Int. J. Nanosci. Nanotechnol., Vol. 11, No. 2, June 2015, pp. 71-82

Model for Thermal Conductivity of Nanofluids Using a General Hybrid GMDH Neural Network Technique

A. Azari*and S. Marhemati

Faculty of Oil, Gas and Petrochemical Engineering, Chemical Engineering Department, Persian Gulf University, Bushehr, I.R. Iran

(*) Corresponding author: azari.ahmad@pgu.ac.ir
(Received: 24 Dec 2014 and Accepted: 10 May. 2015)

Abstract
In this study, a model for estimating the NFs thermal conductivity by using a GMDH-PNN has been investigated. NFs thermal conductivity was modeled as a function of the nanoparticle size, temperature, nanoparticle volume fraction and the thermal conductivity of the base fluid and nanoparticles. For this purpose, the developed network contains 8 layers with 2 inputs in each layer and also training algorithms of least squares regression. The obtained results of the model have shown good accuracy of hybrid GMDH-PNN for estimating the thermal conductivity of NFs. The RMSE of the model for 24 systems containing 211data sets was achieved 0.0224. MAPE for training and validation data setswere3.58 and 3.2%, respectively. Also, the proposed hybrid GMDH-PNN model was compared with different models from the literature. The results showed that the developed model can successively correlate and predict the thermal conductivity of different groups of NFs. Moreover, a remarkable agreement for the model with the experimental data was achieved with respect to the other models from the literature.
Keywords*: Artificial neural network, GMDH-PNN model, Nanofluids, Thermal conductivity.*

1. INRODUCTION

NFs are based on suspensions of nanoparticles in the base fluids such as water, propylene glycol, ethylene glycol and engine oil, firstly described by Choi [1].NFs consist of a new type of heat transfer fluid superior in terms of thermo-physical properties to those conventional fluids[1]. NFs are worthwhile to be applicable in practical heat transfer processes, due to high potential for heat transfer enhancement. The thermo-physical properties of NFs, such as density, viscosity and thermal conductivity are of significant importance in heat transfer application involving heat transfer fluid for thermal engineering[2]. Among the various thermo-physical properties of NFs, most attention was devoted to viscosity and thermal conductivity [3-5] in order to calculate theoretical heat transfer coefficient. Therefore, these properties should accurately be determined because of their influence on NF flow and heat transfer characteristics[6]. Up to now, different models have been developed for the prediction of NFs thermal conductivity, but these correlations can only be used under certain circumstances [7-13].

Over recent years, the ANN has especially found a well famous tool in certain subfields of kinetics, thermodynamics and transport properties where common models and theories fall short to provide accurate predictions [14-18]. Recently, ANNs have been applied to the study of NFs viscosity. Karimi *et al.* [18] developed an optimized ANN to predict NFs viscosity. Their

developed model integrates the concept of GA into an ANN model and has a low MAPE of 2.48%. A diffusional neural network was proposed by Yousefi *et al.* [19] for the estimation of NFs viscosity with an overall MAPE of 3.44%.

The ANN and the GMDH are inductive approach able to establish non-linear connections between a set of input data and its output, without needing sophisticated theory[20]. Based on parallelism and micro-behavior, the information is accumulated on iterations by an element processing network called neurons. These intelligent algorithms were developed in complex systems for modeling, prediction, identification and approximation[20].

Recently, Pazuki *et al.*[21] developed a hybrid GMDH–PNN model to predict the partition coefficients of Penicillin G Acylase in polymer salt aqueous biphasic systems. Abdolrahimi *et al.*[22] proposed a hybrid GMDH–PNN model to investigate the partition coefficients of alkaloids in ionic liquid-based aqueous biphasic systems. Both studies report a considerable decrease in errors generated by the hybrid approach.

Maziar Hakim *et al.*[23] studied the liquid–liquid phase behavior of aromatic compound + liphatic compound + ionic liquid (IL) ternary systems by using two ANNs developed based on back propagation and hybrid GMDH. In their work, the obtained results by the hybrid GMDH model provided a near to accurate prediction of phase behavior with of 7.27%. Araújo Padilha *et al.*[20] investigated the capability of two models ANN and GMDH in predicting the breakthrough curves of rhamnolipids produced by Pseudomonas aeruginosa (AP029-GLVIIA) onto active carbon and Amberlite XAD-2. Finally, they concluded that ANN is a more suitable tool to predict the data of rhamnolipid breakthrough curves than GMDH model to the two porous adsorbents investigated, mainly due to the typical non-linear behavior. Ebtehaj *et al.* [24] used a GMDH model for estimating the discharge coefficient of a rectangular side orifice. They used five structures for the prediction of discharge coefficient based on different dimensionless group of data. The obtained results showed that all models estimate the discharge coefficient fairly accurately. Also their results indicated that not using Froude number parameter has the most effect on the results among the four presented dimensionless models which in some cases led to an over 10% error.

The goal of this research is to add basic information to the knowledge base and propose a general model for prediction of thermal conductivity of NFs under a wide range of circumstances. To this end, a general GMDH-PNN model was developed to estimate the thermal conductivity of twenty four different groups of NFs. These NFs included 6 different materials as the nanoparticles and 5 different base fluids. Systems studied include Al_2O_3, TiO_2, CuO, Cu, AlN and Al as the nanoparticles and water, EG, EO, PG and DIW as the base fluids. The GMDH–PNN correlations were performed on a data set with 211 experimental data [25-34]. The fit for the model was determined by the regression coefficient (R^2) as well as by the MAPE and SSE, for the training and validation data set. Finally, the validity and credibility of the proposed GMDH-PNN model was evaluated with the experimental data sets and other models [9-12] from literature.

2. EXPERIMENTAL DATA

The first step in the modeling of a GMDH neural network is compiling the database for training the network and evaluating the generality of network capability. In the present study, a data set with 211 experimental values for different NFs has been used for the model development. Using the random selection method, 85% of the total data was used for the training of the model and the other was used for the model validation. Table 1 reports all of the studied systems and data sources. The range of the input variables (d_p, T, ϕ, k_b, k_p) for

the training and validation of the hybrid model was listed in Table 2.

Table 1. *Studied systems and data sources.*

NFs group number	NFs		Number of data points	Reference
	Base Fluid	Nanoparticle		
1	DIW	CuO	6	[25]
2	DIW	TiO_2	6	[26]
3	DIW	Al_2O_3	8	[26]
4	Water	CuO	2	[26]
5	Water	Al_2O_3	9	[27]
6	EG	Al_2O_3	3	[27]
7	Water	CuO	1	[27]
8	EG	CuO	4	[27]
9	Water	Cu	2	[27]
10	Water	Al_2O_3	33	[28]
11	Water	Al_2O_3	4	[29]
12	Water	CuO	5	[29]
13	EG	CuO	4	[29]
14	EG	Cu	2	[29]
15	Water	TiO_2	2	[30]
16	EG	TiO_2	3	[30]
17	Water	Al_2O_3	19	[31]
18	EG	AlN*	6	[32]
19	PG	AlN	6	[32]
20	EG	Al_2O_3	10	[33]
21	EO	Al	10	[33]
22	EG	TiO_2	6	[33]
23	EG	Al_2O_3	18	[34]
24	Water	Al_2O_3	42	[34]

Table 2. *Variations range of input and output of hybrid model.*

Properties name (unit)	Properties symbol	Variation range	
		Minimum	Maximum
Nanoparticle diameter (nm)	d_p	8	169
Temperature (K)	T	283.15	411.1
Nanoparticle volume fraction (%)	ϕ(%)	0.01	5
Base fluid thermal conductivity	k_b	0.14035	0.67995
Nanoparticles thermal conductivity	k_p	8.37	401
Nanofluid thermal conductivity	k_{nf}	0.15854	0.77553

3. GROUP METHOD OF DATA HANLING

In a network with multiple inputs and a single output, the relationship between the inputs and the output of the network can be estimated by VKG polynomial[35] according to Equation 1.

$$\hat{y}_n = a_0 + \sum_{i=1}^{M} a_i x_i + \sum_{i=1}^{M}\sum_{j=1}^{M} a_{ij} x_i x_j + \sum_{i=1}^{M}\sum_{j=1}^{M}\sum_{k=1}^{M} a_{ijk} x_i x_j x_k + \ldots \quad (1\text{-a})$$

$$X = (x_1, x_2, ..., x_M) \quad (1\text{-b})$$

$$A = (a_0, a_1, a_2, ...) \quad (1\text{-c})$$

The general equation in the form of VKG can be simplified to a partial quadratic polynomials as Equation 2 consisting of only two variables[36].

$$\hat{y}_n = a_0 + a_1 x_{in} + a_2 x_{jn} + a_3 x_{in} x_{jn} + a_4 x_{in}^2 + a_5 x_{jn}^2 \quad (2)$$

During the construction of a GMDH network, all combinations of the inputs are created and as its source, each layer consists of nodes taking a special pair of inputs (x_i, x_j). A set of coefficients, a_i, is produced by each node. Consequently, based on the training data set, Equation (2) is estimated. Furthermore, the predicted and actual output values are compared using the testing set of data by estimating SSE according to Equation 3[36]:

$$SSE = \sum_{n=1}^{N} (\hat{y}_n - y_n)^2 \quad (3)$$

In order to determine the "best fit" values, the value of SSE should be minimized. This means that the partial derivatives of Equation 3 with respect to each constant coefficient are taken and set equal to zero [36]:

$$\frac{\partial SSE}{\partial a_i} = 0 \quad (4)$$

Solving Equation 4 leads to a system of equations that are solved by the training set of data.

$$Y = [1\ x_i\ x_j\ x_i\ x_j\ x_i^2\ x_j^2] \quad (5)$$

$$X = Y^T Y \quad (6)$$

$$X = \begin{bmatrix} 1 & x_i & x_j & x_i x_j & x_i^2 & x_j^2 \\ x_i & x_i^2 & x_i x_j & x_i^2 x_j & x_i^3 & x_i x_j^2 \\ x_j & x_i x_j & x_j^2 & x_i x_j^2 & x_i^2 x_j & x_j^3 \\ x_i x_j & x_i^2 x_j & x_i x_j^2 & x_i^2 x_j^2 & x_i^3 x_j & x_i x_j^3 \\ x_i^2 & x_i^3 & x_i^2 x_j & x_i^3 x_j & x_i^4 & x_i^2 x_j^2 \\ x_j^2 & x_i^2 x_j & x_j^3 & x_i x_j^3 & x_i^2 x_j^2 & x_j^4 \end{bmatrix} \quad (7)$$

$$A = [a_0\ a_1\ a_2\ a_3\ a_4\ a_5] \quad (8)$$

$$B = (\mathrm{yY})^T \quad (9)$$

Thus the system of equations can be solved according to the following form[36, 37]:

$$\sum_{n=1}^{N} AX = \sum_{n=1}^{N} B \quad (10)$$

4. HYBRID GMDH-PNN MODEL DEVELOPMENT

An ANN provides a very large complex of equations governing its layers and nodes due to its highly complicated structure. Moreover, the configuration of network (including number of layers and nodes, input weights and learning rates and random value of bias) is chosen either arbitrarily or manually and this does not guarantee the best possible network.

In a standard GMDH approach, all pair combinations of inputs are constructed and thus employed for the input layer of the network. Therefore, the produced outputs of the input layer are classified and selected as the inputs for the next layer. This process is repeated continuously as long as each subsequent layer produces a better result than the previous one[36]. Pair selection of inputs results in the exclusion of other variables' effects and thus when the system is highly non-linear, less

precise nodal polynomials estimation is concluded. So, the original GMDH is too simple to model systems of high non-linearity.

In order to alleviate the problems associated with the original approach of GMDH, a number of authors have attempted to hybridize GMDH with some evolutionary optimization techniques. Among such techniques, hybridization of GMDH with ANN is one of the promising ones. The GMDH methodology designs a self-organizing ANN which not only is able to express the system genome, so to speak, by means of simple polynomials, but also uses common optimization algorithms to find the most appropriate configuration.

In this method, each node can take any combination of input variables unless the order of polynomial exceeds two. Moreover, the input of each node can cross over other layers and as a result the complexity of the model is increased. Furthermore, as the number of possible combinations among nodes is increased, the developed model can better predict the system's non-linearity. Therefore, predicted values of the hybrid GMDH-PNN model can be estimated as follows:

$$\hat{y}_n = a_0 + \sum_{i=1}^{M} a_i x_i + \sum_{i=1}^{M}\sum_{j=1}^{M} a_{ij} x_i x_j \qquad (11)$$

5. RESULTS AND DISCUSSION

For the development of the hybrid GMDH-PNN model, different inputs ($1/d_p$, T, ϕ, k_b, k_p) were employed and the NFs thermal conductivity was considered as the model output. One of the most prevalent problems conjunct with neural networks is over-fitting. In an over-fitted neural network, train data are accurately correlated. Using the random selection method, 85% of all data was assigned to the training data set and the remaining to the validation data set. To evaluate the model precision, different errors such as MSE, RMSE, MAE and MAPE were calculated according to the following equations:

$$MSE = \frac{\sum_{i=1}^{N}\left(k_{nf,i}^{Exp} - k_{nf,i}^{Calc}\right)^2}{N} \qquad (12)$$

$$RMSE = \left(\frac{\sum_{i=1}^{N}\left(k_{nf,i}^{Exp} - k_{nf,i}^{Calc}\right)^2}{N}\right)^{1/2} \qquad (13)$$

$$MAE = \frac{\sum_{i=1}^{N}\left|k_{nf,i}^{Exp} - k_{nf,i}^{Calc}\right|}{N} \qquad (14)$$

$$MAPE = \frac{1}{N}\sum_{i=1}^{N}\frac{\left|k_{nf,i}^{Exp} - k_{nf,i}^{Calc}\right|}{k_{nf,i}^{Exp}} \times 100 \qquad (15)$$

In this study, the structure of the hybrid GMDH-PNN model was developed with 2 neural inputs in 8 layers, as shown in schematic Figure 1. As can be seen from the figure, the proposed model has one input layer, seven middle layers and one output layer. Moreover, the figure clearly shows some crossovers between nodes in different layers (dash lines) representing the distinct characteristic of the hybrid GMDH-PNN model.

Table 3 reports the network performance for the optimized hybrid model. The results clearly show that training and validation data set have the same order of magnitude errors. Thus, it can be said that the model was properly developed. Also, generated functions corresponding to each node in each layer together with the total correlation function for NFs thermal conductivity are presented in Table 4.

After the model development, the ability of the hybrid modeling approach for the prediction of the thermal conductivity of different NFs should be evaluated. So, the experimental and predicted values of NFs thermal conductivity are compared in Figures 2 and 3 for the training and validation data sets, respectively.

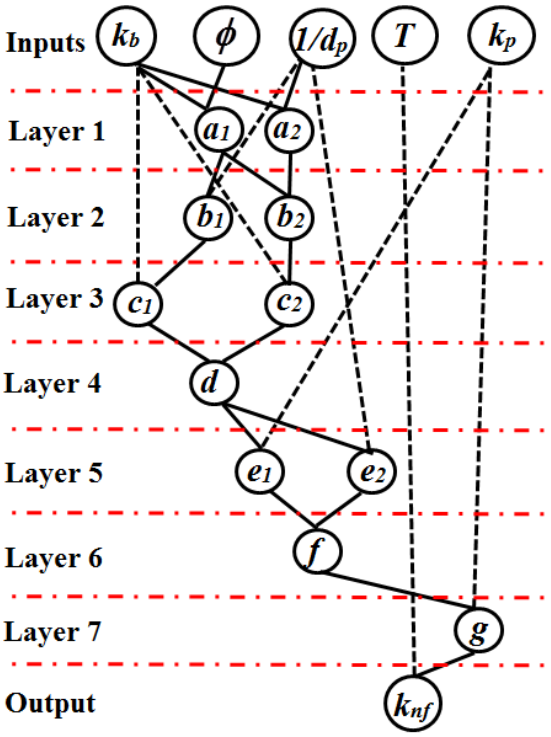

Figure 1. *Architecture of the optimized hybrid GMDH-PNN model.*

As can be seen in the figures, good agreement between the prediction of the hybrid model and the experimental data is observed and R (correlation coefficient) for the training and validation sets of data is in the same order of magnitude. So, the developed hybrid model can be used for the prediction of NFs hermal conductivity data for the aforementioned NFs categories and any kind of NFs. In other word, this hybrid model can be used for any kind of NFs with the range of parameters (minimum and maximum) like Table 2. The hybrid model is based on particle diameter, temperature, nanoparticle volume fraction, base fluid and particle thermal conductivity.

Furthermore, the results of the proposed model for CuO (18 nm)/water NFs at a temperature of 300 K was compared with those of different models from the literature [9-12]. The experimental data for CuO (18 nm)/water NFs at a temperature of 300K was gathered from the literature[38]. Performance criteria of the GMDH-PNN model in comparison with the other models are presented in Table 5 and the results are depicted in Figure 4.

All the input parameters for the different models in Figure 4 and also the experimental condition for the experimental data are as the following: T= 300 K, d_p=18nm, k_b=0.613W/m.K, k_p=20 W/m. K. The results clearly show the reliability and accuracy of the proposed hybrid GMDH-PNN model in predicting NFs thermal conductivity in comparison with the other models from the literature. Nevertheless, the reason for the little deviation may be due to the particle size distribution. Nanoparticles have the actual particle size distribution in the fluid, whereas a number-weighted average particle diameter of 18 nm that was reported in the literature [38] was used in the models input in this study.

On the other hand, Murshed model accounts for the effects of particle size, interfacial layer thickness, volume fraction and thermal conductivity. Thus, the effect of temperature was ignored in the Murshed model[11]. Timofeeva model predicts the thermal conductivity based on effective medium theory and considers the particle shape and surface thermal resistance. This model cannot investigate the effect of temperature and particle diameter for the prediction of thermal conductivity [12]. Kumar model supposes that the thermal conductivity enhancement takes into account the Brownian motion of particles[9]. Therefore, this model expresses the particle thermal conductivity as a function of Brownian motion and assumes that the nanoparticles temperature is the same as fluid temperature. Prasher model considers the effect of the convection of the liquid near the particles due to their Brownian movement for the thermal conductivity prediction. Thus, this model considers the particle diameter and thermal conductivity, fluid thermal conductivity, temperature, interfacial resistance, fluid kinematic viscosity and particle volume fraction [10].

***Table 3**. Performance criteria for the hybrid GMDH-PNN model.*

	MSE	RMSE	MAE	MAPE
Training data	0.00050	0.0224	0.01687	3.58
Validation data	0.00049	0.0223	0.01669	3.20

***Table 4.** Nodal transfer functions for hybrid GMDH–PNN model.*

Layers	Neuron Functions
Layer 1	$a_1 = 0.046054 + 1.021178k_b - 0.002893k_b^2 - 1.8328\phi + 40.39\phi^2 - 0.8703k_b\phi$
	$a_2 = -0.023795 + 1.532286k_b - 0.705609k_b^2 - 1.185457(1/d_p) + 1.320655(1/d_p)^2 + 2.273364k_b(1/d_p)$
Layer 2	$b_1 = -0.010632 - 1.276692(1/d_p) + 3.483926(1/d_p)^2 + 1.179049a_1 - 0.267325a_1^2 + 2.079901(1/d_p)a_1$
	$b_2 = 0.000572 + 0.509404a_2 - 23.36574a_2^2 + 0.507557a_1 - 23.70922a_1^2 + 47.06194a_2a_1$
Layer 3	$c_1 = 0.03888 + 2.895135k_b + 41.33383k_b^2 - 1.86639b_1 + 40.35594b_1^2 - 81.66926k_bb_1$
	$c_2 = 0.10047 + 4.710278k_b + 65.05415k_b^2 - 3.833459b_2 + 64.8477b_2^2 - 129.755k_bb_2$
Layer 4	$d = 0.038249 + 2.475619c_1 - 58.46113c_1^2 - 1.659257c_2 - 54.61134c_2^2 + 113.2715c_1c_2$
Layer 5	$e_1 = 0.007372 - 0.000143k_p + 5.842322e-7k_p^2 + 0.943805d + 0.068799d^2 + 0.000106k_pd$
	$e_2 = 0.006563 - 0.067369(1/d_p) + 0.355567(1/d_p)^2 + 0.974713d + 0.026528d^2 + 0.011504(1/d_p)d$
Layer 6	$f = -0.013424 + 0.655606e_2 - 47.45172e_2^2 + 0.441436e_1 - 42.10731e_1^2 + 89.45111e_2e_1$
Layer 7	$g = 0.002312 - 0.000127k_p + 5.75031e-007k_p^2 + 1.012251f - 0.002848f^2 - 0.000218k_pf$
Output	$k_{nf} = -0.275384 + 0.001477T - 0.000002T^2 + 1.185301\,\mathrm{g} + 0.039599\,\mathrm{g}^2 - 0.000717T\,\mathrm{g}$

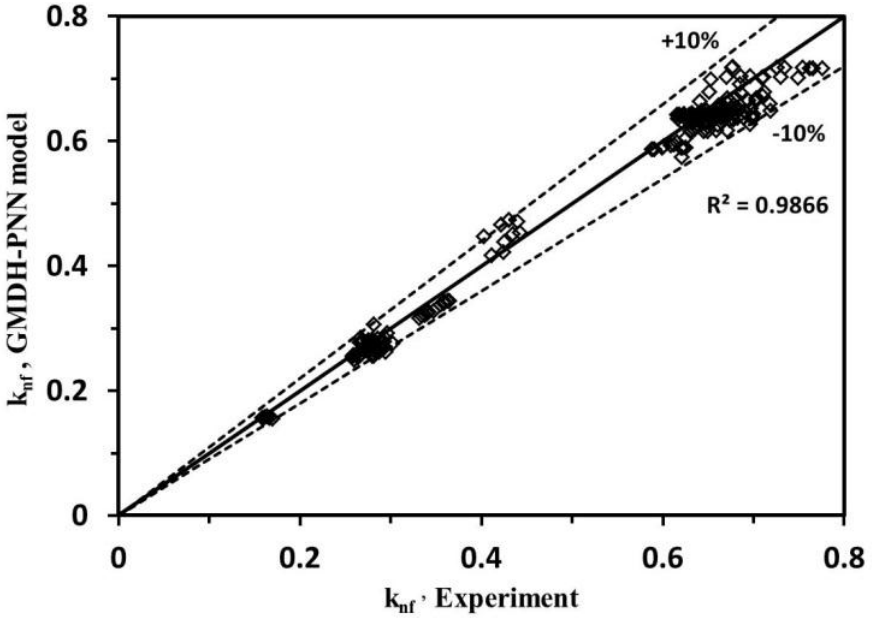

***Figure 2.** Comparison of the experimental and modeling results for the training data set.*

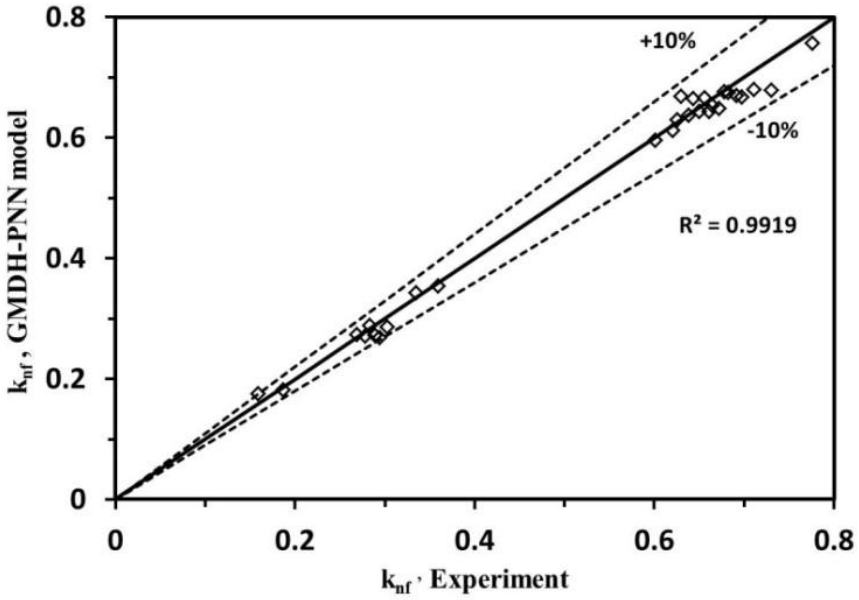

Figure 3. *Comparison of the experimental and modeling results for the validation data set.*

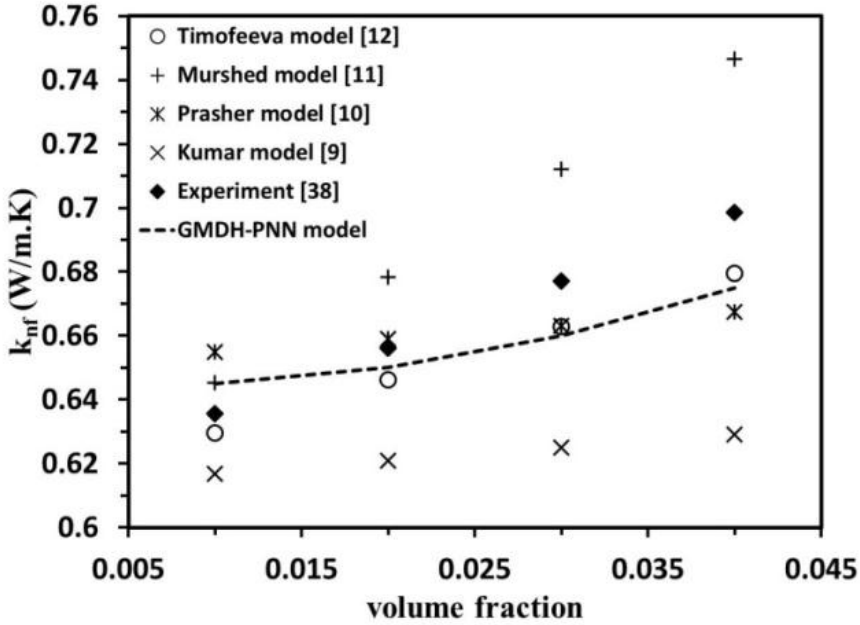

Figure 4. *Comparison of model predictions with the other models from the literature for CuO/water NFs (T= 300 K, d_p=18nm, k_b=0.613W/m. K and k_p=20 W/m.K).*

Table 5. *Performance criteria for comparison of GMDH-PNN model with the other models (the experimental data for the evaluation of the models were gathered from literature [38]).*

Model	MSE*10^3	RMSE*10^2	MAE*10^2	MAPE
Kumar model [9]	2.29	4.79	4.40	6.49
Prasher model [10]	0.39	1.97	1.69	2.51
Murshed model [11]	1.03	3.21	2.87	4.24
Timofeeva model [12]	0.17	1.32	1.23	1.82
GMDH-PNN (this work)	0.24	1.56	1.41	1.98

6. CONCLUSION

A GMDH-PNN model in 8 layers with 2 inputs in each layer was proposed to predict the thermal conductivity of twenty four common NFs (211 sets of data). The objective of the current study was to devise a hybrid GMDH-PNN model to overcome the limitations of ANNs.The schematic diagram of the developed model showed some crossovers between layers representing the distinct characteristic of the hybrid GMDH-PNN. The hybrid GMDH-PNN model can predict the thermal conductivity of NFsby a grand polynomial correlation function of temperature, particle thermal conductivity, particle diameter, particle volume fraction and base fluid thermal conductivity. The regression coefficients for the training and validation set of data were 0.9866 and 0.9919, respectively. Moreover, the MAPEs for the training and validation sets of data were 3.58 and 3.20, respectively. This suggests that the proposed hybrid model can fairly represent the thermal conductivity of NFs. Furthermore, comparison of the estimated thermal conductivity with the experimental values showed excellent agreements between them. Also, the results showed the reliability and accuracy of the proposed hybrid model in predicting NFsthermal conductivity in comparison with the other models from literature.

NOMENCLATURE

A	Vector of weight coefficients
a	Weight coefficient
k	Fluid thermal conductivity, W/mK
M	Number of input variables
N	Number of data sets
T	Temperature, K
X	Vector of input variables
x	Input variable
y	Actual output value
$\hat{y}$	Predicted output value

Greek Symbols

ϕ	Particle volume concentration (volume fraction)

Subscripts

b	Refere to base fluid property
nf	Refere to nanofluid property
p	Refere to nanoparticle property

Superscript

Calc	Calculated value
Exp	Experimental value

ABBREVIATIONS

AI	Artificial Intelligence
AlN	Aluminum Nitride
ANN	Artificial Neural Network
DIW	Deionized Water
EG	Ethylene Glycol
EO	Engine Oil
Exp	Experiment
GA	Genetic Algorithms
GMDH	Group Method of Data Handling
GMDH-PNN	Group Method of Data Handling Polynomial Neural Network
MAE	Mean Absolute Error
MAPE	Mean Absolute Percentage Error
MSE	Mean Squared Error
NFs	Nanofluids
PG	Propylene Glycol
RMSE	Root Mean Squared Error
VKG	Volterra-Kolmogorov-Gabor

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