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Experimental investigation and modeling of thermal conductivity of CuO–water/EG nanofluid by FFBP-ANN and multiple regressions

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Abstract The purpose of this study is to predict the thermal conductivity of copper oxide (CuO) nanofluid by using feed forward backpropagation artificial neural network (FFBP-ANN). Thermal conductivity of CuO nanofluid is measured experimentally using transient hot-wire technique in temperature range of 20–60 °C and in volume fractions of 0.00125, 0.0025, 0.005 and 0.01% for neural network training and modeling. In addition, in order to evaluate accuracy of modeling in predicting the coefficient of nanofluid thermal conductivity, indices of root-mean-square error, coefficient of determination (R^2) and mean absolute percentage error have been used. FFBP-ANN with two input parameters (volume fraction and nanofluid temperature) and one output parameter (nanofluid thermal conductivity) in addition to two hidden layers and one outer layer which purelin, logsig and tansig functions are used was considered as the most optimum structure for modeling with neuron number of 4–10–1. In this study, among common methods of theoretical modeling of nanofluid thermal conductivity, theoretical method of Maxwell and also multivariate linear regression model was used for explaining the importance of modeling and predicting the results using neural network. According to this research, the results of indices and predictions show high accuracy and certainty of ANN modeling in comparison with empirical results and theoretical models.

Keywords Experimental study · Thermal conductivity · Modeling · Artificial neural network · Copper oxide · Nanofluid · Multivariate regression

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Introduction

The idea of dispersing solid particles in fluid in order to increase the fluid thermal conductivity has been developed for a century. James Clerk Maxwell presented a theoretical model for electrical conductivity of solid particles in heterogeneous mixtures and from that time, this classic model of Maxwell was used for studying about thermal conductivity of mixtures of solid particles in fluids. These studies were limited to particles in size of millimeter or micrometer [1]. The research results demonstrated that adding metallic solid particles to base fluid in scale of nanometer led to increasing thermal conductivity and consequently improving physical properties of the fluid [2–5].

Due to the importance of application of nanofluids in heat exchangers, several studies were carried out for evaluating the effect of different types of nanoparticles, whether metallic or nonmetallic, on thermal conductivity coefficient and viscosity [6–8]. In these studies, experimental and theoretical methods were used for measuring thermal conductivity of nanofluids. Although experimental methods have more accuracy and reliability compared to theoretical methods, they are applied with some difficulties considering their need for specific facilities and equipment [9, 10].

Nowadays, ANN is one of the topics of artificial intelligence, which is inspired by human brain performance in identifying phenomena, and can be applied for predicting and modeling phenomena. One of the applications of neural network is predicting and modeling the thermal conductivity of gas, fluid and solid phases of materials [11–15].

Recently, several studies related to modeling and predicting thermophysical characteristics and rheological behavior of nanofluids were carried out by researchers and the results show suitable potential of neural network in modeling [16–24].

According to the research conducted by Papari et al. [25] for determining thermal conductivity of nanofluids, consist of carbon multilayer nanotubes as nanoparticle in oil, distilled water, decene and ethylene glycol, it has been demonstrated that using ANN model leads to more accuracy in comparison with theoretical models. According to this model, the thermal conductivity has led to mean absolute percentage error (MAPE) of 3.26% and the correlation between measured and predicted amounts has been determined to be approximately 0.991.

Furthermore, Hojjat et al. [26] have proven that thermal conductivity of nanofluids including aluminum oxide, copper oxide and titanium oxide nanoparticles is a function of fluid temperature, nanofluid volume fraction and nanoparticle thermal conductivity. The presented model showed a very good agreement compared to experimental method which led to more accuracy in comparison with Hamilton model, which was not capable of evaluating base fluid temperature influence and also the amount of volume fraction.

Additionally, Longo et al. [27] demonstrated that water-based thermal conductivity of titanium oxide and aluminum oxide nanofluid by using neural network and also choosing four input parameters for network training (volume fraction, nanofluid temperature, nanoparticle thermal conductivity and nanoparticle size) is determined more accurate in comparison with the condition of three parameters without nanoparticle size.

Hemmat et al. [28–33] studied the effect of temperature, volume fraction and nanoparticle size on thermal conductivity of several nanofluids. They found that nanofluid temperature has less impact on increase in thermal conductivity compared to other considered parameters. Hemmat et al. [34] presented also a model with high accuracy for predicting thermal conductivity of zirconium oxide based on ethylene glycol considering nanofluid temperature and volume fraction parameters as network input. In this empirical study, nine different volume fractions were evaluated in the range of 0.0625–5%.

Finally, Khosrojerdi et al. [35] used MLP artificial neural network (MLP-ANN) for modeling and predicting thermal conductivity of nanofluid containing grapheme nanoplatelets/deionized water. According to their study, predicting thermal conductivity based on volume fractions and nanofluid temperature using artificial neural network leads to acceptable results compared to “nan” experimental and theoretical results.

Given the previous studies in this regard and with respect to the knowledge of authors, no research has been conducted on modeling of thermal conductivity of nanofluids containing water- and ethylene glycol-based copper oxide using artificial neural networks. Therefore, this study was conducted to evaluate the modeling of the mentioned thermal conductivity of nanofluids under different conditions, such as the number of various neurons in each layer of the neural network and various activation functions. At the end of the assessment of the number of neurons and type of activation function, criteria for selecting the optimal model were identified. After that, the selected model was compared to conventional theoretical methods.

Experimental

In order to prepare nanofluid, CuO nanoparticles with an average diameter of less than 40 nm and density of 6.3 grcm^{-3} and also PVP (polyvinylpyrrolidone), as the surfactant, were dispersed in a 70:30% (in volume) water and ethylene glycolmixture as the base fluid. The nanofluid mixture was then stirred and agitated thoroughly for 30 min using an ultrasonic agitator similar to the one for preparation of nanofluids by Karami et al. [36]. This ensures uniform dispersion of nanoparticles in the base fluid. The photograph of nanofluid samples with densities of 0.00125 and 0.01% is shown in Fig. 1.

In addition, the transient hot-wire technique was used to measure the thermal conductivity of the nanofluids by a KD2 Pro thermal properties analyzer (Decagon devices, Inc., USA), which is shown in Fig. 2 [36]. In order to study the effect of temperature, a thermostat bath was used at temperature range of 20–60 °C. All the measurements (with the accuracy of ±5%) were taken over ten times, and the average values of the measurements were considered. Figure 3 depicts the thermal conductivity of CuO nanofluids versus temperature for different volume fractions. It was found that the thermal conductivity of nanofluids increases with the increase in CuO nanoparticle volume fraction and temperature. Furthermore, nanofluids of high particle volume fractions have resulted in higher thermal conductivity as it shown in Fig. 3. Additionally, more enhancements in thermal conductivity can be

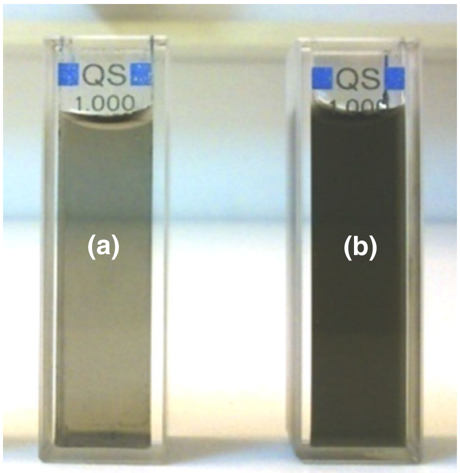

Fig. 1 Comparative photograph of CuO nanofluids with two different volume fractions. (*a*) 0.00125% and (*b*) 0.01%

Fig. 2 KD2 Pro thermal properties analyzer

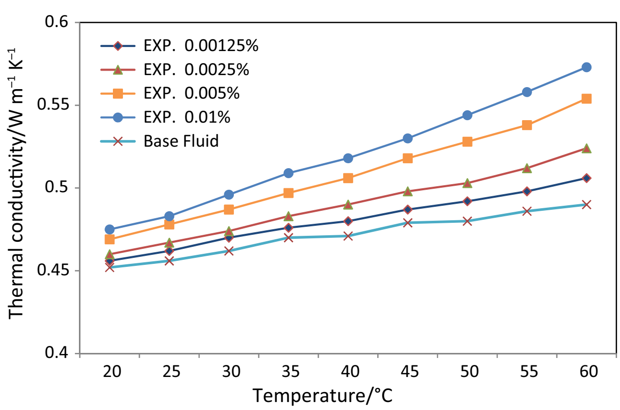

Fig. 3 Thermal conductivity of CuO nanofluids versus temperature for different volume fractions

observed at higher temperatures in comparison with lower temperatures of nanofluids. From the results mentioned above, it can be implied that thermal conductivity of CuO nanofluids is dependent on both particle loading and temperature.

Moreover, from current study, calculated thermal conductivity for water–EG-based CuO nanofluids are correlated with temperature (20 °C $< T <$ 60 °C) and volume fraction ($0 \leq f_v \leq 0.01\%$). This correlation equation can be written as:

$$\frac{k_{nf}}{k_{bf}} = (0.0018 \times T + 0.36)(f_v + 1)^{0.05} \quad (1)$$

This correlation equation has average deviation of 2.8% and standard deviation of 3.6% [36].

Modeling

Feed forward backpropagation (FFBP-ANN)

Artificial neural networks consist of simple functional elements. Their functionality is inspired by biological neural cells of human brain as the connection between them defines network tasks. Artificial neural network enables researchers in order to solve problems, which mathematical modeling is not possible or applicable for them, or there is lack of information for all effective parameters, or there is a very complicated relationship between datasets as this relationship is always difficult to be understood by mathematical models. Hence, neural networks are appropriate tools for fitness of functions and also classification purposes (pattern recognition) [37].

FFBP neural network has one input layer, one output layer and also one or multiple hidden layers, and in each layer there are one or multiple nodes (artificial neurons). The number of nodes in input layer corresponds with the number of input parameters of network, and their number in output layers is also equals to the number of expected outputs from network. However, the number of neurons in hidden layer can vary depends on the number of inputs and outputs and also the relationship complexity among them. The task of an ANN is extracting the relationship between its defined input and output data. There is one weight matrix ($W_{i,j}$) and one bias vector (b_j) per layer and the mentioned matrix and vector influence inputs that are proceeding forward. The values of weights are chosen randomly at first, and during network training, they are modified along with tendency values. The effect of input of each layer can be smaller or bigger by multiplying the input values by weight values that depend on the effect of that layer on network output. Then, in each neuron, the summation of tendencies and weighted inputs are used in an appropriate function for determining output values. After that, final output of network is compared with desirable output and the measured error based on this comparison is used in reverse direction of input movement in order to modify network weights. This will continue until the average network error is less than its allowable defined error. In this case, the network is trained and it can be stabilized and applied as a model for predicting further samples [38].

Generally, a neural network works similar to a function. Equal to the number of input layer neurons, it receives input variables and this is the same as output layer neurons and output values of network. In this study, input parameters include temperature and nanofluid volume fraction which are located in first/initial layer. Based on the assigned weights to neurons and also the number of different neurons in middle layers, thermal conductivity is considered as network output at the end and in last (output) layer. Figure 4 represents a schematic view of ANN for predicting the CuO nanofluid thermal conductivity.

Input parameters of network that are measured experimentally and are used for network training purposes are 28 samples which are normalized in the range of −1 to 1 using Eq. 2 and then are used in the network.

$$y = 2 \times \left(\frac{x - x_{\min}}{x_{\max} - x_{\min}} \right) + 1 \tag{2}$$

Modeling and network training in this research were done based on information derived from experimental measurements and by using the number of neurons and different hidden layers and also by using tangent-sigmoid (tansig) transfer function (Eq. 3), log-sigmoid (logsig) transfer function (Eq. 4) and purelin linear function in output (last) layer (Eq. 5).

$$\mathrm{tansig}(n) = \frac{2}{1 + \exp(-2n)} - 1 \tag{3}$$

$$\mathrm{logsig}(n) = \frac{1}{1 - \exp(-n)} \tag{4}$$

$$\mathrm{purelin}(n) = n \tag{5}$$

Moreover, in current study, modeling was done by using multilayer perceptron (MLP) neural network in MATLAB software. The procedure of data preparation and use is depicted in the following chart (Fig. 5).

Maxwell theory

Maxwell studied thermal conductivity of a much diluted mixture containing spherical particles, regardless of their interactions. By considering spherical particles with equal diameters (their radius is shown by r_{p}) in temperature field of T and temperature gradient of G_{T}, the equation of sustainable situation by solving Laplace differential equation can be derived as below:

$$\nabla^2 T(r) = 0 \tag{6}$$

By assuming a big sphere with radius of R_0 with all spherical particles inside it, from a point with radius of r in this sphere, it can be considered as a system with effective thermal conductivity of K_{EMT} which is surrounded by base fluid with thermal conductivity of K_{f}. Therefore, the function of temperature changes outside of this sphere can be derived from the following equation:

$$T(r) = \left(-1 + \frac{K_{\mathrm{EMT}} - K_{\mathrm{f}}}{2K_{\mathrm{f}} + K_{\mathrm{EMT}}} \frac{r_{\mathrm{o}}^3}{r^3} \right) \vec{G}_{\mathrm{T}} \cdot \vec{r} \tag{7}$$

In addition, temperature change function $T(r)$ can also be derived by using principle of conformity by assuming that all spherical solid particles with radius of r_{p} are surrounded inside the base fluid.

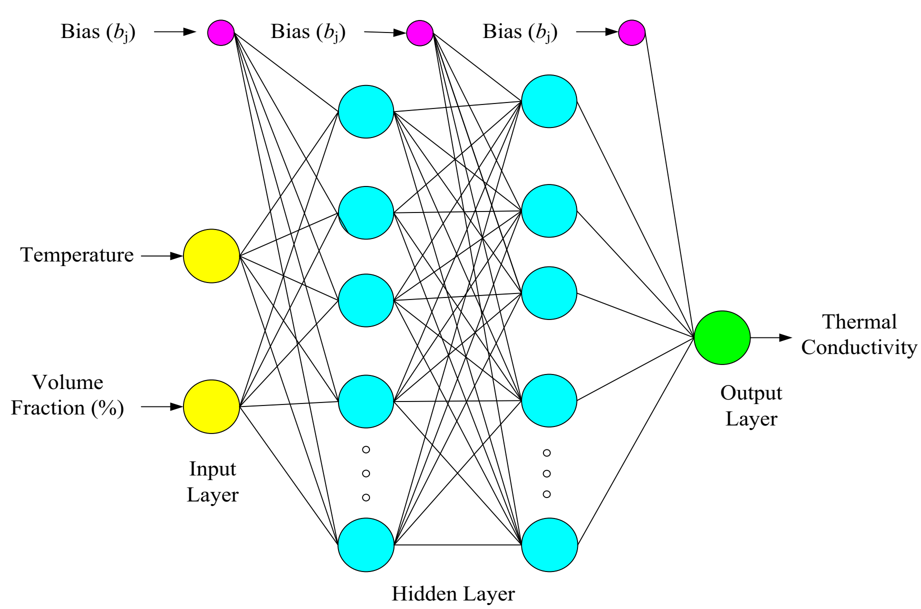

Fig. 4 Schematic view of ANN for predicting the CuO nanofluid thermal conductivity

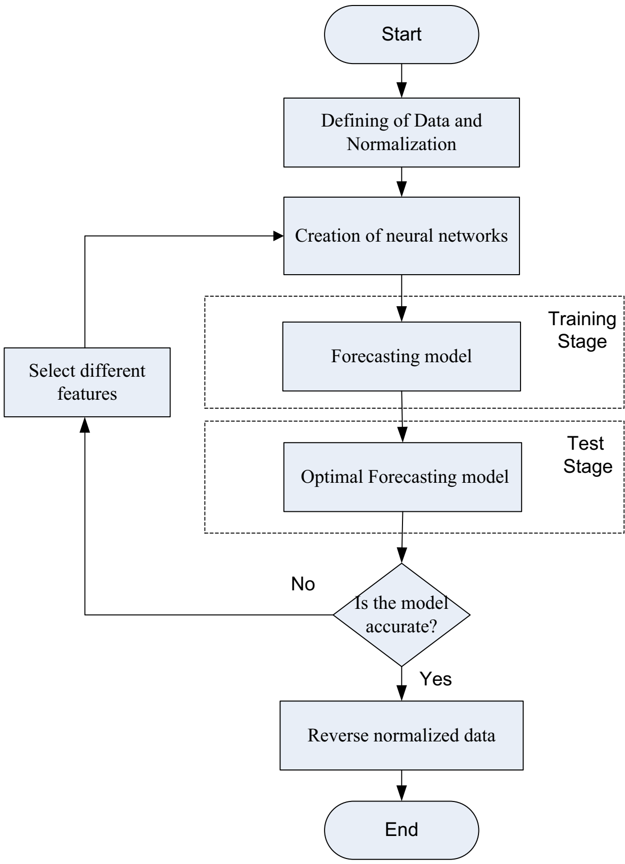

Fig. 5 Flowchart of procedure of ANN modeling

$$T(r) = \left(-1 + \frac{K_p - K_f}{2K_f + K_p}\frac{\varphi r_o^3}{r^3}\right)\vec{G}_T \cdot \vec{r} \quad (8)$$

Therefore, effective thermal conductivity of mixture can be calculated as below:

$$K_{EMT} = \frac{K_p + 2K_f + 2(K_p - K_f)\varphi}{K_p + 2K_f - (K_p - K_f)\varphi}K_f \quad (9)$$

where φ represents the volume fraction of suspended particles in the mixture.

Statistical analysis

In current study, for evaluating the accuracy and performance of model and network, three statistical indices have been used: root-mean-square error (RMSE), mean absolute percentage error (MAPE) and coefficient of determination (R^2). RMSE and MAPE indices are considered as appropriate indices for determining modeling accuracy as more closeness of these two indices to zero leads to high accuracy of modeling. R^2 represents the correlation probability of two data groups in the future as more closeness of this index to zero leads to better modeling performance. Equations used for calculating mentioned indices are defined as below:

$$\mathrm{RSME} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(K_p - K_a)^2} \quad (10)$$

$$\mathrm{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{(K_p - K_a)}{K_a}\right| \times 100 \quad (11)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(K_a - K_p)^2}{\sum_{i=1}^{n}(K_a - \bar{K}_a)^2} \quad (12)$$

where K_p and K_a are predicted thermal conductivity and actual thermal conductivity, respectively. Also, $\bar{K}_a$ and n are mean of actual thermal conductivity in measured period and n number of measured samples, respectively.

Results and discussion

Neural network modeling

According to the procedure of preparing the data and the information for modeling, in the first step of modeling, network was created by downloading experimental data as input parameters. While creating the network, input data were randomly classified into three categories in which 70 and 15% of data were allocated to training and evaluating, respectively, and other 15% was allocated to network testing.

In order to determine the number of neurons and hidden layers, trial and error method was used. Accordingly, by altering the number of layers and neurons in each time of modeling, parameters of network accuracy and validity assessment were estimated. The result of assessing accuracy and validity of model and also the result of statistical indices in each modeling are shown in Table 1.

For modeling and predicting thermal conductivity of CuO nanofluid using MLP neural network, two layers and three hidden layers were used. As only one parameter was considered as network output, one neuron is put in the output layer and its transfer function has been purelin function in all models. In first and second hidden layers, tansig and logsig functions have been used. According to the results in Table 1, increasing the number of neurons in each layer and each transfer function causes enhancement of MAPE index in training part; but this increase in number of neurons leads to lower accuracy and validity in testing part of network. In all created models, R^2 index is in a good state and based on the changes in number of neurons and layer functions, it shows a very small change. Thus, it cannot be used and considered as a factor for determining the most optimum model. In evaluation part of networks,

Table 1 Measurement indices of model accuracy in network training, evaluating and testing based on different conditions

Model	Function	Neurons	Train			Validation			Test		
			MAPE	RMSE	R^2	MAPE	RMSE	R^2	MAPE	RMSE	R^2
ANN											
1	Logsig–purelin	10–1	0.463	0.039	0.994	6.33	0.040	0.996	3.68	0.042	0.996
2	Logsig–purelin	6–1	0.085	0.014	0.999	1.197	0.030	0.981	2.317	0.022	0.999
3	Logsig–purelin	18–1	1.50	0.095	0.999	3.75	0.073	0.979	7.74	0.064	0.989
4	Tansig–purelin	9–1	0.540	0.007	0.999	0.088	0.014	0.998	2.190	0.032	0.995
5	Tansig–purelin	12–1	0.345	0.045	0.997	2.674	0.052	0.996	2.158	0.089	0.982
6	Tansig–purelin	5–1	0.0005	0.016	0.999	2.839	0.018	0.999	0.450	0.034	0.997
7	Tansig–tansig–purelin	4–6–1	0.389	0.015	0.999	0.513	0.026	0.998	5.13	0.052	0.95
8	Tansig–tansig–purelin	5–10–1	0.116	0.013	0.999	0.704	0.033	0.975	5.164	0.041	0.993
9	Logsig–logsig–purelin	6–9–1	0.001	0.002	0.999	0.208	0.020	0.997	0.584	0.024	0.999
10	Logsig–logsig–purelin	4–16–1	1.57	0.017	0.999	3.831	0.042	0.963	3.689	0.074	0.995
11	Logsig–tansig–purelin	4–10–1	0.003	0.006	0.999	0.372	0.015	0.999	0.375	0.058	0.989
12	Tansig–logsig–purelin	6–12–1	1.09	0.10	0.999	1.39	0.021	0.995	0.278	0.023	0.999
13	Tansig–logsig–purelin	4–8–1	0.191	0.010	0.999	0.615	0.025	0.998	0.266	0.021	0.998

varying the number of layers and neurons does not have a significant impact on results. In fact, random increase or decrease in number of layers and neurons can lead to increase or decrease the accuracy and validly of predicted results. All in all, according to the results, using three hidden layers leads to better result in comparison with using two hidden layers in modeling process.

Since increasing the number of neurons leads to increase in calculation/running time and decrease in accuracy and validity of model and also three hidden layer leads to better result compared to two layers, neural network 11 with logsig transfer function and four neurons in first layer and tansig transfer layer with 10 neuron in second layer was chosen as the most optimum model among 13 created models/networks.

In general, accuracy and validity are key factors in all modeling methods. A model is considered as valid and credential when not only its errors in predicting sample data are small, but also its accuracy in performing prediction outside of the sample is high enough and in other words, its predictions can be generalized.

After much deliberation based on performance of network system in training, evaluating and testing parts and ensuring appropriate functionality of modeling, in order to use the achieved information, derived results from the network should be changed from normalized state. The predicted thermal conductivity of CuO nanofluid in different volume fractions and in temperature range of 20–60 °C is measured compared to experimental result and is shown in Fig. 6. Combined set results derived from modeling show that predicted and experimental results have a significant correlation in general. According to the mentioned statistical indices in previous sections, if MAE has a value less than 10% and more specifically has a value closer to 0, the model is considered as more accurate. For combined set, RSME, MAPE and R^2 were measured as 0.002 W m^{-1} K^{-1}, 0.007 and 99.9%, respectively. These statistical indices values show high accuracy and certified results of presented model outputs.

Correlation analysis is a statistical tool for determining the type and strength of relationship between two quantitative variants. Correlation coefficient is the criterion used for determining the correlation between two variants. This coefficient shows strength of relationship and also types of relationship (direct or reverse) and varies between −1 to 1, and also in case there is no any linear relationship, its value

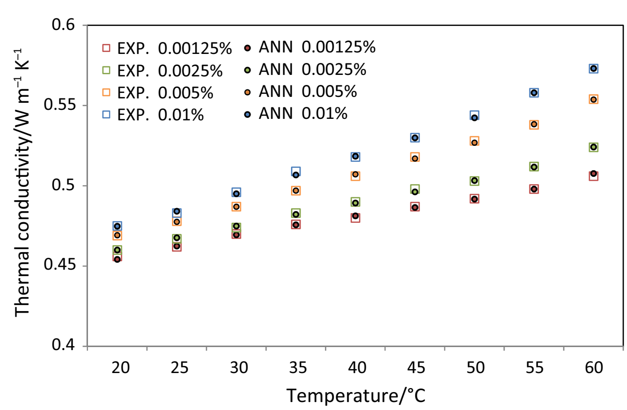

Fig. 6 Comparison of experimental results of CuO nanofluid thermal conductivity and predicted values of ANN model

is zero. Moreover, this coefficient can only measure linear relationship; therefore, the coefficient of correlation of zero means that there is no linear relationship between x and y; but existence of a nonlinear relationship is possible. In Fig. 7, the correlation of the results based on the prediction of optimum model and also experimental measurements of thermal conductivity is demonstrated. According to this figure, most of the values are located on the bisector or its adjacency and this fact shows a good and strong relationship between experimental results and prediction output. Accordingly, based on the derived relationship, it can be concluded that there is a good correlation between experimental and predicted results and there is a linear relationship between datasets.

Theoretical model

Regression is a branch of statistics that its application and use have become common in most of the scientific works. In Engineering Science, regression is used for measuring or estimating the relationship between different variants. As these theoretical relationships, which are presented by researchers, only state some assumptions regarding the behavior of nanofluids thermal conductivity, researchers use statistical data (e.g., observations based on experimental result) in order to test the accuracy and validity of theories and existing relationships. In fact, regression is the most important and fundamental tool that is used in different branches of science, especially in engineering, for studying the relationship between variants. Usually, it is necessary to study and determine the relationship between one variant and multiple variants in different works in which regression is applicable. This will require using multivariate regression. Due to the importance of tow parameters (nanofluid temperature and volume fraction) in predicting thermal conductivity, in this research, multivariate linear regression was used for prediction and estimation of thermal conductivity of CuO nanofluid. According to our investigations and also initial estimation of coefficients of each of the effective parameters in predicting thermal conductivity of nanofluid, the estimated equation can be written as below:

$$K_{\mathrm{nf}} = 0.406 + (0.000445 \times \varphi) + (0.00182 \times T) \quad (13)$$

Based on the derived theoretical relationship from linear regression, thermal conductivity of CuO nanofluid in different volume fractions and in temperature range of 20–60 °C is shown in Fig. 8 compared to the measured experimental results.

Furthermore, Fig. 9 shows the results of correlation between measured results and predicted values by linear regression model. According to this figure, less points are located on bisector or its adjacency in comparison with the correlation figure related to ANN model. This cannot be considered as a good and string relationship between experimental and predicted outputs. According to our studies and the derived relationship, there is a relative correlation with error between predicted values and experimental results.

Finally, in order to assess the accuracy of each of the prediction models, the outputs derived from the results of neural network prediction, Maxwell theory and CuO nanofluid thermal conductivity linear relationships, compared to the experimental results in different volume fractions at 25 °C are demonstrated in Fig. 10. As it appears, the results of neural network model seem to have more accuracy compared to other models. In addition, Maxwell theory shows low accuracy in predicting thermal conductivity of CuO nanofluid by increasing volume fractions.

For better evaluation of the performance and functionality of neural network and also for observing the error between predicted thermal conductivity of CuO nanofluid with different volume fractions at 20–60 °C, the results of

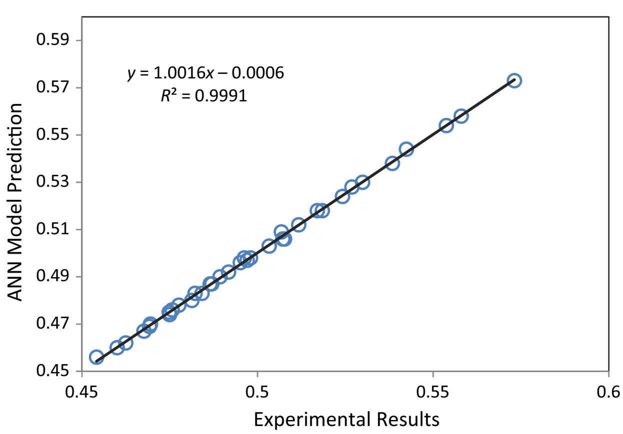

Fig. 7 Correlation chart between measurement results and ANN model

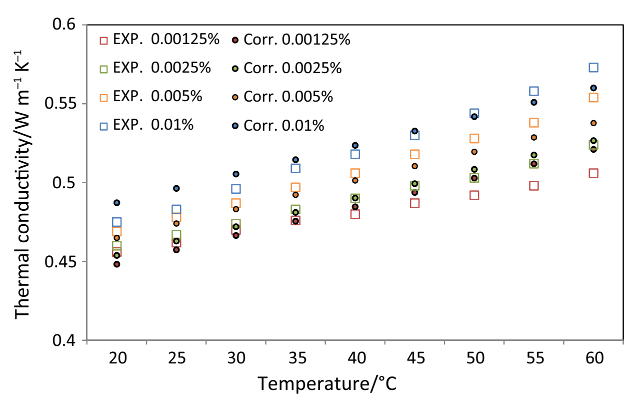

Fig. 8 Comparison of experimental result of thermal conductivity of CuO nanofluid and the predicted values of linear regression

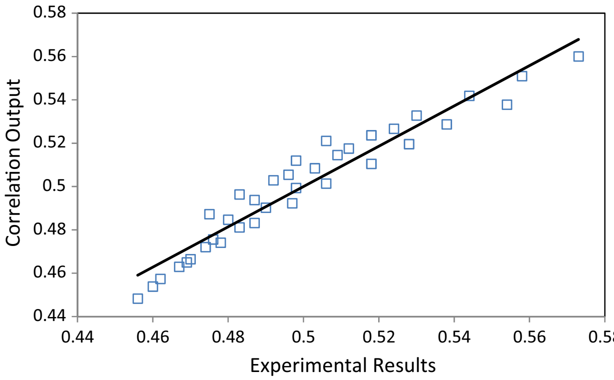

Fig. 9 Correlation diagram between measurement results and linear regression model

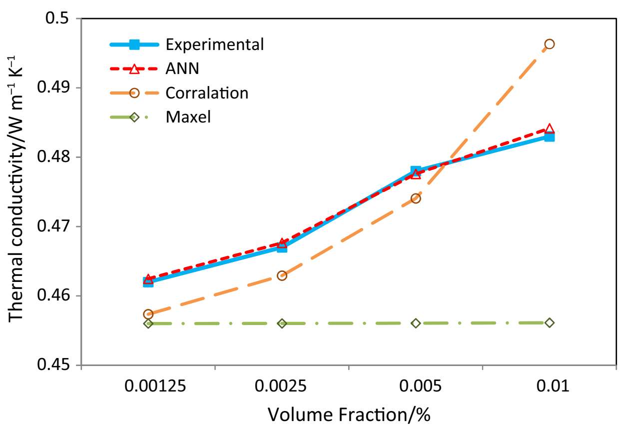

Fig. 10 Comparison between experimental result of thermal conductivity of CuO nanofluid and the predicted values of theoretical models at 25 °C

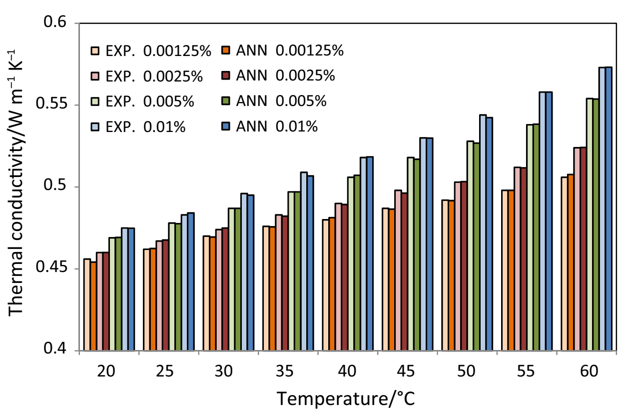

Fig. 11 Comparison between predicted values of ANN model and experimental results for thermal conductivity of CuO nanofluid

modeling and predicted values of ANN model in addition to other experimental and measured values are shown in Fig. 11. As can be seen, the lowest error between measurement results and predicted values can be observed at 55 °C.

Conclusions

Because of the importance of using nanoparticles for increasing thermal properties of common fluids, in current study, feed forward backpropagation artificial neural network (FFBP-ANN) functionality was used and evaluated for predicting thermal conductivity of CuO nanofluid. Accordingly, thermal conductivity of nanofluid with different volume fractions in temperature range of 20–60 °C was measured experimentally. Furthermore, for predicting and modeling these experimental results, FFBP-ANN was used. The modeling results have high accuracy and validity in comparison with theoretical model of Maxwell and also derived relationships and equations based on multivariate linear regression. Due to the fact that performing experiments in laboratories and deriving experimental results requires special facilities and equipment and also can be expensive, using presented model based on artificial neural network (ANN) for predicting and estimating thermal conductivity of CuO nanofluid is suggested by authors.

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