Applications of feedforward multilayer perceptron artificial neural networks and empirical correlation for prediction of thermal conductivity of Mg(OH)$_2$–EG using experimental data\textsuperscript{☆}

Mohammad Hemmat Esfe \textsuperscript{a,*}, Masoud Afrand \textsuperscript{a}, Somchai Wongwises \textsuperscript{b,*}, Ali Naderi \textsuperscript{c}, Amin Asadi \textsuperscript{d}, Sara Rostami \textsuperscript{a}, Mohammad Akbari \textsuperscript{a}

\textsuperscript{a} Department of Mechanical Engineering, Najafabad Branch, Islamic Azad University, Isfahan, Iran

\textsuperscript{b} Fluid Mechanics, Thermal Engineering and Multiphase Flow Research Lab. (FUTURE), Department of Mechanical Engineering, Faculty of Engineering, King Mongkut's University of Technology Thonburi, Bangkok, Thailand

\textsuperscript{c} Faculty of Mechanical Engineering, Semnan University, Semnan, Iran

\textsuperscript{d} Department of Mechanical Engineering, Semnan Branch, Islamic Azad University, Semnan, Iran

A R T I C L E   I N F O

Available online 28 June 2015

Keywords:
Nanofluids
Artificial neural network
Thermal conductivity

A B S T R A C T

This paper presents an investigation on the thermal conductivity of nanofluids using experimental data, neural networks, and correlation for modeling thermal conductivity. The thermal conductivity of Mg(OH)$_2$ nanoparticles with mean diameter of 10 nm dispersed in ethylene glycol was determined by using a KD2-pro thermal analyzer. Based on the experimental data at different solid volume fractions and temperatures, an experimental correlation is proposed in terms of volume fraction and temperature. Then, the model of relative thermal conductivity as a function of volume fraction and temperature was developed via neural network based on the measured data. A network with two hidden layers and 5 neurons in each layer has the lowest error and highest fitting coefficient. By comparing the performance of the neural network model and the correlation derived from empirical data, it was revealed that the neural network can more accurately predict the Mg(OH)$_2$–EG nanofluids’ thermal conductivity.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

In recent years, ultrahigh heat transfer has played an important role in the development of heat-transfer systems and fluids that are required for many applications. The idea of improving the heat-transfer performance of inherently poor conventional heat transfer with the inclusion of solid particles was first introduced by Maxwell [1]. Nanofluid is a novel heat-transfer fluid prepared by dispersing nano-sized particles in base fluid to increase thermal conductivity and heat-transfer performance. The main ideas for improving the heat transfer performance may be listed as follows:

1. The suspended nanoparticles increase the surface area and the heat capacity of the fluid.
2. The suspended nanoparticles increase the effective (or apparent) thermal conductivity of the fluid.
3. The interaction and collision among particles, fluid and the flow-passage surface are intensified.
4. The mixing fluctuation and turbulence of the fluid are intensified.
5. The dispersion of nanoparticles flattens the transverse temperature gradient of the fluid.

Much attention has been paid in the past decade to this type of material because of its enhanced properties and its behavior associated with heat transfer, mass transfer, wetting and spreading, and antimicrobial activities. In addition, the number of publications related to nanofluids has increased in an exponential manner. Because of extensive application of nanofluids [2], recent numerical and experimental studies have concentrated on thermophysical properties [3–7], heat transfer [8–12], and flow behavior of nanofluids.

The neural network is inspired by natural biological systems, and if it is well-trained, it has a very high predictive ability. In recent decades, artificial neural networks have been addressed by researchers in various branches of science due to their high speed in solving complicated equations as compared to conventional methods. The neural network model has been successfully used in various fields of engineering systems modeling [12–16].

Recently, neural networks have been utilized in predicting the nonlinear behavior of the nanofluid thermal conductivity in various thermophysical conditions. Hojat et al. [17] have investigated the impact of nanoparticle concentration and the type of nanoparticles on nanofluid thermal conductivity using the neural network of thermal...
impact. Paperi et al. [18] have predicted nanofluid thermal conductivity containing multi-walled carbon nanotubes (MWCNTs) suspended in oil (oil α-olfin), Decene (DE) distilled water (DW), ethylene glycol (EG) as well as single-walled carbon nanotubes (SWCNTs) in epoxy and poly methyl methacrylate (PMMA) using an artificial neural network. Hammat et al. [19] have presented the relationship between thermal conductivity based on temperature and volume fraction. In addition they have used the neural network to predict ZnO–EG nanofluid thermal conductivity at different temperatures and volume fractions. They have also presented a neural network to estimate the MgO–EG nanofluids’ thermal conductivity using the experimental data [20]. Longo et al. [21], using a neural network and considering various input conditions, predicted the oxide–water nanofluids’ thermal conductivity.

Considering the appropriate performance of neural networks in estimating thermophysical behaviors, the purpose of this study is to provide an artificial neural network model to predict the thermal conductivity coefficient of Mg(OH)2–EG. For this purpose, an MLP feedforward network is used. For the estimation of thermal conductivity coefficient in terms of temperature and solid volume fraction, the empirical correlation is presented.

2. Experiment

The results of experiments conducted to measure the relative thermal conductivity coefficient of nanofluids Mg(OH)2–EG are presented in Fig. 1 at the volume fractions of 0.001, 0.002, 0.004, 0.008, 0.01, 0.015 and 0.02, and temperatures of 24, 35, 45 and 55 °C.

3. Artificial neural network design

An artificial neural network is a computational method that, with the help of a learning process and the use of processors called neurons, tries to present a mapping between the input and the positive environment (output data) by recognizing the intrinsic relationship between the data. Steps to create and select the appropriate neural network model are shown in Fig. 2.

The most common learning is the back-propagation algorithm. The back-propagation algorithm uses supervised learning. In supervised learning, when the input is applied to the network, the network solution is compared with the target solution designed for the network, and then the learning error is calculated and used to adjust the network parameters.

There are several back-propagation algorithms, among which the Lovenberg Marquardt learning algorithm has the best performance in estimating efficiency function [19]. In this study, the Lovenberg Marquardt algorithm is used for training the network. In order to achieve an appropriate structure in nonlinear functions-estimation problems, the tangent sigmoid function is used in the hidden layer and the pure linear function is used in the output layer [22].

In this paper, the created network has two input parameters and one output parameter. The input variable parameters are the volume fraction and temperature and the output variable parameter is thermal conductivity. Therefore, the neural network is designed with 2 neurons in the input layer and 1 neuron in the output layer (Fig. 3). Before training, it is often better to scale the inputs and targets. This is done for the sameness of the data’s impact on network training. These functions’ normalized data are in the range of 1 to −1.

The trained network performance evaluation is performed using defined indices such as the mean square error, mean absolute error, sum-of-squared error, and fitting rate (R). The values of these indices are calculated using the following relations (Table 1).

\[
MSE = \frac{1}{N} \sum_{i=1}^{N} (T_{ij} - P_{ij})^2
\]

\[
MAE = \frac{1}{N} \sum_{i=1}^{N} |T_{ij} - P_{ij}|
\]

![Fig. 1. Relative thermal conductivity of nanofluid versus solid volume fraction at different temperatures.](image)

![Fig. 2. Framework of the methodology used.](image)

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Performance function values for proposed correlation.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSE</td>
<td>6.0489E−06</td>
</tr>
<tr>
<td>MAE</td>
<td>0.0015530159</td>
</tr>
<tr>
<td>SSE</td>
<td>1.6937E−04</td>
</tr>
<tr>
<td>R</td>
<td>0.99926363</td>
</tr>
<tr>
<td>Maximum absolute error</td>
<td>0.0071287366</td>
</tr>
</tbody>
</table>
SSE = \sum_{i=1}^{n} (T_{ij} - P_{ij})^2 \quad (3)

\begin{align*}
R &= \frac{\sum_{i=1}^{n} (T_{ij} - T)(P_{ij} - P)}{\sqrt{\sum_{i=1}^{n} (T_{ij} - T)^2 \sum_{i=1}^{n} (P_{ij} - P)^2}} \\
&= \frac{\sum_{i=1}^{n} (T_{ij} - T)(P_{ij} - P)}{\sqrt{\sum_{i=1}^{n} (T_{ij} - T)^2 \sum_{i=1}^{n} (P_{ij} - P)^2}} \quad (4)
\end{align*}

In these equations, \( T_0 \) is the actual value and \( P \) is the value from the model. \( T \) and \( P \) are the mean experimental values and values predicted by the model for \( N \) data.

### 4. Discussion and conclusions

#### 4.1. Relation

In this paper the Mg(OH\(_2\))–EG nanofluid thermal conductivity is developed using nonlinear regression equations and experimental data based on temperature and volume fraction. To obtain the best-fitting model, the accuracy of the relation is considered. For this purpose, the performance indicators (Eqs. (1)–(4)) are used. Eq. (5) presents the result of regression analysis of thermal conductivity at different temperatures and volume fractions.

\[
K = 0.995 + 4.28\phi + 0.134\phi T - 0.00011T^2 - 0.00908 \sin(0.981 + 0.0201T + 3.02 \times 10^3 \phi^2 + 0.0006917^2 + 2.22 \times 10^3 \phi^3 + 9.78 \times 10^3 \phi T^2 - 2.75 \times 10^3 \phi^3 - 49.8cT - 3.89 \\
\times 10^3 \phi^2 - 8.28 \times 10^3 \phi^3 - 7.6 \times 10^3 \phi T^3) \quad (5)
\]

In this equation, \( K_{nf} / K_B \) is the Mg(OH\(_2\))–EG nanofluid thermal conductivity coefficient. \( \phi \) is the volume fraction and \( T \) is the nanofluid temperature.

The presented empirical relation is provided for the Mg(OH\(_2\))–EG thermal conductivity based on temperature and volume fraction using experimental data. The performance indicators are given in Table 2.

The regression graph of Eq. (5) is presented in Fig. 4. In addition, the data obtained from experiments and the fitting model’s outputs are compared in Fig. 5. Figs. 4 and 5, present the equation comparison, and the experimental results present the maximum absolute error of 0.00713 and a fitting coefficient close to 1, which indicates good agreement between the experimental results and the relation’s outputs. The values of the efficiency functions for the presented relation indicate that this relation has a good ability to estimate thermal conductivity, temperature, and volume fraction.

#### Table 2

The procedure of trial and error to find the optimum number of hidden layers and neurons.

<table>
<thead>
<tr>
<th>Number of hidden layer</th>
<th>Number of neuron in each hidden layer</th>
<th>MSE</th>
<th>MAE</th>
<th>SSE</th>
<th>R</th>
<th>Maximum absolute error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>3.87E–05</td>
<td>0.0049</td>
<td>0.0011</td>
<td>0.99508</td>
<td>0.0138</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>1.26E–05</td>
<td>0.0028</td>
<td>3.54E–04</td>
<td>0.99841</td>
<td>5.70E–03</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>1.99E–05</td>
<td>0.0034</td>
<td>5.57E–04</td>
<td>0.99765</td>
<td>1.05E–02</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>1.65E–05</td>
<td>0.0031</td>
<td>4.63E–04</td>
<td>0.99794</td>
<td>9.70E–03</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>1.54E–06</td>
<td>0.0001</td>
<td>4.31E–05</td>
<td>0.99981</td>
<td>2.70E–03</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>1.77E–06</td>
<td>1.10E–03</td>
<td>4.96E–05</td>
<td>0.99978</td>
<td>3.10E–03</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
<td>1.31E–06</td>
<td>8.90E–04</td>
<td>3.66E–05</td>
<td>0.99983</td>
<td>3.40E–03</td>
</tr>
<tr>
<td>9</td>
<td>9</td>
<td>4.60E–06</td>
<td>6.41E–04</td>
<td>1.29E–04</td>
<td>0.99943</td>
<td>1.10E–03</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>2.48E–06</td>
<td>9.40E–04</td>
<td>6.95E–05</td>
<td>0.9997</td>
<td>3.60E–03</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>1.29E–05</td>
<td>2.70E–03</td>
<td>3.62E–04</td>
<td>0.99847</td>
<td>7.00E–03</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>4.62E–06</td>
<td>0.0016</td>
<td>1.29E–04</td>
<td>0.99943</td>
<td>4.80E–03</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>3.57E–06</td>
<td>9.15E–04</td>
<td>1.00E–04</td>
<td>0.99955</td>
<td>8.60E–03</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>3.14E–07</td>
<td>3.64E–04</td>
<td>8.81E–06</td>
<td>0.99996</td>
<td>1.50E–03</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>6.21E–07</td>
<td>4.34E–04</td>
<td>1.74E–05</td>
<td>0.99992</td>
<td>3.30E–03</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>3.96E–07</td>
<td>5.08E–04</td>
<td>1.67E–05</td>
<td>0.99992</td>
<td>2.20E–03</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
<td>9.73E–07</td>
<td>4.85E–04</td>
<td>2.72E–05</td>
<td>0.99988</td>
<td>2.60E–03</td>
</tr>
<tr>
<td>9</td>
<td>9</td>
<td>3.56E–06</td>
<td>6.22E–04</td>
<td>9.07E–05</td>
<td>0.99959</td>
<td>2.00E–03</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>1.27E–06</td>
<td>3.85E–04</td>
<td>3.55E–05</td>
<td>0.99984</td>
<td>0.0058</td>
</tr>
</tbody>
</table>

Fig. 3. The multilayer perceptions (MLP)-feedforward network.

Fig. 4. The regression graph of the correlation.
4.2. Neural network model

In this study, using an MLP back-propagation network, the Mg(OH$_2$)–EG nanofluids’ thermal conductivity has been modeled at temperatures between 24 and 55 °C and volume fractions between 0.001 and 0.02. A Lovenberg Marquardt algorithm has been devised to train the network. In this method, the allocation of 70% of the data as the training subset, 15% of the data as the validation subset, and 15% of the data as the experimental subset, shows better results in reducing model errors.

After selecting the network’s input and output data; normalizing data; and choosing training algorithms, the activation function, the number of hidden layers, the number of neurons in each hidden layer, the values of training parameters, and the performance function, the network training starts with 1 hidden layer and 2 neurons in the hidden layer. It continues by increasing to 2 hidden layers and 10 neurons in each hidden layer. For better performance evaluation and selecting the optimal network, the performance indicators (Eqs. (1)–(4)) between the network output and optimal output (experimental data) are analyzed. The best number of hidden layers and number of neurons in hidden layers are determined by trial and error and based on the highest fitting correlation and lowest obtained error. Table 2 shows the values of various network performance indicators.

As is clear from Table 2, a network with 2 hidden layers and 5 neurons in each layer has the lowest error and highest fitting coefficient so that the values of MSE, MAE, and SSE equal to 3.14E−07, 3.64E−04, and 8.81E−06, respectively, for this structure of the neural network.

The trained network regression graph is given in Fig. 6. The proper function of the network in predicting thermal conductivity is clearly evident in this graph, in which the fitting coefficient is 0.9996. One of the problems in training neural networks is overfitting. This means that after network training, the error on the training set is reduced to its lowest value by providing the new data as the input error becomes very high. The similarity of the experiment set and validation indicates good results and a lack of overfitting. The obtained fitting coefficients in the prediction of thermal conductivity for training and validation data are 0.99996 and 0.99999, indicating the lack of overfitting and the optimum performance of the neural network.

The experimental results and outputs of the neural network are compared in Fig. 7. The experimental results and outputs of the model fit have good agreement with each other, as the maximum absolute error is equal to 1.50E−03. The results suggest the high accuracy of the MLP artificial neural network with 2 hidden layers and 5 neurons in the hidden layers in predicting Mg(OH$_2$)–EG thermal conductivity.

4.3. Comparison between experimental and model results

The obtained Mg(OH$_2$)–EG nanofluids’ thermal conductivity results from experiments, the fitting model, and the artificial neural network
model are presented in Figs. 8 and 9. The experiments’ and both models’ results have good agreement.

The neural network values of MSE, MAE, and SSE for estimating thermal conductivity are $1.4E-07$, $3.64E-04$, and $8.81E-06$, respectively, and the values for the presented equation equal $6.0489E-06$, $1.55E-03$, and $1.6937E-04$, respectively. As is evident in Figs. 8 and 9, the performance of both models to estimate Mg(OH$_2$)$_2$–EG nanofluids thermal conductivity is good; however, the neural network model is more accurate.

5. Conclusion

In this study, using the MLP neural network and linear regression of the experimental data, the impact of temperature and volume fraction is studied on thermal conductivity. The artificial neural-network modeling results show that sufficient training using the back-propagation error algorithm of the MLP neural network (with 2 hidden layers and 5 neurons in each layer) has a high capability in predicting thermal conductivity. By developing the regression equation, a highly accurate relation for thermal conductivity was extracted based on temperature and volume fraction. By comparing the performance of the neural network model and the relationship derived from empirical data, it was revealed that the neural network can more accurately predict the Mg(OH$_2$)$_2$–EG nanofluids’ thermal conductivity.

The results of the presented models in this paper show that, in the absence of costly and time-consuming tests, these models can be used to analyze the impact of temperature and volume fraction on Mg(OH)$_2$–EG nanofluids’ thermal conductivity.

Acknowledgment

The third author would like to thank the “Research Chair Grant” National Science and Technology Development Agency (NSTDA), the Thailand Research Fund (IRG5780005) and the National Research University Project (NRU) for the support.

References