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A Neural Network Approach to Estimate Non-Newtonian Behavior of Nanofluid Phase Change Material Containing Mesoporous Silica Particles

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P A P E R I N F O

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A B S T R A C T

Neural networks are powerful tools for evaluating the thermophysical characteristics of nanofluids to reduce the cost and time of experiments. Dynamic viscosity is an important property in nanofluids that usually needs to be accurately computed in heat transfer and nanofluid flow problems. In this paper, the rheological properties of nanofluid phase change material containing mesoporous silica nanoparticles are predicted by the artificial neural networks (ANNs) method based on the experimental database reported in literature. Experimental inputs include nanoparticle mass fractions (0-5 wt.%), temperatures (35-55°C), shear rates (10-200 s^{-1}), targets include dynamic viscosities and shear stresses. A multilayer perceptron feedforward neural network with Levenberg-Marquardt back-propagation training algorithm is utilized to predict rheological properties. The optimal network architecture consists of 22 neurons in the hidden layer based on the minimum mean square error (MSE). The results showed that the developed ANN has an MSE of 6.67×10^{-4} and 6.55×10^{-3} for the training and test dataset, respectively. The predicted dynamic viscosity and shear stress also have the maximum relative error of 6.26 and 0.418%, respectively.

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1. INTRODUCTION

Heat transfer enhancement techniques are widely used in many heating and cooling processes to improve the thermal performance of energy systems. With the development of nanotechnology, dispersing high conductive nanostructured materials in a transport medium such as conventional fluids has been considered as a promising method to enhance heat transfer [1]. The fabricated materials are usually called nanofluids which exhibit unique features especially in thermal conductivity and viscosity. Due to the unusual behavior of nanofluids, investigation of nanofluid flow and heat transfer [2] has always been challenging. Nanofluids can be used in many engineering applications including solar collectors [3], automotive [4], heat exchangers [5], and so on.

The rheological properties of nanofluids play an important role in the flow pressure drop inside the ducts, increasing the pumping power and the convective heat transfer [6]. To determine the rheological properties, the relationship between shear stress, shear rate and apparent viscosity is investigated, the result of which determines the Newtonian or non-Newtonian behavior of the nanofluid. Various parameters such as temperature, nanoparticle concentration, nanoparticle size, type of base fluid, surfactant addition, shear stress and shear rate affect the rheological behavior of nanofluids. The viscosity of nanofluids and the effect of various parameters have been measured by many researchers and various models have been proposed for it, some of which are mentioned here. Experimental analysis of more than 30 nanofluids based on water, engine oil and ethylene glycol with the dispersion of Al_2O_3, TiO_2, ZrO_2, CuO, Fe_2O_3, Fe_3O_4, and nanodiamond nanoparticles was performed by Minakov et al. [7]. They investigated the effect of temperature, nanoparticle concentration, nanoparticle size and surfactant addition. The results indicated that the higher the viscosity of the base fluid, the higher the viscosity of the nanofluid. Adding more nanoparticles can also make the nanofluid behavior non-Newtonian. Garoosi [8] presented an experimental model based on a large number of laboratory data. In this model,

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the viscosity of the nanofluids was investigated in terms of volume fraction, type and diameter of nanoparticles, temperature and thermophysical properties of the base fluid. This model gives more accurate output than conventional models such as Brinkman and Maxwell-Garnett models. Bardool et al. [9] developed a model for predicting the viscosity of nanofluids using friction theory and available equations of states. 711 experimental data were used in this study and the error of the developed model was less than 8.1%.

One of the most accurate methods for estimating the thermophysical characteristics of nanofluids is the use of artificial neural networks (ANNs). This method is a machine learning algorithm that has been utilized in thermal applications [10]. Ramezanizadeh et al. [11] have been recently reviewed machine learning methods used in modeling the viscosity of nanofluids. Toghraei et al. [12] experimentally studied the dynamic viscosity of Ag-EG nanofluid. The experiments were performed at the temperature of 25-55°C and a volume fraction of 0.2-2% which 42 experimental data were obtained. These data were used to estimate the dynamic viscosity of the nanofluid by ANN and correlation method. The accuracy of the ANN method compared to correlation was high and its MSE was equal to 0.0012 and the maximum error was 0.0858. Ahmadi et al. [13] evaluated the dynamic viscosity of SiO_2/EG-water nanofluid using the ANN intelligent method. In their study, 160 experimental data extracted from the literature were used. The developed ANN used Multilayer Perceptron (MLP) and Radial Basis Function (RBF) algorithms. Their results demonstrated that the MLP-RNB neural network accurately predicted the dynamic viscosity of the nanofluid and that the MSE and the correlation coefficient were obtained 5.5 and 0.998, respectively. Ali et al. [14] reported the viscosity of EG-water nanofluid and TiO_2 nanotubes in the temperature range of 25-65°C, mass fraction of 0-1% and shear stress of 150-500 s^{-1}. ANN and multivariable correlation methods were used to predict viscosity based on experimental data. The results showed that the ANN method has an accuracy of 0.1981 AAD% and 0.999 R^2 which is very accurate in comparison with the correlation method. Chen et al. [15] utilized 145 measured experimental data to evaluate the viscosity of MWCNTs-TiO_2/SAE50 hybrid nanofluids at different volume fractions, temperatures and shear rates using ANN. In their study, non-Newtonian nanofluid was considered, which follows the power-law model. They used another ANN to predict consistency index and power-law index using temperature and volume fraction. The neural networks used had a hidden layer and a *tansig* activation function whose number of neurons was obtained by trial and error. Hemmat-Esfe et al. [16] proposed an ANN model to compute the viscosity of MWCNT-Al_2O_3/5W50 hybrid nanofluid as a nano lubricant. 174 experimental data in the temperature range of 5°C to 55°C and volume fraction of 0.05 to 1% were used as network inputs. The ANN network was MLP which its accuracy was measured by R^2 and MSE criteria. The results showed that temperature has a greater effect on nanofluid viscosity than other parameters. Ansari et al. [17] proposed a model for predicting the relative viscosity of nanofluids using a feedforward backpropagation network and using various algorithms including Levenberg-Marquardt (LM), Scaled Conjugate Gradient (SCG), Bayesian Regulation backpropagation (BR), and Resilient backpropagation (RP). They used 1620 laboratory data for network training. Shear rate, temperature, nanoparticle density, nanoparticle size, and volume fraction were considered as neural network inputs. The optimized ANN has a hidden layer consisting of 23 neurons and a *tansig* activation function that uses the LM algorithm. MSE and R^2 of this network were 0.00901 and 0.9954, respectively. The viscosity of Tungsten Oxide - MWCNTs/Engine Oil was measured at various temperatures, volume fraction and shear rates by Toghraie et al. [18]. They used an ANN model to predict the dynamic viscosity. The best accuracy was obtained by selecting 39 neurons in their proposed structure. For all data, MSE was 2.409 and MAE was 9.349.

A review of recent researches showed that many researchers have studied the rheological properties of different nanofluids using the ANN predictive method. In this study, the ANN method is used to predict the rheological properties of n-octadecan containing mesoporous SiO_2 nanofluid using 193 experimental measured data. This nanofluid can be considered as a nano-enhanced phase change material (nano-PCM) that can be used for thermal energy storage applications. To the best of our knowledge, no such study has been conducted so far for this material. Moreover, the power-law behavior of this phase change nanofluid is precisely estimated by ANN. An MLP neural network trained by the LM algorithm is used to predict the viscosity and shear stress. Temperature, mass fraction and shear rate are input parameters of the ANN. The ANN structure, i.e. the number of hidden layers and the neurons of each network layer, are optimized based on the minimum MSE and the maximum R. Due to the non-Newtonian behavior of nanofluids in some mass fractions, consistency index and power-law index at various temperatures and mass fractions are obtained according to the network results.

2. EXPERIMENTAL DATABASE

In the present paper, liquid n-octadecane (C_8H_{38}) with melting point of 27.5°C was utilized as the base fluid. Mesoporous SiO_2 particles with the average diameter of 280nm were dispered into the n-octadecane to fabricate nanofluid samples. The nanoparticle mass fractions were.

1%, 3% and 5%. The rheological properties of nanofluids were measured in the temperatures range of 35-55°C and shear rates from 10 s^{-1} to 200 s^{-1}. This includes 193 experimental data were previously reported by Motahar et al. [19]. In this study, these experimental data are used for designing an ANN. Figure 1 shows the viscosity of nanofluids at various mass fractions, temperatures and shear rates.

A fluid is Newtonian if the shear stress is proportional to shear rate, where the viscosity (μ) is the constant of proportionality:

$$\tau = \mu\dot{\gamma} \quad (1)$$

It was reported a non-Newtonian behavior for nanofluid samples with mass fractions of mesoporous SiO_2 greater than 3% [19], the liquid nanofluid can be considered as power-law liquid which is expressed as follows [19]:

$$\tau = K\dot{\gamma}^n \quad (2)$$

where K is the consistency index (in $Pa{\cdot}s^n$), and the exponent n, is the power-law index. For n=1 and K=μ, Equation (2) corresponds to Equation (1), and the fluid behaves Newtonian.

Figure 2 displays shear stress variations with shear rates at different temperatures and nanoparticle mass fractions. It is reported 193 experimental data in Figure 2.

3. ARTIFICIAL NEURAL NETWORKS APPROACH

Artificial neural networks (ANNs) are mathematical tools made by imitating the biological nervous system. The fundamental units of a nervous system are neurons. In solving engineering problems with several inputs, using one neuron is not enough and several neurons should be used. Several parallel neurons form a layer that includes the weight matrix, the bias vector, the transfer function, and the output vector. An ANN consist of several layers. The layer whose output is the network output is called the output layer and the rest of the layers are called hidden layers. If the computing units are interconnected forward, the network is feedforward [20].

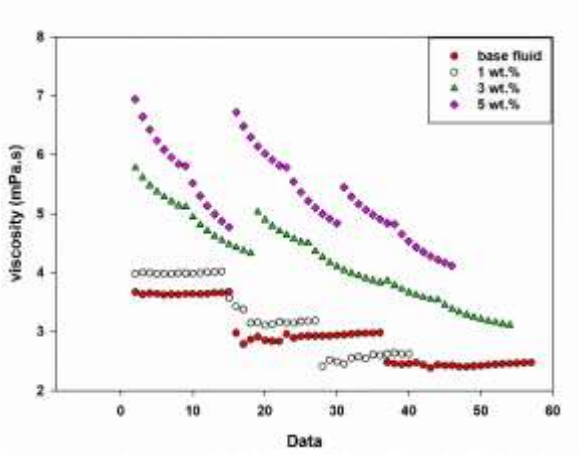

Figure 1. Experimental viscosity data

In this paper, a multilayer perceptron (MLP) is used, which is a common type of feedforward ANN. In general, MLP consists of a hidden layer and an output layer. This network operates very powerfully in regression applications [21].

The transfer function used for the hidden layer is the hyperbolic tangent function (*tansig*) $(f(m) = (e^m - e^{-m})/(e^m + e^{-m}))$ and the transfer function applied to the output layer is linear (*purline*) $(f(m) = m)$[20].

The LM backpropagation algorithm is utilized for solving non-linear least squares problems [22]. In multilayer neural networks, the back-propagation LM algorithm is used for network training. This algorithm has high accuracy and convergence speed in regression problems [23].

To design the structure of the ANN, the number of layers and the number of neurons in each layer are selected by trial and error. The amount of weights and biases is adjusted using the learning algorithm so that the MSE is minimal.

The value of MSE, the correlation coefficient (R) and mean relative error (MRE) used to evaluate the network performance are obtained from the following equations [24, 25]:

$$MSE = \frac{1}{N}\sum_{j=1}^{N}\left(\mu_j^{Exp} - \mu_j^{ANN}\right)^2 \quad (3)$$

$$R = \frac{\sum_{j=1}^{N}\left(\mu_j^{Exp} - \bar{\mu}^{Exp}\right)\left(\mu_j^{ANN} - \bar{\mu}^{ANN}\right)}{\sqrt{\sum_{j=1}^{N}\left(\mu_j^{Exp} - \bar{\mu}^{Exp}\right)^2 \sum_{j=1}^{N}\left(\mu_j^{ANN} - \bar{\mu}^{ANN}\right)^2}} \quad (4)$$

$$MRE = \frac{100}{N}\sum_{j=1}^{N}\left|\frac{\mu_j^{Exp} - \mu_j^{ANN}}{\mu_j^{Exp}}\right| \quad (5)$$

where N is the number of experimental data, and the superscript *Exp* and *ANN* refer to the experimental measured data and the output predicted by ANN, respectively.

4. RESULTS AND DISCUSSIONS

In this work, 193 experimental measured data reported previously [19] are used to predict the rheological properties of n-octadecane/mesoporous SiO_2 nanofluid. These data include nanofluid temperature, mass fraction of nanoparticles and shear rate, which are considered as input parameters of the ANN. The output parameters of the network are viscosity and shear stress, which are used to obtain power-law indices. This data is randomly split

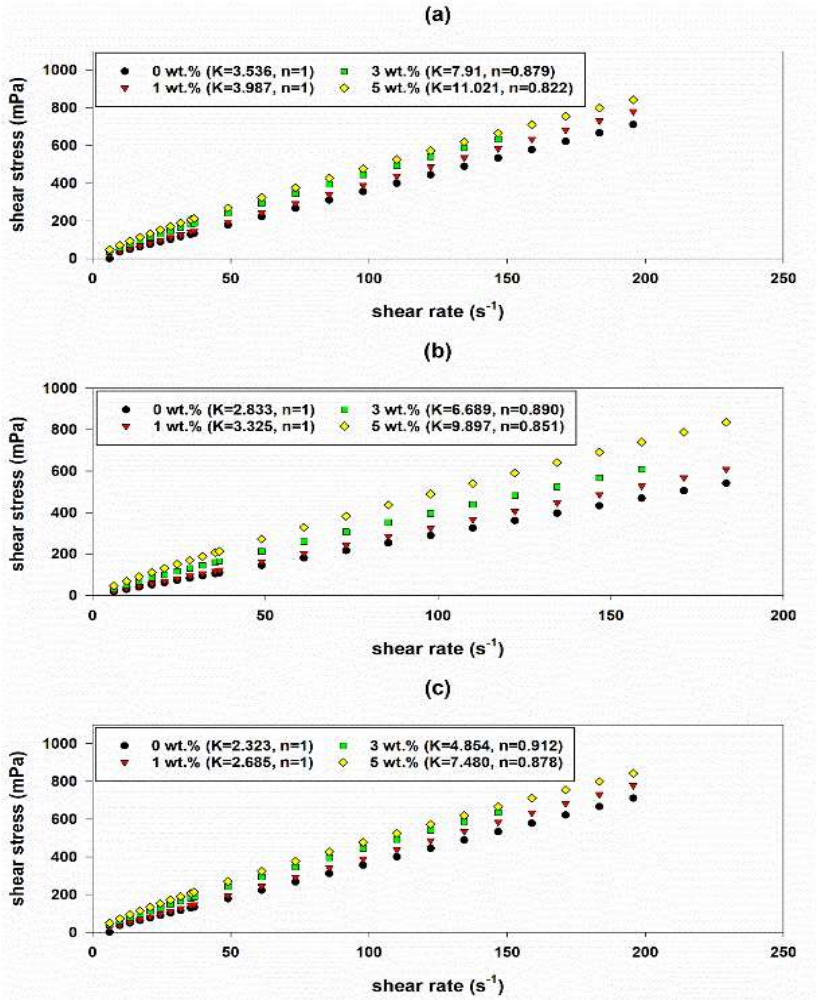

Figure 2. Experimental shear stress-shear rate diagrams (a) 35°C (b) 45°C (c) 55°C

into three categories: training, test, and validation. In the present study, 70% of the data (135 data) are used for training, 15% (29 data) for testing and 15% (29 data) for validation. The trial and error method is used to specify the optimal network structure.

A neural network with a hidden layer whose transfer function is a hyperbolic tangent (*tansig*) is considered. The number of hidden layer neurons varies from 2 to 30. The backpropagation LM algorithm is used to train the network. To increase network reliability and reproducibility, the training cycle is repeated 10 times for each neuron. Network error analysis is performed using MSE and R criteria. In an optimally structured network, the number of neurons in the hidden layer results in the lowest MSE and the highest R. Table 1 lists the MSE and R valuesof ANNs with various numbers of neurons in the hidden layer. As can be seen, when the number of neurons is equal to 22, the least MSE occurs which is bold in Table 1. For the optimal structure, the MSE of training, validation and test data are 6.67×10^{-4}, 4.90×10^{-3}, and 6.55×10^{-3}, respectively. The correlation coefficient for all data is R=0.99999.

Figure 3 shows the optimal network structure. This optimal structure has 3 input parameters (temperature, mass fraction and shear rate). In the hidden layer, there are 22 neurons are delivered to the output layer by multiplying the weights and adding the biases with the input parameters and applying the *tansig* transfer function. There are two neurons in output layer that calculate the targets (dynamic viscosity and shear stress) by applying the *purline* function to its input signal.

Figure 4 shows the measured viscosity and the viscosity calculated by ANN in terms of data number. As can be seen, there is a great compromise between neural network results and experimental measurements. The maximum relative error value between the measured viscosity of n-octadecane/mesoporous SiO_2 nanofluid and the viscosity predicted by the proposed ANN is 6.26%.

Figure 5 compares the amount of laboratory shear stress with the shear stress calculated from the developed neural network. According to Figure 5, it is noted that a very small difference between the experimental values and the values predicted by the ANN can be found, so that the maximum relative error of 0.418% is obtained.

TABLE 1. MSE and R for various neurons numbers

No. of neurons	MSE		R	
	Train	Test	Train	Test
2	31.21446	50.86929	0.999599	0.999373
4	28.81507	47.33163	0.999622	0.999286
6	20.3478	43.0721	0.99974	0.999246
8	1.87313	8.29652	0.999974	0.999914
10	1.57532	2.66298	0.999979	0.999964
12	1.27434	1.82589	0.999982	0.999972
14	1.48E-02	2.14E-02	0.999735	0.999962
16	4.61E-03	1.10E-02	0.999987	0.999973
18	1.17E-02	6.26E-02	0.999992	0.999996
20	2.64E-03	4.10E-02	0.999999	0.999999
22	**6.67E-04**	**6.55E-03**	**0.999999**	**0.999999**
24	3.61E-03	2.45E-02	0.999998	0.999989
26	2.06E-02	2.27E-01	0.999999	0.999999
28	1.68E-02	1.51E-01	0.999894	0.999889
30	1.38E-01	1.50E+01	0.999998	0.999986

Figure 3. Optimal neural network structure

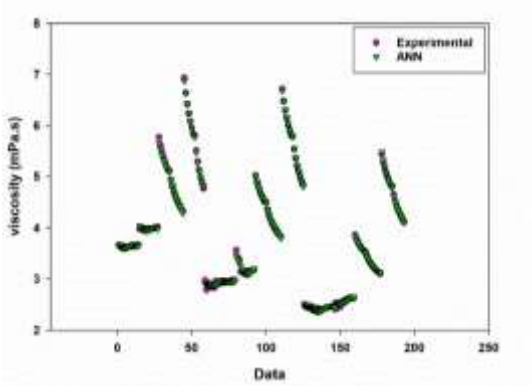

Figure 4. Comparison between experimental viscosity data and ANN results

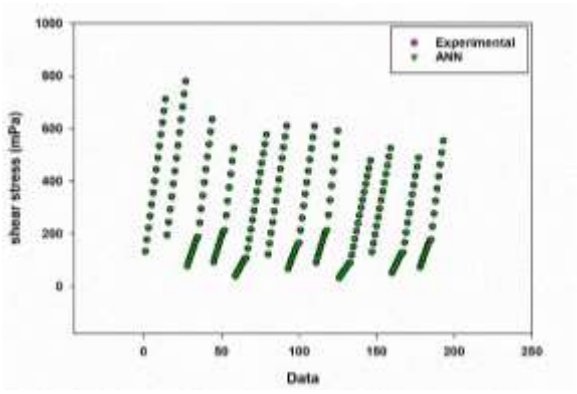

Figure 5. Experimental and ANN results of shear stress vs. number of data

Figure 6 depicts the measured viscosity values of n-octadecane/mesoporous SiO_2 nanofluids in terms of viscosity calculated by the neural network proposed in this study in a parity plot. This diagram compares the distribution of experimental values and modeling results. The line $y = x$ is plotted as a reference. Given the short distance between these points and the reference line, it can be concluded that ANN has made a satisfactory prediction. For all data, the MRE was 0.695 and R=0.99999.

Figure 7 shows the parity plot for comparing experimental shear stress and predicted shear stress by ANN. As evidenced, the points are completely on or near the reference line. The MRE of 0.0177 and R = 0.99999 are obtained for all shear stress data.

As can be seen from the results, the ANN method predicts the viscosity of nanofluid with high accuracy. A comparison between the results of nanofluid viscosity estimated by the ANN and other prediction methods is given in Table 2.

The rheological properties of n-octadecane/mesoporous SiO_2 nanofluids at different temperatures and mass fractions using shear stress calculated with ANN compared to experimental values are given in Table 3. According to the results, there is a

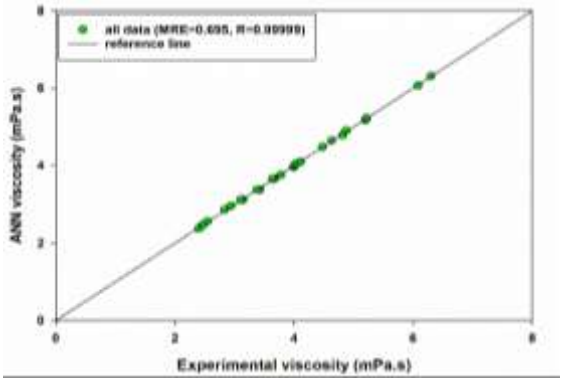

Figure 6. Experimental viscosity in comparison with ANN predicted viscosity

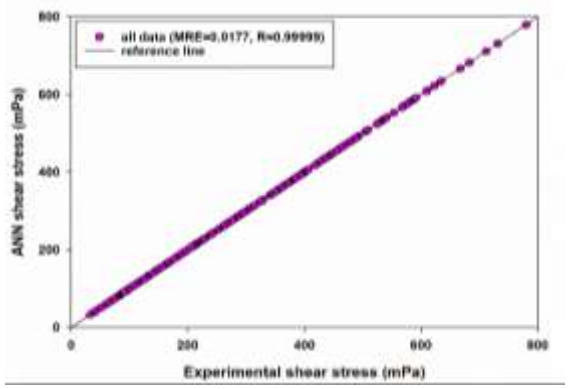

Figure 7. Experimental values shear stress in comparison with ANN shear stress

TABLE 2. Comparison between the ANN and other prediction methods for nanofluid viscosity

Ref.	Nanofluid	T (°C)	Particle loading	Method	Error
[12]	Ag/EG	25-55	0.2- 2 vol%	ANN	0.0314
				Correlation	0.0858
[15]	MWCNTs-TiO_2/ SAE50	25-50	0.125-1 vol%	ANN	0
				Curve fitting	12.25%
[26]	MWCNT/ paraffin	5- 65	0.005-5 wt.%	ANN	0.998 (R^2)
				RSM	0.988 (R^2)

TABLE 3. Rheological parameters predicted by ANN vs. experimental results

		Experimental [19]		Predicted by ANN	
T (°C)	ϕ_m (%)	K (mPa.s^n)	n	K (mPa.s^n)	n
35	0	3.536	1.000	3.636	1.000
	1	3.987	1.000	3.987	1.000
	3	7.91	0.879	7.937	0.878
	5	11.021	0.822	11.049	0.821
45	0	2.833	1.000	2.949	1.000
	1	3.325	1.000	3.325	1.000
	3	6.689	0.890	6.697	0.889
	5	9.897	0.851	9.882	0.851
55	0	2.323	1.000	2.446	1.000
	1	2.685	1.000	2.685	1.000
	3	4.854	0.912	4.854	0.910
	5	7.480	0.878	7.479	0.878

very good agreement between power-law index (n) and consistency index (K) coming from ANN method results and experimental results. It is clear, the maximum relative error of consistency index (K) (or apparent viscosity) is 5.29%, which occurs at 55°C for the base fluid. For non-Newtonian nanofluids, the maximum relative error is 0.341%, which occurs for ϕ_m = 3% and T=35°C. Also, the maximum relative error for power-law index (n) is related to non-Newton nanofluid of ϕ_m = 3% and T=55°C which is equal to 0.219%.

5. CONCLUSIONS

In this study, the rheological properties of n-octadecane/mesoporous SiO_2 nanofluids were predicted using experimental data and the ANN method. The proposed neural network is a feedforward MLP that uses the Levenberg-Marquardt backpropagation algorithm to predict targets. Network input parameters include temperature, mass fraction and shear rate, and network outputs are dynamic viscosity and shear stress. The optimal network architecture was obtained concerning the minimum MSE, which included one hidden layer, 22 neurons in the hidden layer, and a hyperbolic tangent transfer function. The MSE of training, validation and test data were 6.67×10^{-4}, 4.90×10^{-3}, and 6.55×10^{-3}, respectively. The correlation coefficient for all data was obtained as R=0.9999. The proposed ANN predicted dynamic viscosity and shear stress with the maximum relative error equal to 6.26% and 0.418%, respectively. Using the predicted shear stress, power-law index and consistency index were computed for non-Newtonian nanofluids, with a maximum relative error of 0.341% and 0.219%, respectively.

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Persian Abstract

چکیده

شبکه های عصبی مصنوعی، ابزاری قدرتمند برای پیش بینی خواص ترموفیزیکی نانوسیالات و کاهش هزینه و زمان انجام آزمایش هستند. لزجت دینامیکی یک خاصیت مهم درنانوسیالات است که معمولاً نیاز به پیش بینی دقیق آن در مسائل انتقال حرارت و جریان نانوسیالات است. دراین مقاله، خواص رئولوژیکی نانوسیال ان-اکتادکان حاوی نانوذرات مزوپروس سیلیکا به عنوان ماده تغییر فاز دهنده بر اساس داده های آزمایشگاهی موجود در مراجع، توسط یک شبکه عصبی پیش بینی شده است. داده های آزمایشگاهی ورودی شبکه شامل کسر جرمی در بازه صفر تا ۵٪، دماهای مختلف در بازه ۳۵°C تا ۵۵°C و نرخ کرنش برشی از ۱۳ تا ۱۹۶ بر ثانیه و خروجی شامل لزجت دینامیکی و تنش برشی است. گزارش شده است که رفتار نانوسیال با افزایش کسر جرمی به غیرنیوتنی میل می کند. یک شبکه عصبی پرسپترون چندلایه با الگوریتم آموزش لونبرگ-مارکوات برای پیش بینی خواص رئولوژیکی نانوسیال بکار رفته است. بر اساس کمترین خطای میانگین مربعات، ساختار بهینه شبکه شامل ۲۲ نورون در لایه پنهان بدست می آید. نتایج نشان داد شبکه عصبی توسعه داده شده دارای خطای ۰/۰۰۰۶۶۷ و۰/۰۰۶۵۵ برای داده های آموزش و آزمایش است. همچنین، لزجت دینامیکی و تنش برشی پیش بینی شده دارای بیشترین خطای نسبی به ترتیب برابر ۶/۲۶٪ و ۰/۴۱۸٪ است.