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Evaluation of thermal conductivity of COOH-functionalized MWCNTs/water via temperature and solid volume fraction by using experimental data and ANN methods

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Abstract In the present study, the results of several experiments have been used to obtain the thermal conductivity of multi walls carbon nanotubes-water nanofluid. For this purpose, COOH-functionalized MWCNTs nanoparticles have divided into different solid volume fractions in order to disperse in water as the base fluid by different dispersion methods. The thermal conductivity measurement applied in different solid concentrations, up to 1 %, and at the temperatures ranging from 25 to 55 °C. In this paper, based on the experimental data, a new correlation for predicting the thermal conductivity of COOH-functionalized MWCNTs/water nanofluid proposed. After that, for simulating the thermal conductivity of this nanofluid, the artificial neural network is used. For this purpose, multilayer percepetron neural network is used. The network input variables are temperature and solid volume fraction, and the network output variable is thermal conductivity. The results extracted from the artificial neural network show good agreement with the experimental data. The mean square error value is 4.04E−06 that shows excellent performance of artificial neural network to predict thermal conductivity of COOH-functionalized MWCNTs/water nanofluid.

Keywords Thermal conductivity · MWCNTs/water · Artificial neural network · Nanofluid · Correlation

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List of symbols

k	Thermal conductivity, Wm^{-1} K^{-1}
Re	Reynolds number
T	Temperature, K
MSE	Mean square error
RMSE	Root mean square error
MAE	Maximum absolute error
MLP	Feedforward multilayer percepetron

Greek

φ	Solid volume fraction

Subscripts

b	Base fluid
nf	Nanofluid
Pred	Predicted value
Exp	Experimental value

Introduction

In recent years, applications of nanofluids have been developed in different thermal devices such as engine cooling, solar energy, nuclear reactors, cooling of electronic devices, and medical applications [1, 2].

Adding nanoparticles into fluids can be enhanced thermal conductivity of them. Therefore, a more compact system is possible using capable nanofluid. Appropriate type of nanoparticles plays a key role in obtaining a nanofluid with a high efficiency. Improving the heat transfer rate, using nanofluids consists of ultra-fine solid particle instead of usual fluids like water and oil is a proper solution.

A comprehensive model for the enhanced thermal conductivity of nanofluid has been presented by Wang [3]. Ghadimi et al. [4] presented a review of nanofluid stability

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properties and characterization in stationary conditions. Gupta et al. [5] in a comprehensive review presented forced heat transfer characteristics with various nanofluids based on experimental investigation with constant heat flux and constant wall temperature boundary conditions in heat exchangers. Vajjha et al. [6] in a comprehensive evaluation determined the effects on the efficiency of nanofluids as a result of variation of density, specific heat thermal conductivity and viscosity, which are features of nanoparticle temperature and volume fraction.

Between the common nanoparticles, carbon nanotubes (CNTs) because of suitable thermal structure and properties have several advantages. For instance, using CNTs in common fluids makes the heat transfer better. An experimental survey has been done to study the turbulent flow of COOH-functionalized multi-walled CNTs/water nanofluid flowing through a double tube heat exchanger by Hemmat Esfe et al. [7]. Furthermore, Hemmat Esfe et al. [8] assessed the heat transfer features and pressure drop of low concentrations of a COOH-functionalized double-walled carbon nanotube (DWCNTs)/water nanofluid. Phuoc et al. [9] have also investigated thermal conductivity, viscosity and stability of nanofluids including multi-walled carbon nanotubes (MWCNTs) stabilized by cationic Chitosan. Nasiri et al. [10] studied influence of CNT structures on thermal conductivity and stability of nanofluid.

Diameter size, temperature and volume fraction are the factors that have been noticed in the nanofluids researches. In this ground, Hemmat Esfe et al. [11] conducted an experimental study on the thermal conductivity of Al_2O_3–water nanofluid. Using steady-state coaxial cylinders method, the thermal conductivity of Al_2O_3-water nanofluid was measured by Barbes et al. [12]. Using neural network method, Papari et al. [13] conducted a study to predict the thermal conductivity of various nanofluids. Their results showed that there is a great agreement between the results of modeling by neural network method and the other models available in the literature.

Some studies show that the diameter size of nanoparticles has reverse relation with thermal conductivity [14, 15]. Nasiri et al. [10] reported that smaller diameter of nanotubes has occasioned larger thermal conductivity. Furthermore, the most of the studies show that there is a direct relationship between temperature and thermal conductivity fraction [16, 17]. Additionally, there is a nonlinear relation between volume fraction and thermal conductivity of nanofluids in a direct way [7, 18].

Artificial neural network is a new method to predict nonlinear behavior of thermal conductivity ratio. Many researchers have studied an application of ANN in the modeling thermal conductivity in different nanofluids and thermophysical properties [13, 19, 20]. Hemmat Esfe et al. [21] investigated the thermal conductivity of MgO-EG nanofluids using ANN; in addition, they suggested an empirical correlation to calculate the thermal conductivity ratio of MgO-EG nanofluids. A new correlation of dynamic viscosity of ZnO-EG nanofluids at different solid volume fraction and temperature based on experimental measurement has been presented by Hemmat Esfe et al. [16].

The target of the present study is to estimate thermal conductivity ratio of multi-walled carbon nanotubes (MWCNTs)/water nanofluid accurately using correlation and artificial neural networks.

Experimental

Twenty-four data points for MWCNT covering a volume fraction ranging from 0.0005 to 0.01 and a temperature ranging from 25 to 55 °C have been used for developing models (Fig. 1) [22]. Properties of COOH-functionalized MWCNTs are presented in Table 1.

Proposed new correlation

In this study, the thermal conductivity ratio of MWCNT were correlated as a function of solid volume fraction and temperature for the purpose of interpolation. The experimental data used as fitting pattern.

Nonlinear regression equation has employed to develop correlation model. Several equations drive out from nonlinear regression then the precise one chooses among them. In this article, in order to investigate the performance of the model, mean square error (MSE) and root mean square error (RMSE) were selected. The following equations are used to calculate the MSE and RMSE:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{K_{\mathrm{nf}}}{K_{\mathrm{b}}}\bigg|_{\mathrm{Exp,i}} - \frac{K_{\mathrm{nf}}}{K_{\mathrm{b}}}\bigg|_{\mathrm{pred,i}}\right)^2 \quad (1)$$

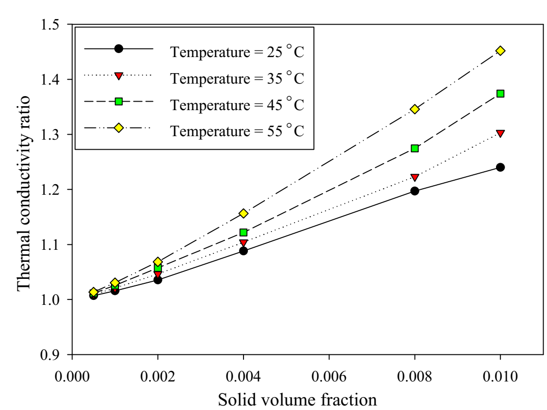

Fig. 1 Thermal conductivity ratio via volume fraction in various temperature

Table 1 Properties of COOH-functionalized MWCNTs

Purity/mass%	>97 (carbon content)
Inside diameter/nm	5–10
Length/um	10–30
Color	Black
True density/g cm^{-3}	2.1

$$\mathrm{RMSE} = \left[\frac{1}{N}\sum_{i=1}^{N}\left(\left|\frac{K_{\mathrm{nf}}}{K_{\mathrm{b}}}\right|_{\mathrm{Exp,i}} - \frac{K_{\mathrm{nf}}}{K_{\mathrm{b}}}\right|_{\mathrm{pred,i}}\bigg|\right)^{2}\right]^{1/2} \quad (2)$$

where N shows the number of experimental data, $\frac{K_{\mathrm{nf}}}{K_{\mathrm{b}}}\Big|_{\mathrm{pred}}$ is the predicted thermal conductivity ratio, and $\frac{K_{\mathrm{nf}}}{K_{\mathrm{b}}}\Big|_{\mathrm{Exp}}$ is the thermal conductivity ratio, which obtained from the experiment.

Artificial neural network modeling

The structure of human's brain has been simulated by artificial neural network in computer. An ANN shows nonlinear relation between inputs and outputs data by a connection between the neurons in pervious and next layers. Modeling complicated relation between data points is possible by using the ANN method.

In this study, thermal conductivity ratio of MWCNT was calculated in terms of temperature and volume fraction. Temperature and volume fraction were used as inputs to predict thermal conductivity ratio of MWCNT, and thermal conductivity ratio is taken into account as the output of the ANN.

Feedforward multilayer percepetron (MLP) was used as structure of ANN. This structure is one of the most applicable structures for prediction [19]. MLP have several layers with various neurons in each of them such as hidden layer and output layer. Neurons in each layer are connected to other neurons by mass coefficient. Outputs of neurons calculate by activation functions. Tangent sigmoid function was used as activation function of hidden layers, and pure linear function was used as activation function of output layer for an accurate prediction. MLP network consists of two hidden layers, and one output layer has been shown in Fig. 2. Each hidden layer has seven neuron, while output layer has one neuron.

In this article, back-propagation algorithm and Levenberg–Marquardt method have been used to predict thermal conductivity ratio of MWCNT. This algorithm commonly used for modeling [19].

Performance function is employed for assessing error during network training process. One of the most usual performance functions used in feedforward neural networks is MSE and RMSE (Eqs. 1 and 2) [13, 23, 24]. In this study, MSE and RMSE have been employed to investigate ANN performance.

Results and discussion

Correlation model

A comparison of the performance functions values for different equation permits to choose the best modeling equation for describing thermal conductivity ratio of MWCNT in terms of solid volume fraction and temperature. According to MSE and RMSE values for various equations, Eq. 3 was chosen as the accurate equation.

$$\frac{K_{\mathrm{nf}}}{K_{\mathrm{b}}} = 0.9975 + 15.82 \times \varphi + 20.42 \times T \times \varphi^2 + 0.005983 \times \varphi \times T^2 - \varphi \times \cos(19.43 \times T \times \varphi) \quad (3)$$

The performance of Eq. 3 via several performance functions has been shown in Table 2.

The thermal conductivity ratio of MWCNT obtained by experimental and correlation has been compared in variety volume fractions and temperatures (Figs. 3, 4).

As it can be seen, the correlation coefficient is very close to one, which shows that there is sufficient adjustment between correlation and experimental data. In addition, maximum error is 0.0055, which occurs in volume fraction 0.01 and temperature 35 °C, which shows that correlation has adequate accuracy to predict thermal conductivity ratio.

ANN model

Thermal conductivity ratio of MWCNT was calculated in solid volume fraction from 0.05 to 1 % and temperature from 25 to 35 °C (Fig. 1). From 24 data points, 18 were used for training and remaining data points were used for testing and validation of network. It is better to normalize data in [−1 1] interval to better network training.

Fourteen networks were used to choose adequate structure. Optimum number of neurons in the hidden layer is selected by trying various network structures and compares their MSE and RMSE values. The ANN structure with lowest MSE and RMSE was selected as the optimum structure. Values of MSE and RMSE for various structures have been shown in Table 3. Based on Table 3, the structure with seven neurons in each hidden layer has the lowest MSE and RMSE value. This structure was chosen as the best structure to predict thermal conductivity ratio in terms of volume fraction and temperature with MSE and RMSE value equal to 4.04×10^{-6} and 0.002, respectively.

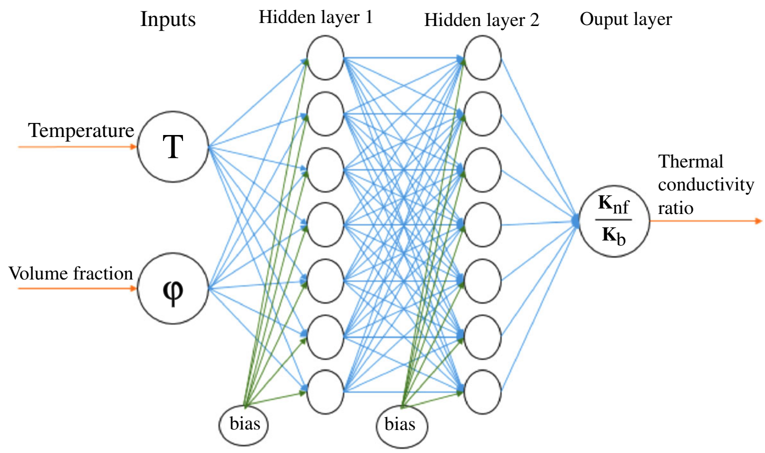

Fig. 2 MLP network consist of two hidden layers and one output layer

Table 2 Performance of correlated model

Mean square error	9.7415238×10^{-6}
Root mean square error	0.0019
Maximum absolute error	0.0055
Correlation coefficient	0.99973063

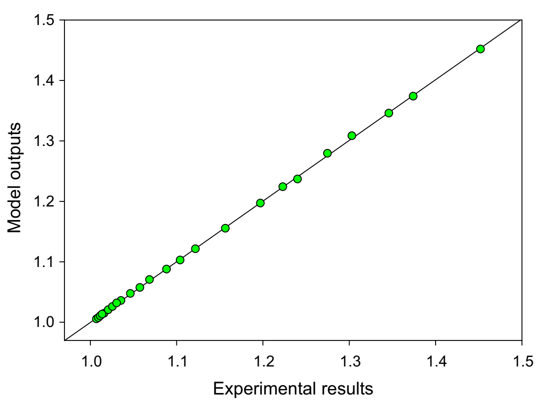

Fig. 3 Regression diagram of correlated model

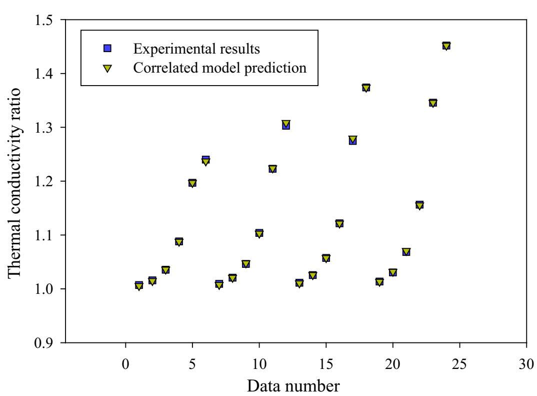

Fig. 4 Comparison between experimental results and correlated model

Table 3 MSE value for various ANN structure

Number of hidden layers	Number of neurons in each hidden layer	MSE	RMSE
1	2	6.36E−05	0.008
1	3	3.61E−05	0.006
1	4	1.61E−05	0.004
1	5	3.27E−05	0.0057
1	6	5.60E−06	0.0024
1	7	3.71E−05	0.0061
1	8	3.00E−05	0.0055
2	2	1.41E−05	0.0038
2	3	1.06E−05	0.0033
2	4	6.08E−05	0.0078
2	5	9.03E−05	0.0095
2	6	4.56E−05	0.0067
2	**7**	**4.04E−06**	**0.002**
2	8	4.91E−05	0.007

The bold value shows best structure with lowest error

Regression diagram of trained neural network has been shown in Fig. 5. This figure shows that there is excellent agreement between experimental results and ANN model outputs.

Figure 6 shows comparison between experimental results and ANN model outputs. The maximum error is 0.0064, which occurs at temperature 25 °C and volume fraction 0.008. As it can be seen, there is good fitness between experimental results and ANN model outputs.

Comparison between experimental results and models

In Figs. 7 and 8, thermal conductivity ratio of MWCNT/water nanofluid obtained by experiment, correlation and ANN model has been compared. It can clearly found that the results of experiment and both models are very close together.

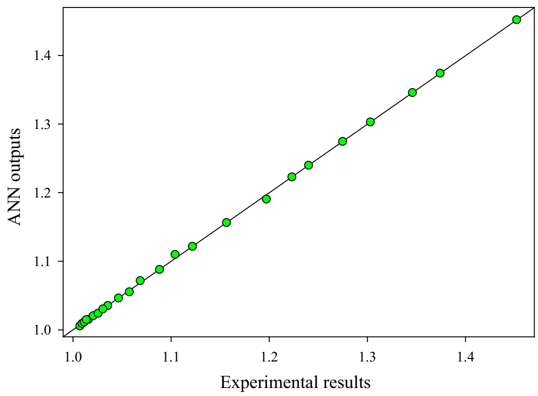

Fig. 5 Regression diagram of trained neural network

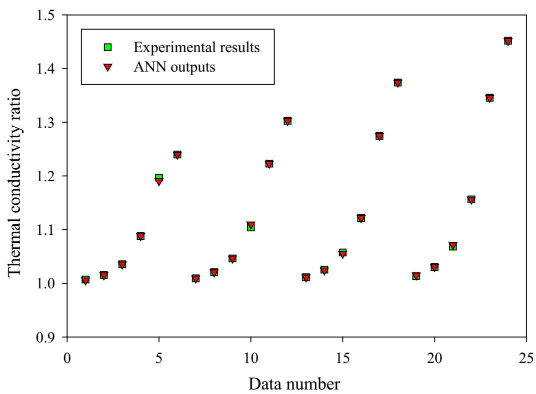

Fig. 6 Comparison between experimental results and ANN model outputs

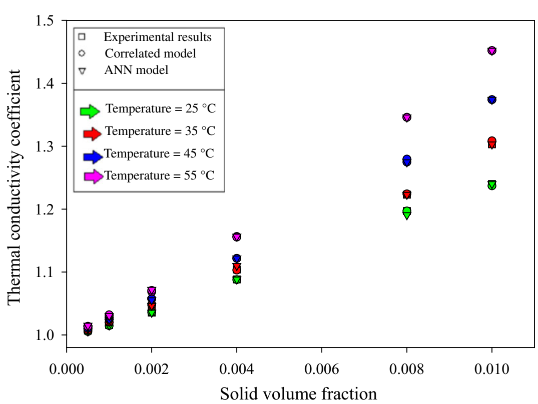

Fig. 7 Comparison between thermal conductivity ratio obtained by experiment, correlation and ANN

As a result, there is sufficient adjustment between experimental results and models outputs. Although ANN model has better performance than correlation, it is possible to use these reliable models to estimate thermal conductivity ratio of MWCNT/water nanofluid, precisely.

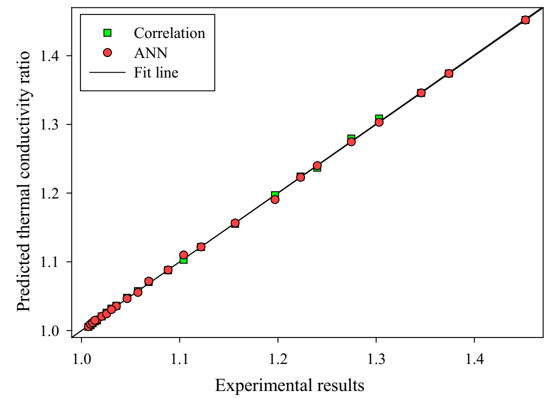

Fig. 8 Parity plot and thermal conductivity ratio prediction for MCWNT

Conclusions

The aim of the present study is to estimate thermal conductivity ratio of multi-walled carbon nanotubes (MWCNTs)/water nanofluid accurately using correlation and artificial neural networks.

It has been suggested an equation (Eq. 3) by nonlinear regression with MSE equal to 9.7415238×10^{-6}, RMSE equal to 0.0019, and the maximum absolute error is 0.0055. Based on performance functions value, this method has an appropriate ability to model thermal conductivity ratio of MWCNTs/water nanofluid, accurately.

Furthermore, artificial neural network has been used to predict thermal conductivity ratio of MWCNTs/water nanofluid. In order to obtain the best structure with lowest performance function, a MLP network with two hidden layers and seven neurons in each hidden layer has been selected as optimal structure. The values of MSE and RMSE are 4.04×10^{-6} and 0.002, respectively. Obviously, it can be found that ANN model has a good ability to predict thermal conductivity ratio of MWCNT in term of volume fraction and temperature with adequate accuracy. In addition, ANN model has better prediction than correlation in order to estimate thermal conductivity ratio.

Therefore, it can be noticed that the presented models have a good ability to estimate thermal conductivity ratio of MWCNTs/water nanofluid. Further studies aimed to elucidate the precise nature of this new class of heat transfer fluids (called as nanofluids) would be of considerable interest. The extension of this paper and our previous work [25–29] affords engineers a good option for nanofluid in applications such as electronics, automotive, and nuclear applications where improved heat transfer or efficient heat dissipation is required. Also, future studies aimed at elucidating the precise nature of nanofluid heat transfer would be of considerable interest.

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