا بين المتغيرات التابعة المتنبئة والحقيقية بدقة ممتازة تصل إلى 996٪ و 998٪ للتوصيل الحراري واللزوجة، على التوالي. في المقابل، يتمتع نموذج *PRM* بقدرة تنبؤية منخفضة وأداء غير مرض مع قيم *RMSE* مرتفعة تبلغ 0.0132 و 0.0201 للتوصيل الحراري واللزوجة، على التوالي.

الكلمات المفتاحية: الموائع النانوية لأكسيد الألومنيوم ، الشبكة العصبية العميقة ذات الانتشار العكسي، شجرة القرار، الانحدار متعدد الحدود، الموصلية الحرارية، اللزوجة.

Introduction

Nanofluids as smart fluids have gained enormous attention from scientists and engineers due to their excellent thermo-physical properties, such as thermal conductivity, thermal diffusivity, viscosity, and the ability to enhance the heat transfer rate compared to their microsized counterparts. Even though base heat transfer fluids such as water, thermal oil, acetone, decene, and ethylene glycol have been usually utilized in several industrial and commercial platforms, including power generation, heating, and cooling processes, they are still unable to achieve the required performance for thermal and mechanical devices due to their low thermal conductivity. However, when nanoparticles are added to the base fluids, the thermo-physical properties of these fluids can be significantly improved by enhancing the thermal conductivity, hence boosting the capability of heat transfer, increasing stability, reducing energy consumption, and speeding up the machine performance [1]. In general, nanofluids research has rapidly grown and exploited in many engineering and industrial applications, including heating and cooling systems [2], solar energy field [3], drug delivery and biomedical technology [4], nuclear reactors [5], thermal processing of food products [6]. In particular, the viscosity and thermal conductivity of nanofluids have been hot research topics in many theoretical and experimental literatures over recent years due to their significant role in the enhancement of heat transfer applications. Further, the viscosity and thermal conductivity have been mostly utilized to understand the heat transfer characteristics and energy transfer mechanisms of nanofluids.

In addition, machine learning and artificial intelligence methods have made enormous evolutions in estimating the thermal conductivity and viscosity of nanofluids. Wang et al. [7] enhanced the accuracy in predicting the thermal conductivity of Cu/Al2O3-EG/W hybrid nanofluids using a genetic algorithm (GA) and a mind evolutionary algorithm (MEA) coupled with a back propagation neural networks (BPNNs). They found that the BPNNs produced higher prediction accuracy compared to binary PRM. Barai et al. [8] predicted the thermal conductivity of rGO nanocomposite-based nanofluids using an artificial neural network (ANN) model. The predicted thermal conductivity was in reasonable agreement with the experimental data and showed a correlation coefficient of 0.956. He et al. [9] modeled the thermal conductivity of ZnO–Ag (50%–50%)/Water hybrid Newtonian nanofluid using ANNs and the surface fitting method. The experimental data sets of nanoparticle volume fraction and temperature were considered as input variables, while thermal conductivity was the output response. It showed that the ANNs provided a good agreement between the simulated and actual data sets with higher precision.

Sharma et al. [10] modeled the thermal conductivity of a TiO2–water nanofluid by ANN models coupled with gradient boosting (GB), support vector regression (SVR), DTR, and random forest (RF). The dataset covers different characteristics of nanofluids, including the size and shape of nanoparticles,

volume fraction of the nanoparticles, temperature, and thermal conductivity. Upon comparative analysis of these algorithms, it was found that the GB model was the optimum algorithm with a high accuracy of 99%. In the current paper, BDNN, DTR, and PRM were applied to accurately predict the thermal conductivity and viscosity of Al_2O_3 nanoparticles dispersed in several base fluids (20:80%, 40:60%, 60:40%) of W–EG mixtures under temperatures between 20 °C and 60 °C and in volume concentrations between 0.3% and 1.5% [11].

Material and Methods

BDNNs Modelling

The focus of this study is on the modeling and estimation of the thermo-physical properties of Al_2O_3 nanoparticles dispersed in several weight concentrations of EG-W base fluids. Hence, thermal conductivity and viscosity were predicted as a function of volume concentrations and temperatures, so for modeling, these two independent key variables were considered input parameters while the thermal conductivity and viscosity were the output responses of the networks. Traditional theoretical techniques and simulations such as Hamilton-Crosse [12,13], Maxwell [14], Einstein model [15], and Bruggeman [16] have their obstacles and challenges for precisely estimating the nanofluids flow features in different media. In these methods, nanoparticles are usually treated as idealized spherical-shaped particles at low-volume concentrations with no interactions between them. For instance, according to the Maxwell model nanoparticles are disconnected and immobile within a continuous environment [14]. Moreover, classical data-driven models of numerical simulations and correlations, such as molecular dynamics (MD) and finite element analysis (FEA) can produce important acuity. However, these models could not be efficiently used for the complex and dynamic behaviour of fluid parameters as the precision of their predictability is still under debate. Further, variation in the nanoparticle concentrations could lead to a change in the thermo-physical characteristics of the nanofluids, which required to be considered in the theoretical simulations.

On the other hand, artificial intelligence approaches illustrated by machine learning methods have interestingly grown in developing trustable prediction models with many benefits in terms of accuracy, credibility, and cost efficiency. These novel models have significant roles in manipulating and training different datasets under several complicated conditions, determining general patterns of simulated data, and yielding higher performance than other correlation algorithms. From an applications perspective, it is highly recommended to design a sophisticated artificial system and machine learning technique to deal with complicated, nonlinear interactions without needing to do certain computing equations of the multi-factorial thermo-physical mechanism of nanofluids. In particular, multilayer perceptron BDNNs are one of the most frequently used artificial intelligence methods due to their efficiency in approximating nonlinear and complex relationships and enhancing the thermal characteristics of nanofluids [17]. Generally, artificial neural networks (ANNs) imitate the synaptic structure of human neurons in manipulating data and receiving rules. In BDNNs, the artificial networks consist of more than one hidden layer of neurons (nodes), and according to the convolution and noise of training data, the hidden layers themselves can contain more than one layer. The nodes are summed up in the first layer and connected to the nodes of the next layer by weight vectors [18]. The output of the network (y_j) can be defined for a group of the input variables (x) as shown in Eq.1 [19].

$$y_j = f\left(\sum_{i=1}^{n} w_{ji} x_i + b_j\right) \quad j = 1,2,\dots\dots, K \qquad (1)$$

Where *xi* describes the input vector, w_{ji} and b are respectively, the weights and biases, *K* represents the number of nodes, and *f* is the activation function. By using the training data, the values of weights and biases are calibrated according to the appropriate loss function, which represents the divergence between predicted and actual data. During an iterative process, the weights of neurons are optimized to minimize the gradient error between the experimental and predicted parameters and get an optimal output. When this target is accomplished, the training procedure is ended, the bias and weight values are maintained constant, and the simulation process of the considered dependent variables is initiated. The learning procedure in multi-layered BDNNs is achieved by adjusting the bias and weight using the back propagation technique and optimization algorithms such as a scaled conjugate gradient, which is adopted in this research by applying the sigmoid function in the hidden layers as an activation function. The sigmoid function is expressed in Eq.2.

$$\sigma(x) = \frac{1}{1+e^{-x}} \qquad (2)$$

In the present study, the trial and error approach was chosen to identify the optimal BDNN architecture. Since the performance and accuracy of the artificial network are extremely influenced by the number of neurons in the hidden layers, several BDNNs are built and trained for each suggested neuron number in the hidden layers, which are considered from 3 to 12 neurons, to find the desired number of neurons in these layers. For each iteration, the performance is further evaluated, in terms of RMSE; hence the desired architecture of BDNN would represent the lowest value of RMSE.

Table 1: The impact of several numbers of neurons on the BDNN performance.

Neurons number	RMSE
3	0.0567
4	0.0473
5	0.0278
6	0.0586
7	0.0722
8	0.0434
9	0.0149
10	0.1074
11	0.1101
12	0.2201

Based on the illustrated results in Table 1 and Figure 1, the optimum neuron set is 9 in the first hidden layers. After developing the promising performance, the thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids can be estimated with high accuracy using a three-layered BDNN with 9 and 2 neurons in the first and second hidden layers, respectively, and one neuron in the output layer. The BDNN architecture is illustrated in Figure 2.

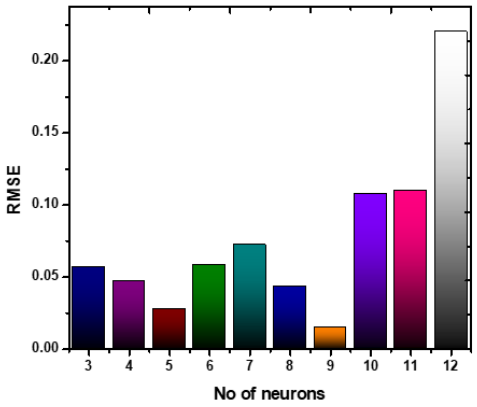


Figure 1: Variation of RMSE with the different number of neurons in the first hidden layer.

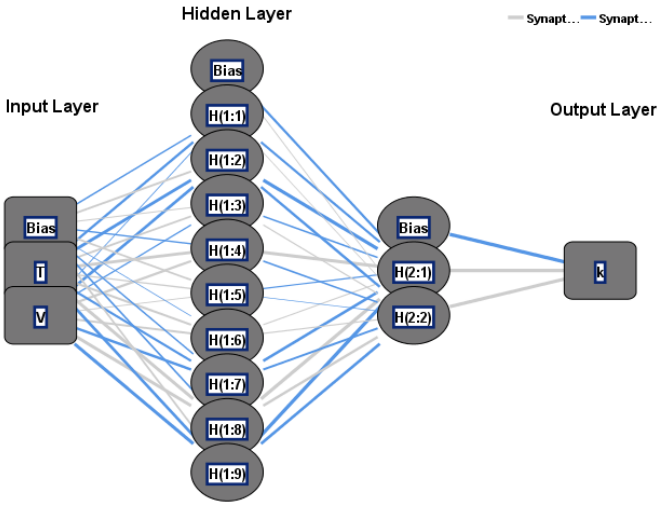


Figure 2**:** The structure of BDNN used for prediction of the thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids.

Machine Learning-Based Modelling

In this research, two different machine learning algorithms, i.e., PRM and DTR are applied as predictive models to simulate the thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids. DTR has become one of the most popular supervised machine learning algorithms for solving regression and classification problems. Due to their clarification, simplicity of utilization, and efficiency in dealing with numerical and categorical variables, the DTR approach is adopted in many fields, including statistics, artificial intelligence learning, pattern recognition, and data mining. The decision tree consists of nodes describing feature tests and branches describing responses to these tests, culminating in leaf nodes that produce the predictive output. In the tree, every node can decide according to the input variables, increasing the model precision through variance reduction [20]. The instance space is divided by the test node into two or more sub-spaces based on a specific discrete function of the input feature values. In this model, each node is classified based on the cost function expressed as [21].

$$J(k, t_k) = \frac{m_L}{m} MSE_L + \frac{m_R}{m} MSE_R \qquad (3)$$

Where k is the splitting feature, t_k is the threshold, MSE is the mean square error and m, m_L and m_R are the total number of training instances, left-node and right-node training instances, respectively. In addition, PRM is one of the most effective machine learning algorithms, which extensively have been used for prediction tasks. In general, PRM is an additional expansion to simple linear regression that provides a good prediction by modelling main properties into higher-order terms of the independent parameters, determining complicity underlying curvature or non-linear patterns. Mathematically, the PRM can be expressed by the following equation [22].

$$y = b_0 + b_1 x_i + b_2 x_i^2 + b_3 x_i^3 + \cdots \ldots . b_k x_i^k + e_i \qquad i = 1,2, \ldots . , n \qquad (4)$$

Where y is the dependent variable, x is the independent predictor variable, b_0 represents the Y-intercept of the regression surface, (b_1-b_n) are the slopes of the regression surface with respect to variable x_i, k is the degree of the polynomial, and e_i is the random error component.

Results and Discussion

As demonstrated previously as presented Figure 2, the best topography of BDNNs applied in the current study has four layers, i.e., one input layer with two neurons, one output layer with one neuron, and two hidden layers with 11 neurons. A systematic strategy to predict the thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids based on various steps starting by gathering experimental data, defining learning algorithms, activation functions, number of hidden layers and neurons, and ending by calculating the performance and regression coefficients of the BDNN models. Therefore, the input datasets of temperature and volume concentrations with regard to the thermal conductivity and viscosity as the network outcomes were trained, tested, and validated. The experimental input data are usually divided into three parts, namely training, testing, and validating, and the training part has more data than the testing in order to validate the generalization ability of models. Some statistical metrics, including RMSE, the correlation coefficient R^2, and relative error (r) are calculated to evaluate the model performance and accuracy and figure out the relationships between the input independent variables and the simulated outcomes of models. Further, these statistical indices can deliver a clear vision of the costs and benefits of the proposed methods, helping to make righteous decisions about the optimization algorithms. The RMSE is estimated by identifying the average distance between the predicted and actual parameters by equation (5).

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}} \qquad (5)$$

The correlation coefficient R2 is another measure of the model's accuracy that can be estimated by equation (6). The perfectly accurate model would be at (R^2 =1).

$$R^2 = \left(\frac{\sum_{i=1}^{n} (y_i - \bar{y}_i)(\hat{y}_i - \bar{\hat{y}}_i)}{\sqrt{\sum_{i=1}^{n} (y_i - \bar{y}_i)^2} \sqrt{\sum_{i-1}^{n} (\hat{y}_i - \bar{\hat{y}}_i)^2}} \right)^2 \qquad (6)$$

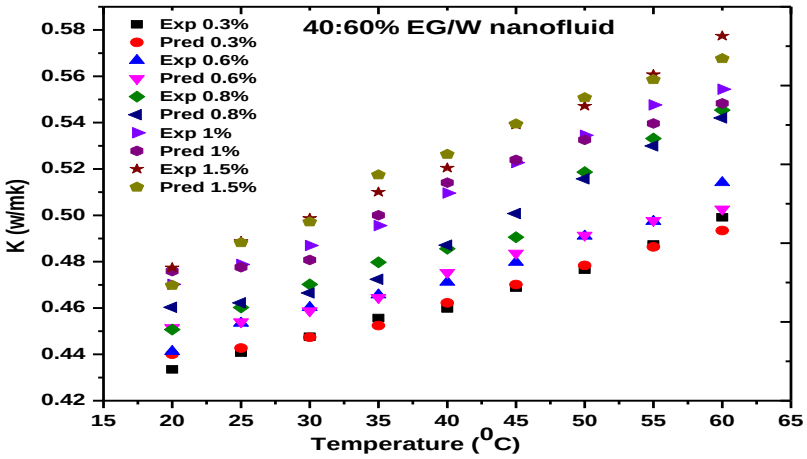
Table 2: The performance evaluation of the three proposed models.

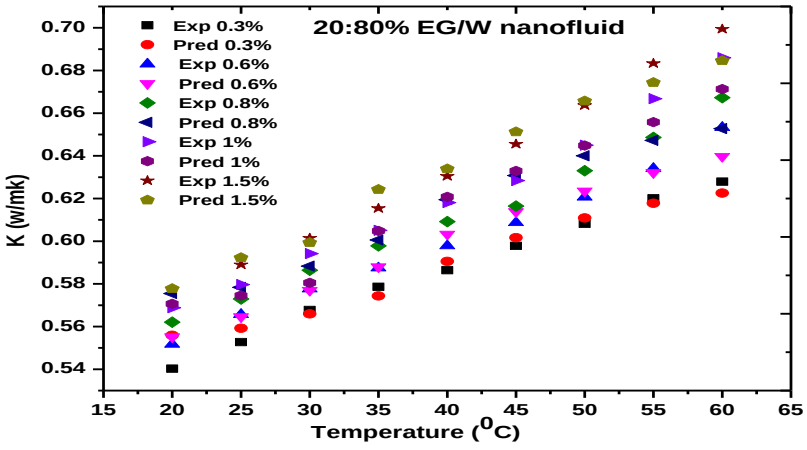
Model	property	EG-W base fluids	RMSE (Test)	R2	r
BDNN	Thermal conductivity	20:80	0.0042	0.99487	0.067
BDNN	Thermal conductivity	60:40	0.0031	0.99602	0.036
BDNN	Thermal conductivity	40:60	0.0051	0.99371	0.075
DTR	Thermal conductivity	20:80	0.0101	0.9549	-
PRM	Thermal conductivity	20:80	0.0132	0.93318	-
BDNN	Viscosity	20:80	0.0021	0.99845	0.012
BDNN	Viscosity	60:40	0.0023	0.99757	0.018
BDNN	Viscosity	40:60	0.0027	0.99584	0.023
DTR	Viscosity	20:80	0.0107	0.9627	-
PRM	Viscosity	20:80	0.0201	0.90828	-

The last index is the relative error (*r*), which can be determined by Eq.7 [23].

$$r = \left|\frac{Actual\ value_{out} - predicted\ value_{out}}{Actual\ value_{out}}\right| \times 100 \qquad (7)$$

Where y_i and $\hat{y}_i$ are the targeted values and predicted values of the thermal conductivity and viscosity respectively, while $\bar{y}_i$ and $\bar{\hat{y}}_i$ are the mean values of targeted and predicted thermal conductivity and viscosity, respectively, and n is the total number of experimental datasets. Detailed predicted results using these statistical indicators for all suggested algorithms are summarized in Table 2.





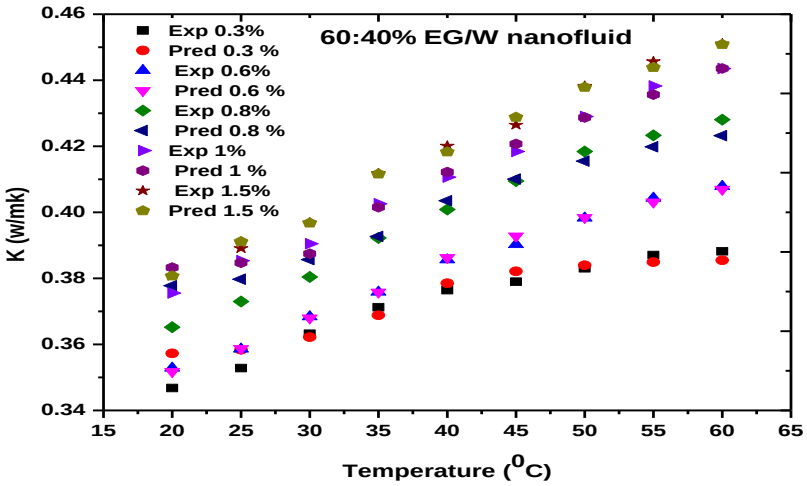
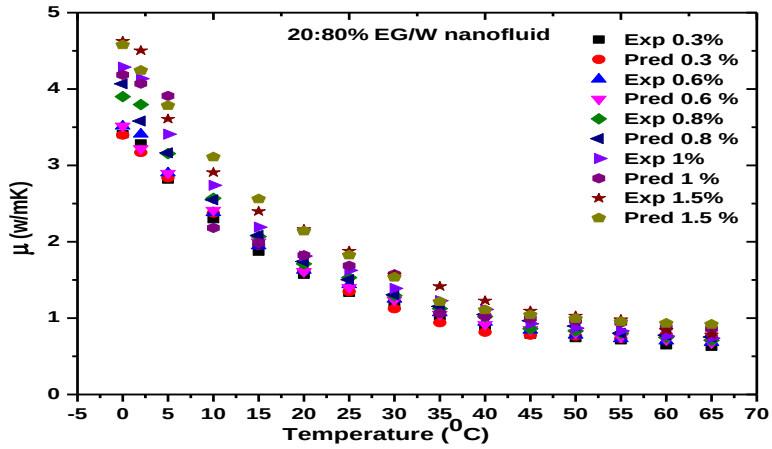
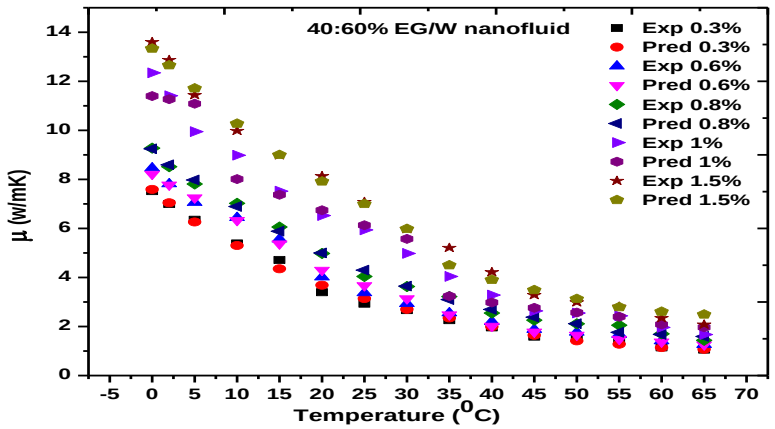


Figure 3: A comparison of the experimental and predicted thermal conductivity of W–EG Al_2O_3 nanofluids at various concentrations using BDNN.





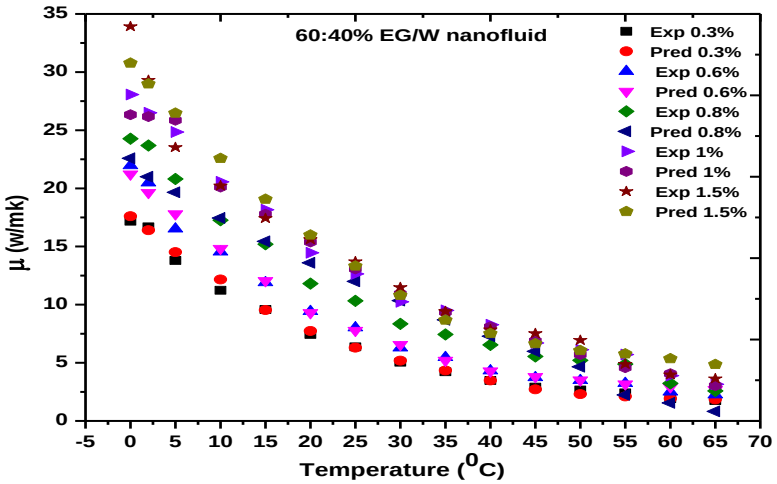
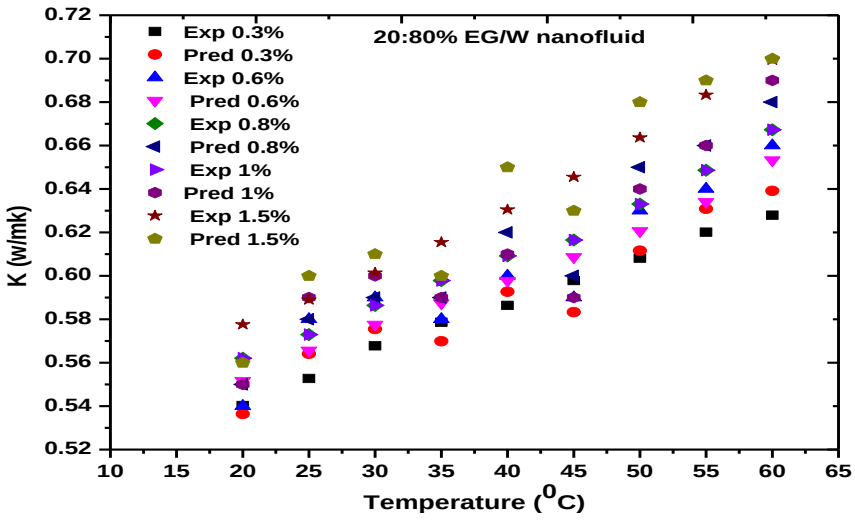


Figure 4: A comparison of the experimental and predicted viscosity of W–EG Al_2O_3 nanofluids at various concentrations using BDNN.

Using the training and test experimental data sets, the performance of all three algorithms is estimated to forecast the thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids. The scatter graphs for the estimated thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids in abroad ranging temperature and particle concentration against the experimental ones using BDNNs are respectively illustrated in Figure 3 and 4. It is obvious from these figures that the predicted and the experimental values of thermal conductivity and viscosity are closely aligned, indicating a significant interrelationship between simulated and targeted values of these thermo-physical properties and confirming the high predictive ability of BDNNs in discovering hidden behavior of the input experimental datasets for thermal conductivity and viscosity. In addition, quantitatively evaluated indices represented in Table 2 showed that the BDNNs provide the best performance with higher accuracy and reliability in terms of low RMSE and relative error values and high R^2 values near to one, and subsequently referring to perfect estimation results using the training datasets.



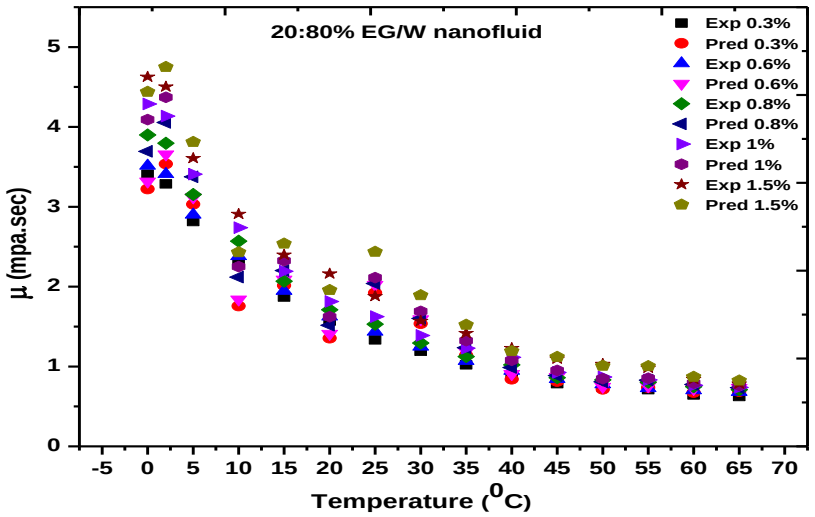
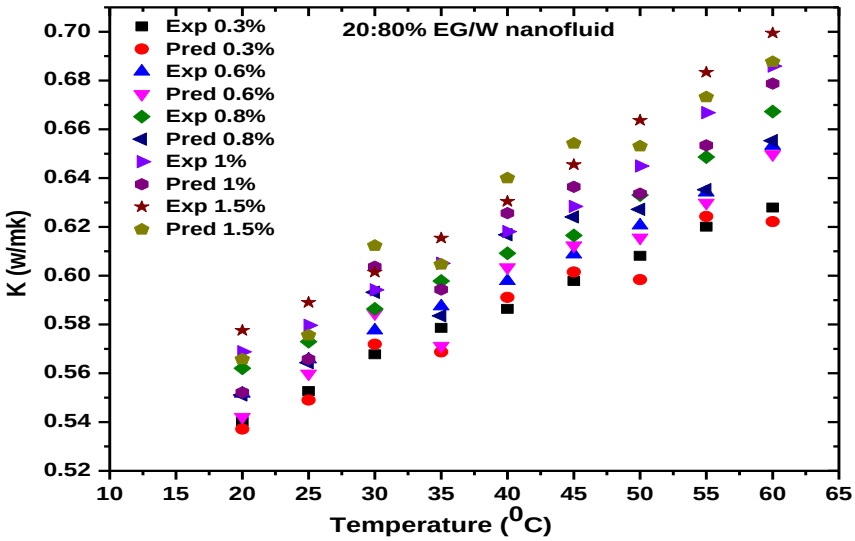


Figure 5: A comparison of the experimental and predicted thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids at various concentrations using the DTR model.

Furthermore, a comparison of the experimental and predicted thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids at various concentrations using the DTR algorithm is illustrated in Figure 5. It can be seen that most points of experimental and predicted parameters are clustered within a stated interval but, some points are dispersed which influence the model accuracy. However, the DTR still performs well according to the model evaluation results represented by estimated indices.



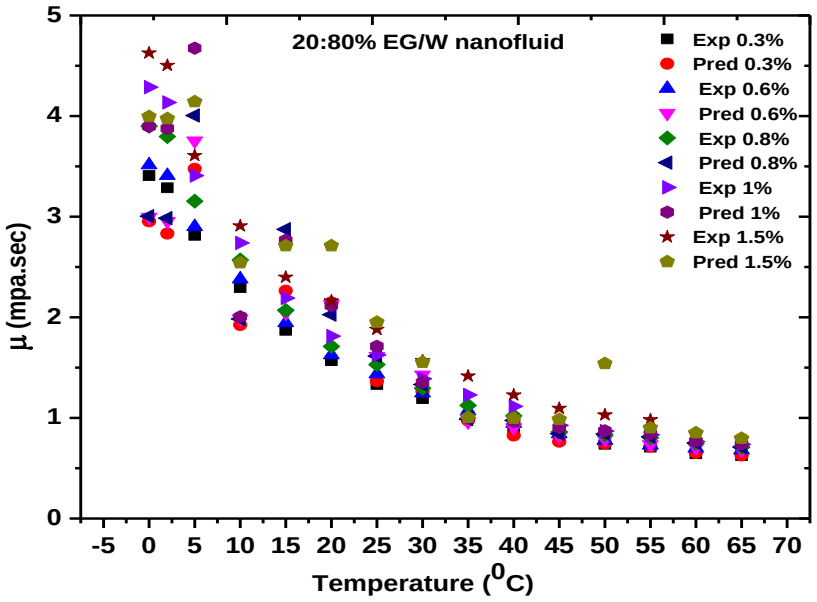
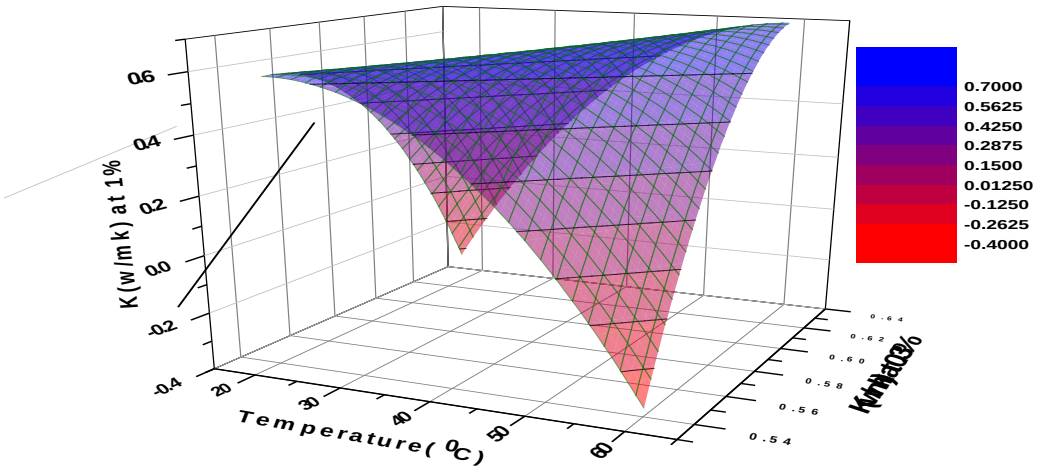


Figure 6: A comparison of the experimental and predicted thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids at various concentrations using the PRM.

The DTR provides satisfactory performance with lower RMSE of 0.0107 and 0.0101 and higher R^2 of 0.9627 and 0.9549 for viscosity and thermal conductivity, respectively. In general, the obtained result from BDNN and DTR models confirmed that these two algorithms provide superior learning efficiency and a powerful ability to address the complex connections among the experimental independent variables and thermo-physical properties of W–EG Al_2O_3 nanofluids. Further, the experimental and predicted thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids at various concentrations using PRM algorithm are compared and illustrated in Figure 6. The PRM showed a lower level of precision in estimating the thermo-physical properties of W–EG Al_2O_3 nanofluids with slightly higher RMSE of 0.0132 and 0.0201 and lower R^2 of 0.9331and 0.9082 for thermal conductivity and viscosity, respectively compared to BDNN and DTR models (see Table 2).



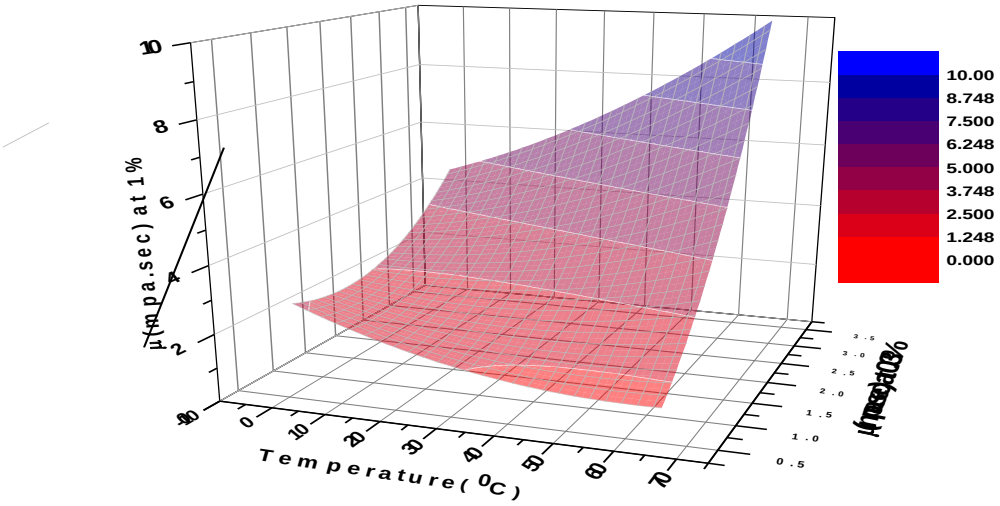


Figure 7: 3D-surface plots of the predicted thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids by BDNN.

To further grasp patterns and insights hiding within complicated nonlinear relationships of thermo-physical properties, the variation of the predicted thermal conductivity and viscosity of W–EG Al_2O_3 nanofluids with temperatures between 0 °C and 60 °C for the volumetric concentration of 0.3% and 1% is visualized by 3D surface plots as shown in Figure 7. Based on represented data of the nanofluids properties it found that W–EG Al_2O_3 nanofluids have a significant and strongly temperature and volumetric concentration-dependent thermal conductivity. Thus, an increase in volume concentrations and temperatures increased the thermal conductivity of nanofluids. In addition, it can be clearly noticed that the thermal conductivity of W–EG Al_2O_3 nanofluids is not only enhanced by the temperature and volumetric concentration but it is also improved by the base fluids. As higher thermal conductivity base fluids can efficiently produce higher thermal conductivity nanofluids than lower thermal conductivity base fluids. Therefore, the most significant enhancement of thermal conductivity of nearly 32.26% was accomplished at EG/W base nanofluid of 20:80% and the particle concentration of 1.5% at a temperature of 60 °C. In a similar way, the viscosity of W–EG Al_2O_3 nanofluid increases as particle concentrations increase however it reduces with an increase of temperatures. Hence, the best enhancement of the nanofluids viscosity of approximately 2.58 times was found at the highest particle concentration of 1.5% and a temperature of 0 °C. Similarly, higher viscosity base fluid can develop higher viscosity nanofluids than lower viscosity base fluids.

Conclusion

In this research, a simulation strategy based on different data-driven techniques, including BDNNs, DTR, and PRM, is conducted to efficiently predict the thermal conductivity and viscosity of W–EG Al_2O_3 nanofluid. To find an optimized architecture of BDNN with lower values of RMSE, which is later selected to train the input data, several structures were examined using a trial-and-error approach. Additionally, the performance of these algorithms was evaluated by various statistical indices to identify the most applicable and reliable model in estimating the thermo-physical properties. Amongst these proposed models, the BDNNs were the superior model with a higher predictive accuracy of 0.99602 and 0.99845 for thermal conductivity and viscosity, respectively. Besides, the accuracy of the predictability for The DTR is lower than that of BDNNs; however, it still performs well with overall R^2 of 0.9627 and 0.9549 for viscosity and thermal conductivity, respectively. On the other hand, the PRM showed the highest RMSE values, indicating less precision in predicted variables. Due to the capability and simplicity of the proposed BDNNs in processing the multivariate nonlinear features of nanofluids, it suggested using it for investigating other different properties, for instance, size and shape of particles, clustering of particles, the fluid temperature and their effect on the thermal conductivity and viscosity of nanofluids.

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